

*Supporting Information*

**Stereochemical model and origins of selectivity for rhodium-catalyzed  
hydroselelenation of styrene**

Chunhui Shan\*, Xi Luo, Xiaoling Luo and Rong Long\*

College of Chemistry, Chongqing Normal University, Chongqing 401331, P. R. China.

E-mail: [chunhui.shan@cqu.edu.cn](mailto:chunhui.shan@cqu.edu.cn); [longrong@cqu.edu.cn](mailto:longrong@cqu.edu.cn)

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## 1. Complete reference for Gaussian 16

Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

## 2. Another possible mechanism

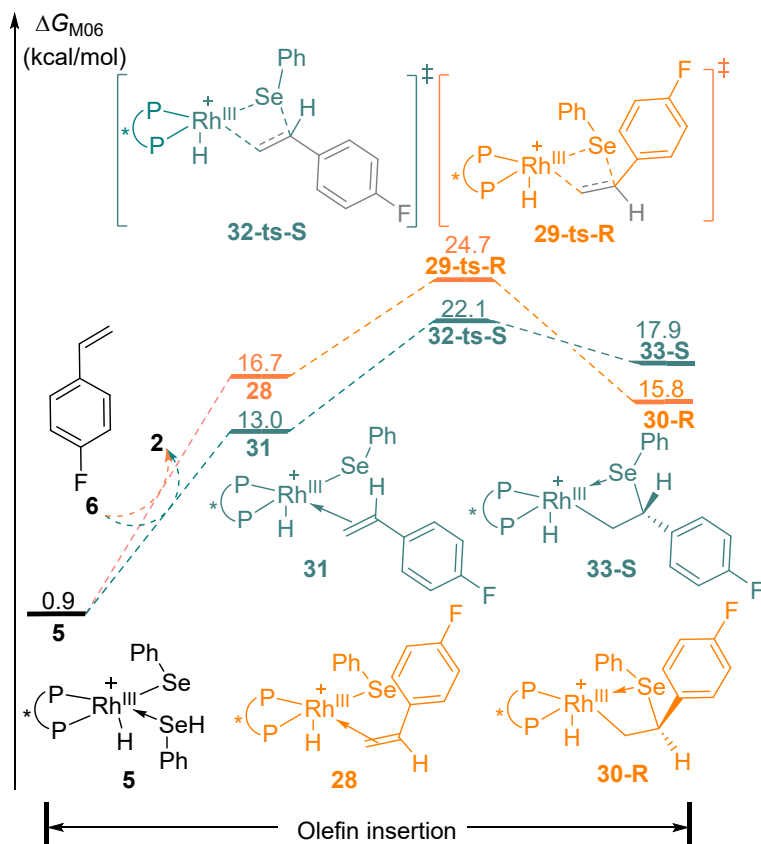


Fig. S1. Free-energy profiles of the of rhodium-catalyzed olefin insertion step. Values are given in kcal/mol.

When the five-coordinated Rh(III)-H species **5** is generated, there are other pathways to be considered. As shown in Figure S1, the ligand exchange of selenol with *para*-fluorostyrene **6** forms the alkene-coordinated intermediate **28** with an endergonic energy of 15.8 kcal/mol. Then unsaturated C-C double bond in intermediate **28** is inserted into the Rh-Se bond via transition state **29-ts** with an energy barrier of 8.0 kcal/mol to yield R-configuration alkyl Rh(III) **30**. The activation free energy of **29-ts** is 24.7 kcal/mol, which is 4.3 kcal/mol higher than that of **8-ts**, indicating that this pathway is unfavourable.

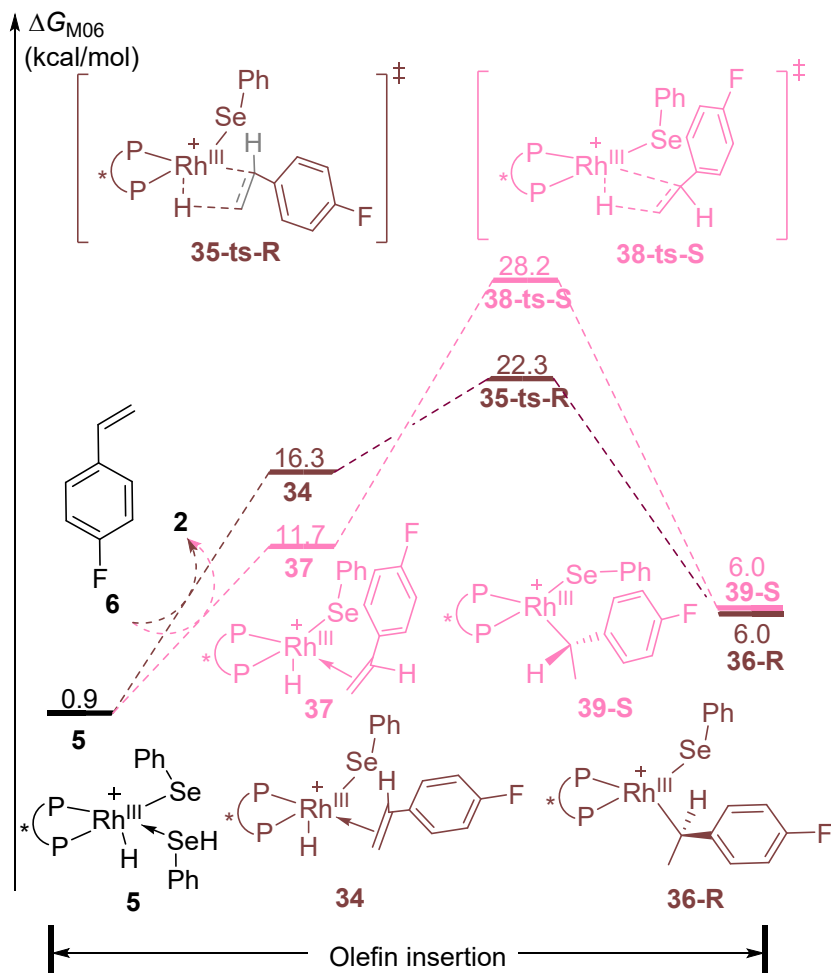


Fig. S2. Free-energy profiles of rhodium-catalyzed olefin insertion step. Values are given in kcal/mol.

When the five-coordinated Rh(III)-H species **5** is generated, there are other pathways to be considered. As shown in Figure S2, the ligand exchange of selenol with *para*-fluorostyrene **6** forms the alkene-coordinated intermediate **34** with an endergonic energy of 15.4 kcal/mol. Then unsaturated C-C double bond in intermediate **34** is inserted into the Rh-Se bond via transition state **35-ts** with an energy barrier of 6.0 kcal/mol to yield R-configuration alkyl Rh(III) **36**. The activation free energy of **35-ts** is 22.3 kcal/mol, which is 1.9 kcal/mol higher than that of **8-ts**, indicating that this pathway is unfavourable. Therefore, this pathway can also be excluded.

### 3. DFT benchmark of different methods of energy difference between 16-ts-S and 10-ts-R

Table S1. DFT benchmark of different methods of energy difference of 16-ts-S and 10-ts-R.

Single-point calculations	$\Delta\Delta G^\ddagger_{16\text{-ts-S}-10\text{-ts-R}}$
M06	0.8
wB97XD	0.8
B3LYP-D3	0.4
M06L	1.1

To further confirm the reliability of our approach, we have performed additional calculations using different levels of theory, such as wB97XD, B3LYP-D3 and M06-L with the 6-311+G(d) and SDD basis sets. These calculations were carried out for solvation single-point energy calculations based on the gas-phase structures optimized using B3LYP-D3/6-31G(d)-LANL2DZ level of theory. The results are shown below. Computational results suggest that, in addition to the B3LYP-D3 calculated value, which is slightly smaller, the energy difference between 16-ts-S and 10-ts-R is in close agreement with the data obtained using M06. The enantioselectivity observed in the experiment is 92:8, meaning the energy difference between 16-ts-S and 10-ts-R is approximately 1.5 kcal/mol, which is in close agreement with the energy difference we calculated. Therefore, the energy difference between 16-ts-S and 10-ts-R, as presented in the manuscript, is reliable.

### 4. Regioselectivity of the olefin insertion step

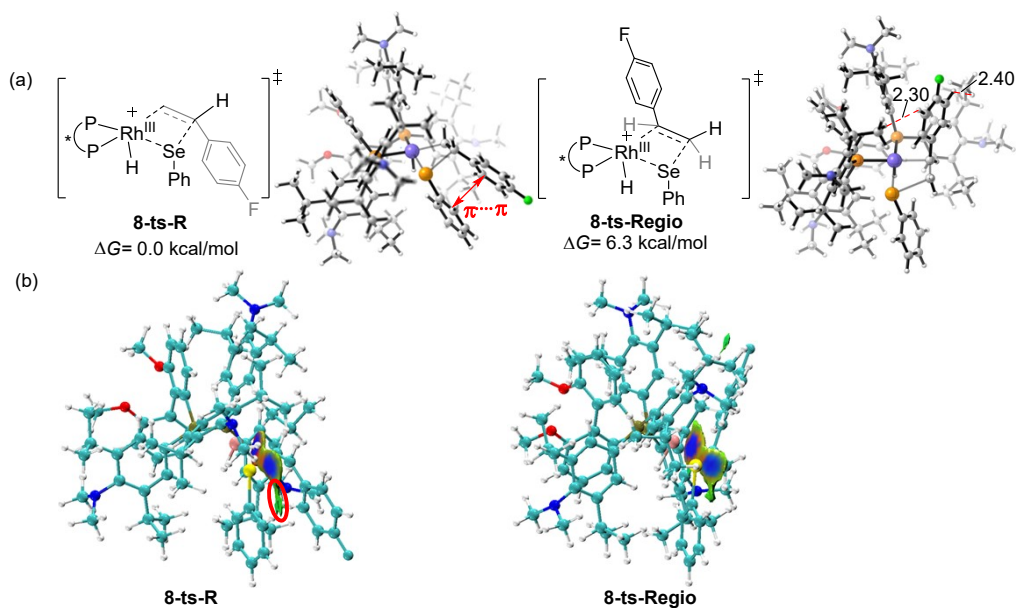


Fig. S3 (a) the structures of **8-ts-R** and **8-ts-Regio**; (b) IGMH analysis of **8-ts-R** and **8-ts-Regio**.

The olefin insertion step can produce two regioisomers, such as **8-ts-R** and **8-ts-regio**. The relative free energy of the transition state **8-ts-Regio** is 6.3 kcal/mol higher than that of **8-ts-R**. IGMH analysis indicated that there was a weak interaction between the fluorophenyl group of *para*-fluorostyrene and the phenyl group of selenol in transition state **8-ts-R**, thereby facilitating its stability and lowering the activation energy. Furthermore, the structural information of **8-ts-regio** shows that the distances between the hydrogen atoms of the isopropyl group and the phenyl group of selenol are 2.30 and 2.40 Å, respectively. This also indicates the presence of steric hindrance, but unfortunately, it is not displayed in the IGMH. Therefore, the  $\pi$ -stacking and steric effects may jointly influence the regioselectivity of the olefin insertion step.

### 5. Free energy profiles for the $[\text{Rh}(\text{cod})\text{Cl}]_2$ catalyzed selenol oxidative addition step

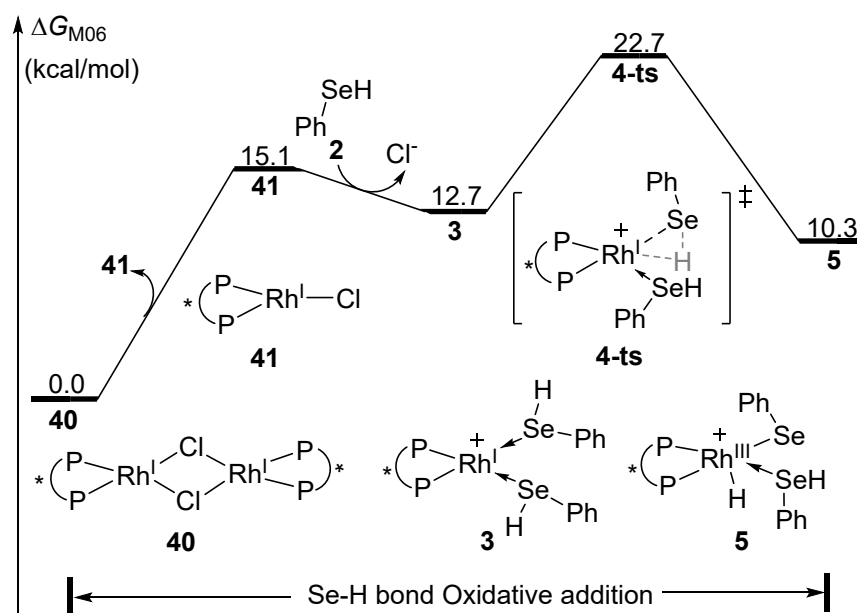


Fig. S4 Free energy profiles for the  $[\text{Rh}(\text{cod})\text{Cl}]_2$  catalyzed selenol oxidative addition step. Values are given in kcal/mol.

The free energy profiles for the  $[\text{Rh}(\text{cod})\text{Cl}]_2$  catalyzed selenol oxidative addition step are shown in Fig. S4. The calculated free energy profiles for the whole catalytic cycle start with the rhodium chloride dimer **40**, which is derived from complexation of  $[\text{Rh}(\text{cod})\text{Cl}]_2$ . Dissociation of rhodium chloride dimer gives rhodium monomer **41** with an endergonic energy of 15.1 kcal/mol. The ligand exchange of chloride ion with two molecules of selenols **2** yielded the selenols-coordinated intermediate **3**. Subsequently, the oxidative addition of selenol **2** occurs via a three-membered-ring transition state **4-ts** to generate five-coordinated Rh(III)-H species **5** with an activation energy of 22.7 kcal/mol. The relative free energy of the Rh(III)-H species **5** is 10.3 kcal/mol, which is 9.4 kcal/mol higher than that of the same intermediate

in the corresponding step in Fig. 1 of the article, resulting in a higher activation energy for the subsequent reductive elimination step. Therefore,  $[\text{Rh}(\text{cod})\text{Cl}]_2$  is not favorable for the hydroselenation reaction as a catalyst, which is consistent with the experimental observations.

## 6. Cartesian coordinates and energies of optimized structures

<b>1</b>				H	0.96970700	-2.42724700	-0.92576700
B3LYP-D3 SCF energy: -4201.535106 a.u.				H	3.52317000	-0.60420300	1.97263000
B3LYP-D3 enthalpy: -4199.678770 a.u.				H	4.40001800	-0.59150100	-0.56154200
B3LYP-D3 free energy: -4199.914019 a.u.				H	2.06486400	2.96774200	-1.10440800
M06 SCF energy in solution: -4200.530173 a.u.				H	-1.02179400	2.33575400	-0.83539300
				H	-3.30379600	0.65742000	2.37117500
Cartesian coordinates				H	-4.33351400	0.88233200	-0.41186200
ATOM	X	Y	Z	H	-2.52331000	-2.98701300	-0.81240200
C	0.02211000	1.30282600	3.61520200	N	-6.80324600	-2.54196700	-2.33650800
C	0.36523200	0.55225200	2.46580400	C	-7.98245300	-2.71764900	-1.50196700
C	1.22675000	1.13642500	1.51449600	H	-7.67896400	-3.10823300	-0.52559900
C	1.75081600	2.41781500	1.75030500	H	-8.57075400	-1.79859600	-1.33233400
C	1.40253700	3.13302700	2.89180100	H	-8.64611600	-3.45464400	-1.97033200
C	0.52736000	2.58698000	3.82459100	C	-7.04723700	-2.19377200	-3.72785500
C	-0.16806400	-0.84824500	2.43083800	H	-6.10409900	-2.23722600	-4.28240600
C	-1.20134500	-1.29212400	1.57946100	H	-7.73294700	-2.92791500	-4.16802000
C	0.30081300	-1.72568700	3.44086800	H	-7.48556200	-1.19156700	-3.88136300
C	-1.79360900	-2.54605400	1.80700200	N	-3.03936500	5.28359700	2.03072800
C	-0.25468500	-2.99543600	3.61208400	N	6.40466700	3.08982900	-2.54300900
C	-1.32283700	-3.38435800	2.81025000	N	3.39208500	-5.18105500	1.93392500
P	1.61020000	0.25559800	-0.06902000	C	-2.56357000	5.68148200	3.34683100
P	-1.68519600	-0.29761100	0.09149200	H	-2.36811700	6.76178500	3.34771600
C	2.20359600	-1.38616800	0.47421900	H	-3.26245700	5.47103400	4.17439500
C	1.69387000	-2.53604000	-0.12347900	H	-1.62252000	5.16485700	3.55960200
C	3.13618300	-1.50466000	1.51095100	C	-4.29321300	5.88790100	1.60782600
C	2.05037700	-3.81203800	0.32681700	H	-4.47968800	5.64633100	0.55635300
C	3.55656900	-2.75618000	1.96076600	H	-5.17159000	5.55881800	2.19203400
C	2.98973700	-3.92217700	1.37654000	H	-4.22042700	6.97856000	1.69928100
C	3.09590400	1.10633100	-0.74162500	C	6.74748300	2.72547200	-3.90915200
C	4.30860100	0.43316800	-0.90156800	H	7.34400900	3.52948700	-4.35685100
C	3.00258000	2.42673700	-1.20509000	H	7.32322000	1.78764200	-4.00505000
C	5.42124200	1.04768800	-1.49108600	H	5.82958000	2.61829900	-4.49636900
C	4.08844700	3.07853800	-1.79379700	C	7.51333600	3.47360400	-1.68197200
C	5.31568800	2.38370300	-1.93678100	H	8.22717600	2.66180700	-1.45722800
C	-2.11922800	1.36339400	0.72198400	H	8.07395300	4.28600500	-2.16021300
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C	-2.94320900	1.53125900	1.83630100	C	2.48030000	-5.75521500	2.91021000
C	-1.96805200	3.77886800	0.46013700	H	1.57663700	-6.21369700	2.46786800
C	-3.31722900	2.80918000	2.27075200	H	3.00271500	-6.52880200	3.48597800
C	-2.79143300	3.93914900	1.60164300	H	2.14978100	-4.97531500	3.60402000
C	-3.28371200	-0.99130900	-0.50276900	C	4.07958500	-6.14754400	1.08980000
C	-4.38607600	-0.15768500	-0.71252700	H	4.71702600	-5.61880700	0.37563500
C	-3.37339400	-2.32314100	-0.93021800	H	4.72432200	-6.77680500	1.71707900
C	-5.55696300	-0.62377500	-1.32524200	H	3.41537700	-6.81915300	0.52038900
C	-4.53259000	-2.83688900	-1.51387400	C	-6.67932100	0.37845500	-1.57401300
C	-5.64002700	-1.97876400	-1.71868900	H	-7.52023500	-0.14833500	-2.02593000
H	2.45387400	2.85983900	1.05886100	C	-6.23025000	1.46211600	-2.57425800
H	1.81657800	4.12410200	3.05232500	H	-5.39898900	2.05421800	-2.17243800
H	-2.64016400	-2.86978300	1.22096900	H	-5.89995600	1.01425000	-3.51841200
H	-1.79229500	-4.35105800	2.96915200	H	-7.05564200	2.14944300	-2.79227200

C	-7.18419800	1.00884300	-0.26372600	H	-0.36816000	5.76484100	1.52444300
H	-8.02803300	1.67924200	-0.46247000	C	-1.04819800	4.73670400	-1.72971100
H	-7.51502800	0.24140200	0.44453100	H	-0.20502900	4.04333400	-1.83902000
H	-6.39906800	1.59702900	0.22365500	H	-1.90250400	4.31715000	-2.27394400
C	-4.55723600	-4.30005200	-1.93300200	H	-0.75776200	5.67326700	-2.21758400
H	-5.55539100	-4.49364700	-2.33443700	C	4.62307000	-2.86845700	3.04846500
C	-3.53155700	-4.58072000	-3.04805300	H	4.29353200	-3.64196700	3.75236300
H	-2.50240500	-4.44286700	-2.69223800	C	4.84744500	-1.56594000	3.83369400
H	-3.62106100	-5.61506500	-3.39914900	H	5.35773400	-0.81254500	3.22070500
H	-3.68389200	-3.91518600	-3.90544600	H	3.90947200	-1.12771000	4.18481900
C	-4.33143400	-5.23586800	-0.73114100	H	5.48734500	-1.76179200	4.70076400
H	-3.33108600	-5.10419600	-0.29855300	C	5.96531100	-3.33895700	2.45020300
H	-5.06721200	-5.05030300	0.05927400	H	6.32866600	-2.61652300	1.70928500
H	-4.42077900	-6.28359000	-1.04022900	H	6.72444000	-3.42288600	3.23661900
C	3.92191500	4.51336000	-2.27408200	H	5.86964100	-4.31187600	1.96546300
H	4.87951600	4.80821800	-2.71072200	C	1.42064400	-5.02174100	-0.35854000
C	3.61780400	5.46533100	-1.10284000	H	1.59272000	-5.89948300	0.26713700
H	2.65861700	5.22714600	-0.62773200	C	-0.10558800	-4.89000500	-0.52227100
H	4.39758100	5.40916000	-0.33501600	H	-0.37213500	-4.08831400	-1.22166700
H	3.56259000	6.50161900	-1.45577200	H	-0.52351000	-5.82075500	-0.92216000
C	2.84396300	4.62049000	-3.36892500	H	-0.58942000	-4.67078800	0.43357900
H	2.79666000	5.64321500	-3.75992500	C	2.08867700	-5.27266700	-1.72510800
H	3.05897500	3.94582600	-4.20564600	H	1.94026900	-4.41099700	-2.38796200
H	1.84760400	4.37206200	-2.98288400	H	3.16689000	-5.42979800	-1.62261100
C	6.70438400	0.23171800	-1.60806800	H	1.65805800	-6.15417500	-2.21404000
H	7.45043000	0.83142600	-2.13057100	Rh	-0.09905900	-0.07868000	-1.68020400
C	7.27375500	-0.09867200	-0.21482900	C	-1.14671600	-1.45275500	-3.14309900
H	6.57220900	-0.71088300	0.36416100	H	-1.69476600	-2.12124300	-2.49110800
H	8.21175300	-0.65825600	-0.30478300	C	-1.71202500	-0.20978300	-3.36712900
H	7.47249400	0.81383300	0.35787900	H	-2.63519000	0.01391100	-2.83862400
C	6.48918800	-1.04746900	-2.43924500	C	-1.37066400	0.70479300	-4.52942200
H	5.78402500	-1.73174600	-1.95270400	H	-2.26179800	1.28056800	-4.80125600
H	6.09654600	-0.80959400	-3.43429600	H	-1.11805100	0.10400400	-5.40837600
H	7.43682400	-1.58327100	-2.56480300	C	-0.22839200	1.68650900	-4.19816200
H	0.24874000	3.14726200	4.70986700	H	0.20111500	2.09958000	-5.12397900
H	0.11217800	-3.66425300	4.38028800	H	-0.64381100	2.53944400	-3.65106500
O	1.29659100	-1.24248500	4.23558700	C	0.87866000	1.10431100	-3.34847800
O	-0.82628700	0.69863600	4.49634400	H	1.45602900	1.85060800	-2.81529800
C	1.65676700	-1.98458200	5.39454300	C	1.43881100	-0.15966400	-3.42994000
H	2.14685700	-2.93026200	5.12999200	H	2.38986900	-0.30607300	-2.92283600
H	2.36455200	-1.35983400	5.94081500	C	1.05999600	-1.22262500	-4.44686800
H	0.78268300	-2.18595200	6.02653600	H	1.94085000	-1.83685700	-4.66181200
C	-0.67008300	0.99909600	5.88030200	H	0.78739600	-0.74328900	-5.39199700
H	-1.07449500	1.98493700	6.13609500	C	-0.07916000	-2.14352500	-3.96155200
H	-1.23953400	0.23738100	6.41667600	H	-0.54743400	-2.65354200	-4.81751400
H	0.38616500	0.94742800	6.17027500	H	0.34799300	-2.93635200	-3.33744500
C	-4.27936300	2.93178600	3.44889200				
H	-4.56559300	3.98005600	3.54787600				
C	-5.58009900	2.14259000	3.21134100				
H	-5.39642200	1.06639200	3.11710500				
H	-6.26907500	2.28837300	4.05106100				
H	-6.08258800	2.47864300	2.29848800				
C	-3.60526300	2.50545200	4.76450000				
H	-3.27062200	1.46470200	4.71404500				
H	-2.72625600	3.12659800	4.96717700				
H	-4.29974200	2.60863600	5.60623300				
C	-1.38162500	4.99327200	-0.25222600				
H	-2.12539700	5.79476000	-0.20909500				
C	-0.12845500	5.49137300	0.49365300				
H	0.63420900	4.70532300	0.52230400				
H	0.29764800	6.36902800	-0.00656800				

## 2

B3LYP-D3 SCF energy: -241.459530 a.u.

B3LYP-D3 enthalpy: -241.354246 a.u.

B3LYP-D3 free energy: -241.394161 a.u.

M06 SCF energy in solution: -241.427090 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.12893700	0.00001200	0.00951700
C	-0.82573500	1.21208000	0.00219100
C	-2.22274400	1.20864400	0.00080700
C	-2.92204700	-0.00002800	0.00248600
C	-2.22274000	-1.20864200	0.00094700
C	-0.82568200	-1.21203600	0.00244700

H	-0.28014200	2.15030200	-0.00335000
H	-2.76250600	2.15188000	-0.00248100
H	-4.00868800	-0.00000300	-0.00034200
H	-2.76242300	-2.15192300	-0.00217800
H	-0.28010900	-2.15027100	-0.00271700
Se	1.85135800	-0.00010100	-0.04540400
H	2.03499800	0.00327500	1.44442900

### 3

B3LYP-D3 SCF energy: -4372.437014 a.u.

B3LYP-D3 enthalpy: -4370.557251 a.u.

B3LYP-D3 free energy: -4370.810935 a.u.

M06 SCF energy in solution: -4371.557048 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z
C	-0.29928200	4.38590200	-1.07873600
C	0.18542000	3.23117800	-0.42911800
C	1.05156500	2.37057800	-1.13050700
C	1.44996800	2.68669400	-2.43835000
C	0.97024600	3.84031200	-3.05407700
C	0.08868400	4.68767300	-2.38770200
C	-0.17878700	3.03717800	1.00833100
C	-1.03596100	2.01911800	1.46673300
C	0.35881700	3.94929200	1.94592000
C	-1.38061500	1.94755300	2.82616300
C	0.02169300	3.86287800	3.30023000
C	-0.85934500	2.87106700	3.72575400
P	1.60463900	0.81573700	-0.31111100
P	-1.55525700	0.66885400	0.31758600
C	2.59627800	1.38906200	1.10816800
C	2.41443300	0.80433500	2.35872100
C	3.55510100	2.39647900	0.94861800
C	3.18856600	1.18788900	3.46175100
C	4.35645800	2.79888000	2.01663300
C	4.18117800	2.17576400	3.28220400
C	2.78250900	0.00193200	-1.45497300
C	4.06137500	-0.37535800	-1.04059700
C	2.31292500	-0.45466100	-2.69407500
C	4.86050700	-1.22529400	-1.81836800
C	3.10448400	-1.24661300	-3.52898300
C	4.37566200	-1.67494900	-3.06853900
C	-2.40989400	1.48958900	-1.06823200
C	-2.10168500	1.09074200	-2.37194500
C	-3.36937600	2.48305000	-0.86550800
C	-2.73902000	1.65802800	-3.47543000
C	-4.04916400	3.06254700	-1.94378600
C	-3.70988400	2.66699400	-3.25905300
C	-2.81222700	-0.27115000	1.26717300
C	-4.19394300	-0.12663300	1.13849300
C	-2.31653900	-1.18895200	2.20317400
C	-5.07722600	-0.84899400	1.95640800
C	-3.15643800	-1.89015700	3.06514900
C	-4.55570900	-1.68391900	2.97471400
H	2.14296300	2.04919200	-2.97251500
H	1.28334900	4.08045600	-4.06591900
H	-2.04860200	1.17441500	3.18378700
H	-1.13115400	2.81246400	4.77566500
H	1.63254600	0.06108200	2.48222100
H	3.67097800	2.86508300	-0.02255700
H	4.43997300	-0.01977900	-0.08778000

H	1.30878100	-0.18959100	-3.01189900
H	-1.31458100	0.35833000	-2.51613200
H	-3.58794800	2.81520100	0.14524300
H	-4.59723900	0.54529800	0.38823000
H	-1.24097000	-1.32694000	2.28097200
N	-5.38118700	-2.31886800	3.95224300
C	-6.23614700	-1.49506400	4.79212400
H	-5.75228600	-0.52919100	4.96255300
H	-7.24344900	-1.30570000	4.38447700
H	-6.36254100	-1.98697300	5.76539100
C	-5.87505000	-3.65267300	3.66371100
H	-5.06835900	-4.26498500	3.25080600
H	-6.21860200	-4.12280500	4.59298600
H	-6.71817100	-3.66934700	2.94718600
N	-4.29437400	3.25941900	-4.42532000
N	5.10797100	-2.57168300	-3.91223800
N	5.04723200	2.61244000	4.33996800
C	-4.04636800	4.67073400	-4.67282500
H	-4.12073800	4.86607600	-5.75042300
H	-4.74199400	5.35933100	-4.16266200
H	-3.02933600	4.91810100	-4.35267300
C	-5.60301100	2.76815800	-4.82720500
H	-5.62034900	1.67569000	-4.75603100
H	-6.43985800	3.16099100	-4.22174600
H	-5.78886400	3.04395500	-5.87243900
C	5.25185700	-3.94720000	-3.45841300
H	5.45315800	-4.59162400	-4.32334900
H	6.06284000	-4.10946200	-2.72685300
H	4.31554700	-4.27852600	-2.99856800
C	6.23892700	-2.01844900	-4.64198500
H	7.14875500	-1.87012400	-4.03347700
H	6.49718800	-2.69082000	-5.46902300
H	5.95692000	-1.05022700	-5.06797300
C	4.46830300	3.53312000	5.30532600
H	3.77592300	3.06136400	6.02593200
H	5.27249000	4.01157700	5.87722400
H	3.91726500	4.31830100	4.77572800
C	5.99861200	1.65398400	4.88521800
H	6.37516200	1.01836000	4.07857800
H	6.84980500	2.19727100	5.31499200
H	5.59321700	0.99533400	5.67239300
C	-6.57522700	-0.71669900	1.69912000
H	-7.09217500	-1.44734600	2.32493800
C	-6.92762200	-1.05930100	0.23818400
H	-6.48742100	-0.34336100	-0.46569500
H	-6.57100500	-2.05984600	-0.03294900
H	-8.01389900	-1.03655400	0.09551600
C	-7.09522200	0.68390200	2.07305000
H	-8.17836800	0.74920800	1.91876300
H	-6.88442500	0.92100900	3.12090100
H	-6.62227200	1.45340900	1.45248900
C	-2.52882300	-2.82901000	4.08577500
H	-3.34115100	-3.26775700	4.67068900
C	-1.75548700	-3.96638100	3.38982600
H	-0.90685300	-3.57583900	2.81356500
H	-1.35774900	-4.66690500	4.13361500
H	-2.39442800	-4.52243000	2.69727300
C	-1.61836400	-2.06097700	5.06279700
H	-0.76399100	-1.60885000	4.54434200
H	-2.16772500	-1.25867500	5.56796500
H	-1.22068200	-2.73714900	5.82844200



C	2.57390500	-1.63382000	-4.90368700	H	7.08055000	2.54345700	2.42263400
H	3.39510500	-2.12404900	-5.43289400	C	2.91923000	0.50520300	4.79911700
C	2.14768000	-0.39448800	-5.71284300	H	3.57434300	0.94437200	5.55207700
H	1.28351400	0.11075500	-5.26606300	C	1.47391500	0.73920100	5.27459800
H	2.96349400	0.33395300	-5.78217400	H	0.74223400	0.32516500	4.57235500
H	1.86468900	-0.68618800	-6.73059200	H	1.31202400	0.26330900	6.24868600
C	1.41906900	-2.64655700	-4.79747600	H	1.26231900	1.80878000	5.37072600
H	1.01520700	-2.87831500	-5.78958400	C	3.24342400	-0.99953300	4.72646700
H	1.76402900	-3.58381300	-4.34988900	H	2.59374300	-1.51301200	4.00740700
H	0.59692700	-2.26272300	-4.18144300	H	4.28177300	-1.16577200	4.41812200
C	6.20966600	-1.65229300	-1.25076500	H	3.09758100	-1.47190200	5.70470400
H	6.72766900	-2.24980100	-2.00168900	Rh	0.08226100	-0.81949100	-0.07257900
C	7.10965500	-0.44304000	-0.93407000	C	-2.41222600	-3.89905100	-0.49372700
H	6.68102700	0.18725200	-0.14605500	C	-3.69838800	-3.64468900	-0.01719300
H	8.09232400	-0.78201100	-0.58738200	C	-4.42461400	-4.68624100	0.56272000
H	7.25687600	0.18230700	-1.82134900	C	-3.85549600	-5.95429500	0.70244900
C	6.01683800	-2.54312400	-0.00719200	C	-2.55494700	-6.18479200	0.24750300
H	5.54634000	-1.98294900	0.81055800	C	-1.83030300	-5.16124600	-0.36647500
H	5.38254500	-3.40792600	-0.23417800	H	-4.13484000	-2.65415100	-0.09091300
H	6.98175700	-2.91338600	0.35716300	H	-5.43621500	-4.49821400	0.90822700
H	-0.28322300	5.57841000	-2.88060200	H	-4.42403800	-6.75898600	1.15953700
H	0.43242100	4.55927200	4.02079000	H	-2.10368200	-7.16754600	0.35113600
O	1.20625000	4.88667500	1.43949600	H	-0.83712400	-5.35724900	-0.75393400
O	-1.14772400	5.16485700	-0.35196400	Se	-1.38544400	-2.49335100	-1.42067100
C	1.79716100	5.81885300	2.33432900	H	-2.58869600	-1.66148600	-1.70714700
H	2.43705000	5.31224900	3.06882600	C	1.73188600	-4.26618100	-0.04099800
H	2.41015500	6.47706100	1.71736600	C	1.61874800	-5.45645900	0.67903400
H	1.03785600	6.41525600	2.85634800	C	1.54314400	-6.66991500	-0.01167100
C	-1.22399800	6.54891000	-0.67498200	C	1.58564600	-6.68604400	-1.40713100
H	-1.74581600	6.72217300	-1.62362800	C	1.70028200	-5.48681800	-2.11707500
H	-1.79786100	7.01175600	0.12954900	C	1.76793500	-4.26811200	-1.43763500
H	-0.22188200	6.99271500	-0.72127700	H	1.58767700	-5.44130500	1.76399800
C	-5.13096100	4.09630300	-1.64817300	H	1.45425500	-7.59913200	0.54379100
H	-5.66227200	4.31264300	-2.57664900	H	1.52700600	-7.62932200	-1.94213300
C	-6.17627200	3.55702600	-0.65310200	H	1.72690800	-5.49898500	-3.20261200
H	-5.74486200	3.40043200	0.34214500	H	1.84215100	-3.33386000	-1.98451600
H	-7.00020000	4.27101400	-0.54334800	Se	1.75791800	-2.56608700	0.95714200
H	-6.59422100	2.60299800	-0.99416800	H	3.08531500	-2.11506800	0.43890000
C	-4.51604100	5.41341200	-1.14084500				
H	-3.91295000	5.24468000	-0.24205700				
H	-3.86235500	5.85374000	-1.90016800				
H	-5.30030600	6.14093300	-0.90171100				
C	-2.34674200	1.23478000	-4.88585900				
H	-3.20604000	1.42610900	-5.53444100				
C	-1.18587700	2.11040200	-5.39525200				
H	-0.30264600	1.98582200	-4.75875300				
H	-0.91433500	1.83698300	-6.42175700				
H	-1.46049000	3.16999800	-5.38173100				
C	-1.98856200	-0.25622100	-4.99571700				
H	-1.05994800	-0.49840200	-4.46515900				
H	-2.78240800	-0.89438400	-4.59064600				
H	-1.83489000	-0.52930800	-6.04538800				
C	5.43633100	3.85577200	1.81316100				
H	5.51199200	4.42661800	2.74428200				
C	5.13061400	4.83556300	0.66849000				
H	5.24101100	4.36110700	-0.31418300				
H	4.11207600	5.23180700	0.73116200				
H	5.83289500	5.67551600	0.69983700				
C	6.80366600	3.18168200	1.57961000				
H	6.77641900	2.56368500	0.67313700				
H	7.58892900	3.93575700	1.45059900				

**4-ts**  
B3LYP-D3 SCF energy: -4372.422439 a.u.  
B3LYP-D3 enthalpy: -4370.544479 a.u.  
B3LYP-D3 free energy: -4370.794743 a.u.  
M06 SCF energy in solution: -4371.542833 a.u.  
Imaginary frequency: -403.80 cm<sup>-1</sup>

Cartesian coordinates

ATOM	X	Y	Z
C	0.10272700	1.30294700	3.81850600
C	0.37887200	0.52053400	2.67593300
C	1.17802500	1.06960600	1.65501800
C	1.69001000	2.36922100	1.79575300
C	1.41247000	3.11857600	2.93550100
C	0.61874600	2.59371600	3.95104000
C	-0.17909600	-0.86354900	2.64674200
C	-1.16928600	-1.28340800	1.73531300
C	0.26956800	-1.77226100	3.63648200
C	-1.72255100	-2.56944500	1.85972300
C	-0.27100700	-3.05628300	3.73117600
C	-1.28088100	-3.43635500	2.85188200
P	1.54335700	0.09891900	0.11700900

P	-1.66216500	-0.22666300	0.28337700	C	6.30403500	4.88570800	-0.99527900
C	2.25184800	-1.45783100	0.76458300	H	7.14119200	4.56188600	-0.35326000
C	1.82153200	-2.66769500	0.22155200	H	6.63524700	5.77257600	-1.55009700
C	3.16856800	-1.47009100	1.82114800	H	5.47803700	5.18373700	-0.34284400
C	2.29023200	-3.89463700	0.70415000	C	2.97206900	-5.77056200	3.28244100
C	3.70176400	-2.66685300	2.30004400	H	2.12654500	-6.33618800	2.84993000
C	3.25419400	-3.89213900	1.73806300	H	3.58763600	-6.47348900	3.85683100
C	2.91403700	1.09782400	-0.59960900	H	2.55733100	-5.03290800	3.97766700
C	4.23173200	0.97813000	-0.15954300	C	4.57962300	-5.97560700	1.43779900
C	2.59416500	2.12826900	-1.49231800	H	5.14762900	-5.37450400	0.72169200
C	5.22243200	1.88620100	-0.55264100	H	5.29568300	-6.53669200	2.05216600
C	3.56698400	3.00948400	-1.97022800	H	3.98569400	-6.70950000	0.86761800
C	4.88866800	2.90869600	-1.46874200	C	-7.01636800	-0.59409600	0.30958800
C	-2.06386600	1.42866000	0.95524300	H	-7.83337000	-1.12381800	-0.18228600
C	-1.57798200	2.55332700	0.28157600	C	-7.23486900	0.90524000	0.05052900
C	-2.86265800	1.60514000	2.08817800	H	-6.45736200	1.52166800	0.51507600
C	-1.89439700	3.84666400	0.69710100	H	-7.23197100	1.12252500	-1.02019800
C	-3.22074400	2.88629400	2.52851600	H	-8.19861200	1.22055100	0.46614600
C	-2.71513400	4.01309400	1.83941700	C	-7.10674600	-0.91363600	1.81604600
C	-3.26016600	-0.98489100	-0.23500000	H	-8.07008300	-0.58526600	2.22319800
C	-4.50892900	-0.46788600	0.11094300	H	-7.00407300	-1.98828900	2.00058900
C	-3.20672400	-2.18574000	-0.95675800	H	-6.31326300	-0.40120300	2.37013200
C	-5.69581800	-1.12531400	-0.24210400	C	-4.24097900	-4.19491000	-2.07100900
C	-4.36480100	-2.86144600	-1.34666700	H	-5.25220700	-4.48529900	-2.36797200
C	-5.62568200	-2.31755500	-0.99861100	C	-3.37490400	-4.10622400	-3.33869400
H	2.31542900	2.79896000	1.02462500	H	-2.33225400	-3.85743500	-3.10736600
H	1.81449600	4.12293800	3.02943700	H	-3.37596100	-5.06775500	-3.86445700
H	-2.50636800	-2.90024800	1.19331200	H	-3.74980300	-3.34108600	-4.02716500
H	-1.72502700	-4.42392400	2.93927900	C	-3.69827600	-5.27170000	-1.11008100
H	1.08358500	-2.64475700	-0.57552300	H	-2.68393300	-5.02579200	-0.77076000
H	3.44605800	-0.53387000	2.28878400	H	-4.33476700	-5.36860900	-0.22299700
H	4.49962000	0.18206200	0.52255600	H	-3.65719300	-6.24761300	-1.60750200
H	1.56243000	2.25332600	-1.80709200	C	3.19605400	4.09196700	-2.97655800
H	-0.91575800	2.39612600	-0.56353100	H	4.10886800	4.33565700	-3.52798000
H	-3.20635400	0.73592400	2.64137200	C	2.74810900	5.37524900	-2.25027700
H	-4.57065000	0.45502900	0.67380400	H	1.85693300	5.18708800	-1.64200500
H	-2.23950700	-2.61813900	-1.19973800	H	3.53659000	5.74969200	-1.59059000
N	-6.79006000	-3.02409400	-1.44461900	H	2.50555600	6.16394300	-2.97225900
C	-7.52569000	-3.80919500	-0.46559600	C	2.13024000	3.64183800	-3.99005400
H	-6.81700800	-4.31560000	0.19730600	H	2.01003300	4.40301100	-4.76848800
H	-8.22090200	-3.22485500	0.16210500	H	2.40689400	2.69937400	-4.47698600
H	-8.11163300	-4.57788700	-0.98472800	H	1.14708700	3.50188400	-3.52449300
C	-7.58207000	-2.39976100	-2.49077800	C	6.58959900	1.79543200	0.12047000
H	-6.91346700	-1.99014400	-3.25461600	H	7.26784800	2.49017500	-0.37687700
H	-8.21309500	-3.16050500	-2.96617400	C	6.46912800	2.23948500	1.59326700
H	-8.24372500	-1.58371700	-2.14793300	H	5.81614100	1.55883000	2.15362700
N	-2.97692100	5.36009800	2.25217200	H	7.45198800	2.24044500	2.07829200
N	5.83497500	3.87921500	-1.93730300	H	6.04616500	3.24685600	1.67209300
N	3.80138700	-5.09489300	2.29727200	C	7.22961300	0.40143500	0.02245600
C	-2.46217600	5.80117800	3.53869100	H	6.61159000	-0.36994100	0.49579900
H	-2.28756600	6.88458400	3.50586600	H	7.37789300	0.11169700	-1.02017300
H	-3.12684000	5.59852900	4.39602300	H	8.20339600	0.39963600	0.52498800
H	-1.50417200	5.30814500	3.73019100	H	0.39875800	3.18282100	4.83425100
C	-4.25071200	5.93430400	1.85053400	H	0.07573100	-3.75255100	4.48453200
H	-4.45403900	5.67645500	0.80566300	O	1.24271400	-1.31316100	4.47314800
H	-5.11130900	5.59658500	2.45605900	O	-0.70292900	0.73120000	4.75945200
H	-4.19709200	7.02727400	1.92679100	C	1.60281300	-2.11189000	5.59257500
C	6.81914600	3.40854000	-2.89859700	H	2.10905200	-3.03446300	5.28068400
H	7.29979200	4.27200100	-3.37353100	H	2.29618000	-1.50869900	6.18007300
H	7.61489200	2.77441500	-2.46750400	H	0.72682000	-2.36100300	6.20465500
H	6.31457500	2.83025700	-3.67959600	C	-0.47086000	1.07044600	6.12324700

H	-0.84750700	2.07029400	6.36820200
H	-1.02198500	0.33452400	6.71219500
H	0.59816700	1.01046400	6.36002100
C	-4.13355000	3.02299600	3.74344800
H	-4.45108700	4.06470700	3.81335600
C	-5.41175200	2.17699900	3.60923600
H	-5.18856000	1.10459600	3.62128900
H	-6.08951400	2.37792800	4.44652200
H	-5.94401300	2.40124800	2.67862200
C	-3.38397300	2.67000800	5.04062300
H	-3.03288000	1.63399300	5.01328700
H	-2.50801100	3.31375900	5.17336400
H	-4.03752900	2.79537900	5.91178000
C	-1.31840900	5.06008900	-0.02650000
H	-2.02331700	5.88454300	0.11272500
C	0.00981000	5.48744600	0.62699400
H	0.76085600	4.69708200	0.52407700
H	0.39929200	6.39644500	0.15381600
H	-0.12618600	5.68608900	1.69427300
C	-1.13050700	4.84987000	-1.53670700
H	-0.38281100	4.07849400	-1.75597000
H	-2.06601700	4.56212600	-2.02836100
H	-0.77817100	5.77625700	-2.00300700
C	4.77430200	-2.65022900	3.38649800
H	4.54625400	-3.46006800	4.08899400
C	4.83915400	-1.33164200	4.17513400
H	5.26259400	-0.52125900	3.56789800
H	3.85371300	-1.00626500	4.51962000
H	5.49182400	-1.45245900	5.04636200
C	6.16023400	-2.94945200	2.77790300
H	6.42508000	-2.18417100	2.03764800
H	6.93061800	-2.94346200	3.55789600
H	6.17954200	-3.92496400	2.28836200
C	1.75443800	-5.17563900	0.06894400
H	2.06603600	-6.02035400	0.68523100
C	0.21623300	-5.21140800	0.01459300
H	-0.18731100	-4.42257200	-0.63112800
H	-0.12379600	-6.17223800	-0.38836300
H	-0.21711500	-5.07661100	1.00880800
C	2.34666400	-5.37785200	-1.33969400
H	2.00559900	-4.58852200	-2.02081500
H	3.44178900	-5.35989100	-1.32298900
H	2.02759700	-6.33843800	-1.76000900
Rh	-0.11838500	-0.27740500	-1.41377900
C	3.44530400	-0.90439800	-3.16110400
C	4.33765400	-0.03169500	-3.78880600
C	5.70943600	-0.24219100	-3.64349200
C	6.18136100	-1.32016400	-2.89025200
C	5.28116500	-2.17440700	-2.25260800
C	3.90716900	-1.97105500	-2.38867500
H	3.97186500	0.79264100	-4.39151000
H	6.40952900	0.42799100	-4.13307900
H	7.24980000	-1.49412800	-2.80363300
H	5.64115500	-3.00422300	-1.65093500
H	3.21133300	-2.63495800	-1.89476300
Se	1.52564500	-0.78870800	-3.56950900
H	1.18802700	0.57146000	-2.91393400
C	-3.42971200	0.60564600	-3.15853800
C	-4.67561800	0.15293700	-3.59069000
C	-5.78481900	0.99090000	-3.45341400
C	-5.64263900	2.25736900	-2.88274000

C	-4.39169100	2.68763000	-2.43529300
C	-3.27628300	1.86150400	-2.57642600
H	-4.78216600	-0.83371100	-4.02932000
H	-6.75926300	0.64910100	-3.79011100
H	-6.50848300	2.90446900	-2.77746100
H	-4.28018300	3.66260600	-1.96953900
H	-2.30408700	2.18492800	-2.23023900
Se	-1.88064300	-0.59285900	-3.38902700
H	-1.21093200	0.25529900	-4.42777900

## 5

B3LYP-D3 SCF energy: -4372.445771 a.u.

B3LYP-D3 enthalpy: -4370.565478 a.u.

B3LYP-D3 free energy: -4370.818016 a.u.

M06 SCF energy in solution: -4371.562589 a.u.

## Cartesian coordinates

ATOM	X	Y	Z
C	0.05835700	1.93439700	3.47546000
C	0.37627000	0.97846500	2.48612300
C	1.18924900	1.37049200	1.40204800
C	1.67103000	2.68718400	1.33251800
C	1.35869700	3.60566200	2.33107000
C	0.55149100	3.23909000	3.40319900
C	-0.14213900	-0.40725100	2.69093900
C	-1.12320300	-0.99525900	1.86785300
C	0.32839400	-1.13430500	3.81081600
C	-1.62077800	-2.27467300	2.16870100
C	-0.15934400	-2.41401000	4.08971300
C	-1.14106300	-2.96838200	3.27298800
P	1.65388300	0.16901700	0.06987600
P	-1.70106500	-0.13617700	0.33539300
C	2.36928500	-1.23042600	0.99402800
C	2.01992500	-2.54251100	0.68369000
C	3.26553600	-0.98772500	2.04296500
C	2.56596800	-3.62662400	1.38193200
C	3.87048100	-2.03900800	2.73027000
C	3.51923500	-3.37320700	2.39304900
C	2.98560700	1.05838800	-0.81323900
C	4.30188000	1.06309200	-0.35057400
C	2.63584400	1.91390900	-1.86223500
C	5.26028200	1.93025400	-0.88598000
C	3.57094700	2.76700300	-2.44945900
C	4.90231500	2.76898000	-1.96636100
C	-2.24551600	1.52982800	0.85392200
C	-1.84699500	2.65831600	0.13342900
C	-3.08792800	1.69742300	1.95883500
C	-2.29912000	3.93733700	0.46051700
C	-3.57627100	2.96008400	2.31509600
C	-3.16632100	4.09118100	1.56902400
C	-3.18260300	-1.10224700	-0.15578800
C	-4.48986200	-0.74022800	0.16030100
C	-2.95526700	-2.32366200	-0.81078300
C	-5.57188700	-1.57681600	-0.15680300
C	-4.00510800	-3.16016900	-1.18593300
C	-5.33261700	-2.77067600	-0.87130200
H	2.30359000	2.99636900	0.51076800
H	1.74505800	4.61828700	2.26877000
H	-2.38741600	-2.72686100	1.55441800
H	-1.53593900	-3.95360100	3.50298500
H	1.31942200	-2.73143200	-0.12156800

H	3.48159900	0.03402400	2.32924500	H	-2.20579900	-5.18114200	-0.53267000
H	4.59321400	0.40199700	0.45545000	H	-2.28491600	-6.07171400	-2.06349200
H	1.61978200	1.90480800	-2.24106500	C	3.12761400	3.66800600	-3.59379000
H	-1.14489200	2.54417900	-0.68460600	H	3.98392700	4.29331700	-3.85914600
H	-3.36343600	0.83346100	2.55608600	C	1.96855900	4.58957700	-3.17045000
H	-4.68116200	0.19228100	0.67761500	H	1.06206400	4.01819200	-2.93463600
H	-1.93598100	-2.63387600	-1.01803900	H	2.22853400	5.17733000	-2.28242800
N	-6.38060300	-3.64765500	-1.30378500	H	1.71666800	5.28578300	-3.97855700
C	-6.94137900	-4.54679900	-0.30561400	C	2.75126100	2.84074500	-4.83679600
H	-6.13203400	-4.97241500	0.29651100	H	2.44239300	3.49705000	-5.65862000
H	-7.66110400	-4.06821200	0.38170500	H	3.60294200	2.24403200	-5.18020900
H	-7.45859300	-5.37135400	-0.81104700	H	1.92322800	2.15233700	-4.62396400
C	-7.32032100	-3.14416000	-2.29319700	C	6.62669700	1.99166800	-0.20852900
H	-6.78109500	-2.53945000	-3.02751800	H	7.21907400	2.76505000	-0.69922700
H	-7.77534800	-3.99262600	-2.81905500	C	6.47989100	2.41710500	1.26630300
H	-8.14044600	-2.52737000	-1.88517100	H	5.93789100	1.66335100	1.84900400
N	-3.57779000	5.42354100	1.89240000	H	7.46628000	2.54565700	1.72631400
N	5.83754200	3.63286200	-2.61852500	H	5.93369300	3.36299400	1.35337600
N	4.16351500	-4.41641100	3.13772000	C	7.40089000	0.66811600	-0.32636300
C	-3.11491900	5.99980000	3.14451900	H	6.84640700	-0.16128200	0.12869600
H	-3.09273400	7.09312200	3.05180900	H	7.57653400	0.40792100	-1.37360000
H	-3.73403500	5.75365100	4.02444000	H	8.36972700	0.74508800	0.18023600
H	-2.09442100	5.65590400	3.34103900	H	0.30522000	3.96089700	4.17372800
C	-4.89956600	5.83279000	1.44643000	H	0.21110700	-2.97616900	4.93775000
H	-5.05501600	5.49826100	0.41514100	O	1.26252000	-0.51150600	4.58093900
H	-5.72982600	5.43844700	2.05970500	O	-0.75671000	1.50930100	4.48252900
H	-4.96418900	6.92748000	1.46094200	C	1.64448000	-1.12444000	5.80679900
C	6.98646400	3.03089900	-3.27775000	H	2.20229200	-2.05310900	5.63217400
H	7.30962700	3.68063300	-4.10121500	H	2.29558500	-0.40829700	6.30918400
H	7.86056600	2.86413900	-2.62487300	H	0.77196000	-1.33021600	6.43932200
H	6.69180100	2.06604400	-3.69856800	C	-0.54866000	2.06475700	5.77792700
C	6.06553900	4.93231100	-2.00768200	H	-0.91697100	3.09467000	5.84969200
H	6.71876500	4.90136200	-1.11652500	H	-1.12163700	1.44086900	6.46635800
H	6.53014700	5.60301500	-2.74062600	H	0.51455000	2.03454400	6.04412300
H	5.10684100	5.36897700	-1.70828300	C	-4.53263600	3.07074100	3.49863100
C	3.38532200	-5.00270800	4.21709500	H	-4.93751400	4.08385800	3.51419800
H	2.59367300	-5.69632500	3.87966800	C	-5.73104400	2.11439600	3.36375300
H	4.05337500	-5.55647800	4.88771600	H	-5.42053900	1.06632200	3.43454700
H	2.90630300	-4.20602100	4.79676500	H	-6.45327100	2.29496000	4.16768600
C	5.02555200	-5.34732200	2.42089900	H	-6.24544700	2.25044600	2.40609900
H	5.54082600	-4.81708500	1.61494800	C	-3.79675300	2.84055600	4.83070100
H	5.78469500	-5.73765300	3.11082000	H	-3.33233100	1.84938500	4.85464300
H	4.50368800	-6.21146800	1.97705100	H	-3.00305300	3.58140800	4.96903400
C	-6.95086200	-1.21720500	0.39019900	H	-4.49168500	2.92118300	5.67451600
H	-7.67945100	-1.91517300	-0.02304500	C	-1.82543800	5.13684400	-0.35327300
C	-7.41247100	0.19721500	0.00407900	H	-2.46048800	5.98024100	-0.07072000
H	-6.72659500	0.96817000	0.37287100	C	-0.37631900	5.50623200	0.01276400
H	-7.47696400	0.30458700	-1.08172000	H	0.31077800	4.68812000	-0.23130600
H	-8.40082700	0.40043900	0.43141600	H	-0.05611300	6.39738600	-0.53966800
C	-6.96301000	-1.41048200	1.92046200	H	-0.28256900	5.71116800	1.08409300
H	-7.96005500	-1.20443000	2.32634600	C	-1.95745500	4.92245000	-1.87067300
H	-6.68730300	-2.43567000	2.19077400	H	-1.29379000	4.12785300	-2.23358000
H	-6.25391900	-0.73315000	2.40810700	H	-2.98229500	4.66303100	-2.15680500
C	-3.72915900	-4.45908500	-1.93555500	H	-1.68079400	5.83776200	-2.40537800
H	-4.50185600	-5.17340800	-1.63618200	C	4.93070600	-1.75397800	3.79017800
C	-3.87840600	-4.24410600	-3.45502500	H	4.78230700	-2.47052100	4.60563200
H	-3.13250900	-3.52831800	-3.82092400	C	4.86076200	-0.33328200	4.37444100
H	-3.73091100	-5.18738300	-3.99315800	H	5.22265400	0.41452900	3.65837000
H	-4.87550100	-3.86716000	-3.70174900	H	3.84322500	-0.05104600	4.65737300
C	-2.35879800	-5.07630800	-1.61288700	H	5.50278500	-0.26385600	5.25904900
H	-1.53018100	-4.48133200	-2.01689000	C	6.34004100	-2.00242700	3.21284100

H	6.52864900	-1.33341600	2.36361700
H	7.10559500	-1.80612300	3.97260500
H	6.45545900	-3.03329900	2.87182000
C	2.12739800	-5.03258600	0.98058700
H	2.54806100	-5.74197200	1.69434400
C	0.59867300	-5.20272800	1.03615400
H	0.08873100	-4.54203500	0.32652600
H	0.32553600	-6.23334100	0.78208900
H	0.21435300	-4.97686500	2.03472000
C	2.66529000	-5.39708100	-0.41721300
H	2.23737900	-4.74369100	-1.18689900
H	3.75572500	-5.30200000	-0.46313900
H	2.40282700	-6.43012000	-0.67230700
Rh	-0.07978700	-0.38104000	-1.34586100
Se	1.37091400	-1.66090000	-2.97521000
C	3.31651800	-1.43700100	-2.89272000
C	3.92610800	-0.62412100	-3.85628400
C	4.10871800	-2.16486000	-1.99742300
C	5.31739800	-0.55166400	-3.93024400
H	3.31436900	-0.06346900	-4.55416300
C	5.50032300	-2.08450500	-2.07395600
H	3.64842300	-2.79655600	-1.24948300
C	6.10879300	-1.28637300	-3.04450900
H	5.78101700	0.06618500	-4.69485800
H	6.10821200	-2.65620500	-1.37744600
H	7.19175500	-1.24431900	-3.11649900
H	-0.25918300	1.12218200	-1.56112400
C	-3.45135000	0.26173400	-3.18988400
C	-4.61974400	-0.37896500	-3.60358000
C	-5.84112000	0.28645800	-3.47247700
C	-5.88944900	1.56897300	-2.92372300
C	-4.71449100	2.19029900	-2.49686300
C	-3.48828300	1.53980100	-2.63506100
H	-4.58148900	-1.37616900	-4.02868000
H	-6.75437700	-0.19987000	-3.80247200
H	-6.84172000	2.08114700	-2.82360800
H	-4.74714600	3.17936400	-2.04992800
H	-2.57839400	2.02338200	-2.30753500
Se	-1.74423200	-0.69838800	-3.42199100
H	-1.09665300	0.33846400	-4.27260000

## 6

B3LYP-D3 SCF energy: -408.884183 a.u.

B3LYP-D3 enthalpy: -408.750038 a.u.

B3LYP-D3 free energy: -408.791482 a.u.

M06 SCF energy in solution: -408.707820 a.u

Cartesian coordinates

ATOM	X	Y	Z
C	0.98304800	-1.22190000	0.00025700
C	-0.39756300	-1.05394800	0.00043300
C	-0.97891100	0.22896300	0.00028600
C	-0.11661200	1.33981500	0.00001000
C	1.26954700	1.19094700	-0.00016000
C	1.79899200	-0.09310100	-0.00005200
H	1.43741500	-2.20721500	0.00034200
H	-1.03095100	-1.93558300	0.00074700
H	-0.54023400	2.34116400	-0.00008600
H	1.93676200	2.04640700	-0.00036400
F	3.13865100	-0.25416600	-0.00029800
C	-2.43334400	0.45413100	0.00039800

H	-2.72747300	1.50400100	0.00131500
C	-3.40361800	-0.46916800	-0.00065900
H	-3.20302900	-1.53728600	-0.00175900
H	-4.44957700	-0.17842900	-0.00059000

## 7

B3LYP-D3 SCF energy: -4539.849992 a.u.

B3LYP-D3 enthalpy: -4537.941146 a.u.

B3LYP-D3 free energy: -4538.195187 a.u.

M06 SCF energy in solution: -4538.822115 a.u

Cartesian coordinates

ATOM	X	Y	Z
C	0.34019300	-4.22942400	1.14486700
C	-0.08184500	-2.88505300	1.09236900
C	-0.85632400	-2.46300500	-0.00658000
C	-1.18926700	-3.36983200	-1.02527100
C	-0.76461400	-4.69372900	-0.94769800
C	-0.00214600	-5.13030500	0.13195000
C	0.29300200	-2.00242300	2.23748000
C	1.24208500	-0.96737100	2.13063200
C	-0.28638300	-2.27072800	3.49982900
C	1.60292100	-0.22548900	3.26649000
C	0.04913000	-1.49926700	4.61677900
C	1.00081400	-0.48989100	4.49227700
P	-1.50054400	-0.74060600	-0.09753000
P	1.83191500	-0.43540600	0.46122700
C	-2.50414200	-0.55718900	1.40671200
C	-2.51481900	0.61509400	2.15520300
C	-3.31346500	-1.63362600	1.79850400
C	-3.29709300	0.73225000	3.30964400
C	-4.16968900	-1.52663100	2.89381600
C	-4.16002700	-0.32979700	3.65948600
C	-2.61936000	-0.73796100	-1.53835900
C	-3.99572200	-0.88984200	-1.39776200
C	-2.07565100	-0.53549900	-2.81602200
C	-4.84586400	-0.84786600	-2.50991000
C	-2.89583800	-0.41526600	-3.93692700
C	-4.29906700	-0.56068800	-3.77942300
C	2.47716100	-1.90698800	-0.39777800
C	2.13759800	-2.11218100	-1.73631600
C	3.35084700	-2.80046700	0.23025800
C	2.66484700	-3.17907400	-2.46699500
C	3.90403800	-3.88027700	-0.46664900
C	3.54192000	-4.08226900	-1.82126500
C	3.26805900	0.66614700	0.74864800
C	4.55927100	0.31655800	0.35020600
C	3.05833400	1.92773300	1.32811300
C	5.63980400	1.19218900	0.52182300
C	4.12422400	2.78732600	1.60514600
C	5.43048600	2.42297000	1.18369400
H	-1.79246900	-3.05200600	-1.86600300
H	-1.03329200	-5.39164500	-1.73479400
H	2.35361100	0.55088500	3.20371200
H	1.27777200	0.09483900	5.36470700
H	-1.91029300	1.45672100	1.84461000
H	-3.27921500	-2.55593200	1.23170100
H	-4.42381900	-1.03884600	-0.41380800
H	-1.00078700	-0.42687800	-2.92880100
H	1.42674700	-1.44556200	-2.21419900
H	3.60404200	-2.65246100	1.27607800

H	4.73419200	-0.64368100	-0.11991400	H	-0.15084800	-0.00460000	-4.84892400
H	2.05274000	2.23078600	1.60458300	H	-0.77365900	-1.59013600	-5.33429900
N	6.48651900	3.34696200	1.45654200	H	-0.55550700	-0.30401200	-6.53495800
C	7.56942000	2.93728500	2.33776500	C	-2.38327600	1.51284000	-5.43540100
H	7.17274700	2.28591800	3.12196000	H	-1.94430800	1.83305200	-6.38772300
H	8.39652300	2.40685600	1.83636300	H	-3.42087400	1.85609000	-5.40246200
H	7.99366600	3.82729800	2.81986600	H	-1.84354300	2.00398300	-4.61627600
C	6.86158800	4.25382100	0.38242300	C	-6.32929800	-1.11625800	-2.28059800
H	5.96265300	4.60983900	-0.12948100	H	-6.83313300	-1.12014200	-3.24815900
H	7.38060100	5.12354700	0.80339500	C	-6.55003000	-2.50937700	-1.65886500
H	7.52542900	3.79866200	-0.37485200	H	-6.10168300	-2.58266200	-0.66091400
N	4.01556900	-5.19257400	-2.59045100	H	-7.62166000	-2.71365200	-1.55561700
N	-5.10044000	-0.38323800	-4.95199600	H	-6.10998500	-3.29558600	-2.28249800
N	-5.06301300	-0.26533000	4.77155400	C	-6.97455500	-0.01472700	-1.41868400
C	3.57582900	-6.52326400	-2.20282500	H	-6.52655100	0.01969900	-0.41836900
H	3.62017300	-7.18594900	-3.07635100	H	-6.84606900	0.97221900	-1.87546200
H	4.16978100	-6.99267300	-1.39939300	H	-8.04773700	-0.20158800	-1.29859300
H	2.53461100	-6.47247200	-1.86841000	H	0.32701100	-6.16195200	0.18528000
C	5.35734900	-5.09271900	-3.14265600	H	-0.41143200	-1.68456500	5.57900300
H	5.50344100	-4.09254100	-3.56361000	O	-1.16877000	-3.30544800	3.54013700
H	6.16538100	-5.27502700	-2.41150700	O	1.09915800	-4.57648800	2.22084900
H	5.47011000	-5.82205400	-3.95386200	C	-1.74861100	-3.64940600	4.79277400
C	-6.06861600	0.70509300	-4.96522700	H	-2.38101500	-2.83685200	5.16954900
H	-6.23979700	1.01777200	-6.00315700	H	-2.36751400	-4.52707600	4.60552000
H	-7.05008400	0.45585600	-4.52779700	H	-0.98031800	-3.89692300	5.53585600
H	-5.66160300	1.55863600	-4.41566400	C	0.96322500	-5.90195100	2.72870400
C	-5.51191000	-1.59464900	-5.64564600	H	1.45697200	-6.64094500	2.08769400
H	-6.34115700	-2.13407800	-5.15342400	H	1.45477900	-5.89903600	3.70314800
H	-5.83492900	-1.33875200	-6.66190300	H	-0.09530800	-6.16218500	2.84672600
H	-4.66171900	-2.28060000	-5.72151800	C	4.88375500	-4.79642400	0.25982300
C	-4.50230100	-0.56100200	6.08005000	H	5.30344500	-5.49246300	-0.46766700
H	-3.86618300	0.24343400	6.49153200	C	6.06698000	-4.00955500	0.85207200
H	-5.31751900	-0.74137500	6.79080000	H	5.74350700	-3.30984400	1.63121800
H	-3.89758500	-1.47251800	6.02544800	H	6.79104300	-4.69557600	1.30569900
C	-6.08826000	0.77155700	4.76160000	H	6.58351600	-3.43536500	0.07516700
H	-6.42649200	0.93607000	3.73476200	C	4.16964900	-5.62895600	1.33922500
H	-6.94737100	0.42923600	5.35261000	H	3.68771100	-4.98480200	2.08174200
H	-5.76710600	1.74280000	5.17218300	H	3.39221400	-6.25595600	0.88970800
C	7.00522300	0.76638300	-0.00726600	H	4.88106700	-6.28379000	1.85525800
H	7.67040400	1.63082400	0.03422700	C	2.27405400	-3.34606400	-3.92906300
C	6.94009100	0.32579800	-1.48238700	H	2.88892600	-4.15521400	-4.33089700
H	6.35528100	-0.59277400	-1.60990300	C	0.80109200	-3.77226500	-4.06163700
H	6.48812500	1.10277000	-2.10886100	H	0.12879500	-3.02482500	-3.62460500
H	7.94948700	0.12668400	-1.85931300	H	0.53030500	-3.89786100	-5.11645700
C	7.61410200	-0.34311400	0.87115200	H	0.62041000	-4.72033000	-3.54471000
H	8.60531900	-0.62925000	0.50110100	C	2.56003900	-2.07235400	-4.74521400
H	7.71847400	-0.01779300	1.91126400	H	1.93253300	-1.23182100	-4.42490800
H	6.97997800	-1.23617300	0.86206500	H	3.60740000	-1.76482300	-4.64929000
C	3.87730700	4.07592200	2.37983300	H	2.35084000	-2.24530200	-5.80684700
H	4.86211400	4.44498400	2.67856900	C	-5.13531200	-2.66097500	3.22674000
C	3.21633700	5.15273300	1.50258200	H	-5.16143600	-2.76467400	4.31725500
H	2.21518500	4.84520500	1.18637600	C	-4.73116800	-4.01675600	2.62368200
H	3.11279800	6.09167700	2.05907900	H	-4.88428600	-4.03540200	1.53724900
H	3.81198500	5.35704400	0.60574500	H	-3.68075800	-4.25963700	2.81220800
C	3.05082400	3.82932800	3.65558700	H	-5.35358600	-4.81168000	3.04799300
H	2.03011800	3.49698000	3.42853700	C	-6.56353000	-2.29879100	2.76814500
H	3.51790300	3.06804400	4.29086400	H	-6.59063500	-2.14624600	1.68200200
H	2.97083100	4.75400800	4.23831700	H	-7.26096800	-3.10878600	3.01172000
C	-2.30522900	-0.02088800	-5.28527700	H	-6.91690300	-1.38681200	3.25313100
H	-2.93580500	-0.45699000	-6.06520000	C	-3.16302800	2.01254400	4.12789500
C	-0.86784100	-0.51304900	-5.50630900	H	-3.74361600	1.89814500	5.04452500

C	-1.70123900	2.24950900	4.55788000	P	-1.90046300	-0.18295600	-0.35316400
H	-1.05515500	2.45108000	3.69689000	C	2.14834800	-1.52058500	-1.42415500
H	-1.64105800	3.11745800	5.22435700	C	2.19746000	-0.48388300	-2.35160600
H	-1.29595800	1.37762400	5.08268100	C	2.75050500	-2.74750400	-1.72666700
C	-3.71921200	3.22854300	3.36140100	C	2.80100800	-0.65281500	-3.60291400
H	-3.16109400	3.40465000	2.43560100	C	3.40485800	-2.94429800	-2.94243700
H	-4.77235900	3.08137700	3.09894600	C	3.41899700	-1.88882900	-3.89512500
H	-3.64167600	4.13438600	3.97352200	C	2.62087100	-1.20159600	1.44088100
Rh	0.09312400	0.81450100	-0.53613400	C	3.97196300	-1.18389300	1.10436600
C	-1.43999600	3.98850100	0.00970900	C	2.24907000	-0.91223200	2.76206700
C	-2.01774700	5.20825200	-0.37769700	C	4.95868000	-0.88369300	2.05351500
C	-1.78333900	6.37243000	0.35350400	C	3.19790800	-0.59194300	3.73320400
C	-0.97050700	6.34509500	1.48972500	C	4.57065000	-0.57199300	3.37478800
C	-0.39854600	5.13680000	1.88770400	C	-2.80221200	-1.21535300	0.84475400
C	-0.62497000	3.97093200	1.15206900	C	-2.41240400	-1.15055400	2.18655900
H	-2.64423500	5.24850600	-1.26356800	C	-3.88046200	-2.02514600	0.48366300
H	-2.22945800	7.30744300	0.02570800	C	-3.05654200	-1.90019600	3.16939300
H	-0.78956200	7.25276400	2.05798100	C	-4.58857300	-2.75393200	1.44804500
H	0.22891800	5.09460300	2.77390300	C	-4.14487900	-2.72454100	2.79072400
H	-0.16439600	3.04437900	1.47870500	C	-3.06253600	1.11264200	-0.92686600
Se	-1.89952400	2.40486200	-1.04730500	C	-4.41474500	1.12136800	-0.58426600
H	-0.19435500	1.16393900	0.91358400	C	-2.56626600	2.14900400	-1.72987600
C	1.40357900	5.90987400	-1.43279000	C	-5.27457100	2.13753900	-1.02504000
C	1.60993300	4.54883100	-1.61010400	C	-3.40170200	3.13688500	-2.24958200
C	0.88611700	3.82746100	-2.57710000	C	-4.77489800	3.13574700	-1.89217100
C	-0.05041800	4.51546500	-3.36941000	H	1.37461400	-3.30576700	2.31770400
C	-0.26163200	5.88141000	-3.21073900	H	-0.00686200	-5.29524700	2.77228400
C	0.46231900	6.55346000	-2.23271500	H	-2.31642500	0.26433500	-3.22146500
H	1.93072000	6.47443500	-0.67314900	H	-1.61674300	-0.93881900	-5.23977500
H	2.32625700	4.03806100	-0.97571700	H	1.73982800	0.46612600	-2.10437500
H	-0.62452300	3.97026400	-4.11216800	H	2.70093700	-3.55004000	-1.00003800
H	-0.98597800	6.42303600	-3.80902700	H	4.26894600	-1.38322600	0.08079000
F	0.23467600	7.86362200	-2.03778300	H	1.19423500	-0.90582200	3.03403700
C	1.05701800	2.39267500	-2.78355800	H	-1.57264900	-0.51991300	2.46390900
H	0.39004000	1.95928200	-3.52717600	H	-4.17786300	-2.08608600	-0.55902700
C	1.97673900	1.57013300	-2.20866900	H	-4.81145500	0.33988400	0.05310800
H	2.74011400	1.93666000	-1.53058200	H	-1.50857600	2.17323500	-1.97605700
H	2.12618400	0.56556500	-2.59076100	N	-5.59063900	4.17822800	-2.43312200

### 8-ts-R

B3LYP-D3 SCF energy: -4539.839616 a.u.

B3LYP-D3 enthalpy: -4537.933400 a.u.

B3LYP-D3 free energy: -4538.186627 a.u.

M06 SCF energy in solution: -4538.810124 a.u.

Imaginary frequency: -98.89 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z
C	-1.41261000	-4.33349500	-0.16374600
C	-0.65442600	-3.17597100	-0.43158500
C	0.35639700	-2.80342200	0.47697300
C	0.58529100	-3.57528500	1.62648600
C	-0.18857600	-4.70602800	1.87825100
C	-1.18953100	-5.09017200	0.98967200
C	-0.90923400	-2.47299100	-1.72816200
C	-1.54471700	-1.21959200	-1.84460900
C	-0.53480800	-3.15635400	-2.91132600
C	-1.80356000	-0.68205300	-3.11702900
C	-0.76545600	-2.59521100	-4.16983700
C	-1.41262300	-1.36581000	-4.26198900
P	1.31155100	-1.25924700	0.16869000

P	-1.90046300	-0.18295600	-0.35316400
C	2.14834800	-1.52058500	-1.42415500
C	2.19746000	-0.48388300	-2.35160600
C	2.75050500	-2.74750400	-1.72666700
C	2.80100800	-0.65281500	-3.60291400
C	3.40485800	-2.94429800	-2.94243700
C	3.41899700	-1.88882900	-3.89512500
C	2.62087100	-1.20159600	1.44088100
C	3.97196300	-1.18389300	1.10436600
C	2.24907000	-0.91223200	2.76206700
C	4.95868000	-0.88369300	2.05351500
C	3.19790800	-0.59194300	3.73320400
C	4.57065000	-0.57199300	3.37478800
C	-2.80221200	-1.21535300	0.84475400
C	-2.41240400	-1.15055400	2.18655900
C	-3.88046200	-2.02514600	0.48366300
C	-3.05654200	-1.90019600	3.16939300
C	-4.58857300	-2.75393200	1.44804500
C	-4.14487900	-2.72454100	2.79072400
C	-3.06253600	1.11264200	-0.92686600
C	-4.41474500	1.12136800	-0.58426600
C	-2.56626600	2.14900400	-1.72987600
C	-5.27457100	2.13753900	-1.02504000
C	-3.40170200	3.13688500	-2.24958200
C	-4.77489800	3.13574700	-1.89217100
H	1.37461400	-3.30576700	2.31770400
H	-0.00686200	-5.29524700	2.77228400
H	-2.31642500	0.26433500	-3.22146500
H	-1.61674300	-0.93881900	-5.23977500
H	1.73982800	0.46612600	-2.10437500
H	2.70093700	-3.55004000	-1.00003800
H	4.26894600	-1.38322600	0.08079000
H	1.19423500	-0.90582200	3.03403700
H	-1.57264900	-0.51991300	2.46390900
H	-4.17786300	-2.08608600	-0.55902700
H	-4.81145500	0.33988400	0.05310800
H	-1.50857600	2.17323500	-1.97605700
N	-5.59063900	4.17822800	-2.43312200
C	-6.70366000	3.82642500	-3.30101400
H	-6.43253000	2.95259600	-3.90064700
H	-7.64757000	3.60209000	-2.77617800
H	-6.89900600	4.66022400	-3.98758000
C	-5.78633900	5.35136200	-1.59595600
H	-4.83485100	5.63472900	-1.13424600
H	-6.12636300	6.18923700	-2.21659100
H	-6.52617900	5.20700800	-0.78780800
N	-4.73885500	-3.51759900	3.82381500
N	5.50697300	-0.19665000	4.39226900
N	4.06722300	-2.15997800	-5.14584300
C	-4.68415500	-4.96544000	3.69416100
H	-4.70713900	-5.41695300	4.69440100
H	-5.50975000	-5.40879100	3.11158100
H	-3.74137100	-5.24759400	3.21520500
C	-5.93538900	-2.98708300	4.45936400
H	-5.80714000	-1.91588900	4.64541300
H	-6.85708600	-3.11985000	3.86468700
H	-6.08562900	-3.48538400	5.42484400
C	6.15060200	1.10146600	4.25721100
H	6.51495700	1.42626500	5.23988700
H	7.00656900	1.12188300	3.56019100
H	5.41497100	1.83310100	3.90805500

C	6.31863200	-1.25673100	4.96978300	H	-3.15693600	-6.52096100	-0.53587300
H	7.16684800	-1.58009700	4.34028200	H	-3.18195300	-6.08188400	-2.25807400
H	6.72716600	-0.91583100	5.92897500	H	-1.63861900	-6.56204200	-1.48746400
H	5.68913400	-2.13157900	5.16141900	C	-5.82604800	-3.53355900	1.01517300
C	3.19158900	-2.52647500	-6.24692100	H	-6.33118100	-3.89459700	1.91255600
H	2.63925200	-1.67596900	-6.68725400	C	-6.83006600	-2.62976900	0.27490900
H	3.78389900	-2.99095700	-7.04457300	H	-6.43122000	-2.28395300	-0.68557000
H	2.45465900	-3.25944700	-5.90079900	H	-7.75468400	-3.17973000	0.06680200
C	5.23066100	-1.36813500	-5.52068300	H	-7.08497200	-1.74724000	0.87234100
H	5.80474200	-1.11906500	-4.62390400	C	-5.45364500	-4.75698300	0.16008300
H	5.87358000	-1.96509600	-6.18044500	H	-4.91380000	-4.45279300	-0.74197800
H	4.99847600	-0.42687300	-6.04657600	H	-4.80594700	-5.43980200	0.71962400
C	-6.72454500	2.11362300	-0.55204100	H	-6.35311200	-5.30669800	-0.14006100
H	-7.18400500	3.06731500	-0.81876800	C	-2.55605700	-1.87991000	4.60883700
C	-6.83249100	1.98192600	0.97928200	H	-3.41638700	-2.06046000	5.25934200
H	-6.46898600	1.00998000	1.33314900	C	-1.56447400	-3.03844500	4.83262500
H	-6.25482700	2.76251600	1.48648500	H	-0.69856100	-2.93766000	4.16852200
H	-7.87916200	2.07322800	1.29060000	H	-1.20651400	-3.04836000	5.86871100
C	-7.51543500	0.99309700	-1.25436200	H	-2.03833000	-4.00168500	4.62178200
H	-8.56373100	1.00034400	-0.93428100	C	-1.92656900	-0.54002200	5.02049100
H	-7.48961700	1.10644900	-2.34297800	H	-0.97794300	-0.35535800	4.50227500
H	-7.09603800	0.01112500	-1.00885000	H	-2.59542600	0.30329500	4.81259700
C	-2.82125100	4.17208400	-3.20424300	H	-1.70356300	-0.54424800	6.09267200
H	-3.65716400	4.79069900	-3.54114600	C	4.13450900	-4.25537400	-3.22205000
C	-1.79834500	5.08457200	-2.50503900	H	3.95656500	-4.51501500	-4.27158800
H	-0.91925500	4.51908300	-2.17298700	C	3.66263800	-5.42796300	-2.34678500
H	-1.44504900	5.86424200	-3.19011200	H	3.99934100	-5.31596200	-1.30888200
H	-2.23716700	5.57739400	-1.62968000	H	2.57290200	-5.52085000	-2.33132900
C	-2.19513100	3.50158200	-4.44205400	H	4.08624400	-6.36549100	-2.72252100
H	-1.33166000	2.87878800	-4.17408200	C	5.65609400	-4.06561600	-3.04963000
H	-2.92225500	2.86279300	-4.95574500	H	5.88947600	-3.76957600	-2.01901900
H	-1.84735700	4.25982100	-5.15318600	H	6.18577000	-5.00233400	-3.25910300
C	2.73137300	-0.21445300	5.13184300	H	6.04175800	-3.29845800	-3.72420600
H	3.63146000	-0.00882400	5.71689800	C	2.77737400	0.52151600	-4.57688900
C	1.96646300	-1.36438500	5.81036200	H	3.09547200	0.16187900	-5.55698700
H	1.04797300	-1.61766800	5.26898100	C	1.36227700	1.10302000	-4.76088200
H	2.58211500	-2.26918900	5.86457100	H	0.98573100	1.56415300	-3.84010800
H	1.68129400	-1.08552100	6.83144500	H	1.37207800	1.87875600	-5.53517000
C	1.88792900	1.07575900	5.09758100	H	0.64916200	0.32672100	-5.05342100
H	1.60636500	1.38058000	6.11209800	C	3.76477000	1.61731200	-4.12875700
H	2.44352800	1.89604900	4.62911500	H	3.48158500	2.02245600	-3.15075600
H	0.96146100	0.93226500	4.52648000	H	4.78400900	1.22553800	-4.04851500
C	6.40914500	-0.86041100	1.58473500	H	3.77316000	2.44730600	-4.84519600
H	7.04986900	-0.66819400	2.44625100	Rh	0.03044700	0.74260100	0.53370300
C	6.83888900	-2.21761700	0.99587100	C	0.24687300	6.72419800	0.67438500
H	6.26834500	-2.46488000	0.09264200	C	-0.07636100	5.37781100	0.79818200
H	7.89933400	-2.19361700	0.72060900	C	0.29155400	4.64316900	1.94091000
H	6.69087300	-3.02744300	1.71873900	C	1.00539800	5.30380800	2.96220300
C	6.63717000	0.28205500	0.57511600	C	1.33168000	6.64943700	2.85606100
H	6.04140800	0.13373600	-0.33332400	C	0.94850400	7.33951400	1.70590000
H	6.35416700	1.24954500	1.00387400	H	-0.02338800	7.29525000	-0.20680700
H	7.69211600	0.32992100	0.28146300	H	-0.61245300	4.89315500	-0.00554000
H	-1.78785300	-5.97261300	1.18754800	H	1.31411900	4.74553900	3.84250800
H	-0.45832800	-3.10837400	-5.07249800	H	1.87417800	7.17229700	3.63623000
O	0.04883900	-4.37385000	-2.73357400	F	1.27233800	8.63767400	1.59135900
O	-2.36661100	-4.65430800	-1.08575500	C	-0.00548700	3.21914200	2.07622000
C	0.34116400	-5.15678200	-3.88415700	C	-0.97573000	2.49408300	1.25986800
H	1.12879200	-4.69286300	-4.49134500	C	2.37924300	3.53682300	-0.08057100
H	0.69870000	-6.11646600	-3.50939300	C	3.19873200	4.61905100	0.27270200
H	-0.55398000	-5.31676900	-4.49835300	C	3.41528400	5.65909700	-0.63099700
C	-2.59092900	-6.03897300	-1.34114300	C	2.82081400	5.63101600	-1.89501300



C	2.01130700	4.55171200	-2.25295100	H	2.01002700	-1.39471500	3.21518000
C	1.79102200	3.50852800	-1.35130800	H	0.86348400	-2.81562700	4.86345900
H	3.65063500	4.65799400	1.25885400	H	-1.52420100	0.42423100	2.39477700
H	4.04431200	6.49660500	-0.34295800	H	-3.90216200	-2.47809000	0.35553900
H	2.99184800	6.44197200	-2.59695200	H	-4.64189800	0.09439500	-0.10314100
H	1.54971600	4.51314600	-3.23583800	H	-1.43316200	0.51830000	-2.91850800
H	1.15843800	2.67703200	-1.63693900	H	1.37683800	-0.28580100	-2.39155300
Se	2.10297300	2.15919500	1.27189600	H	3.08488300	-3.47220800	-0.08731500
H	0.18908200	1.25079000	-0.88155100	H	4.54954900	-1.45935400	0.14569200
H	-1.43608000	3.06598400	0.45812900	H	1.96368700	1.08806200	2.42771600
H	0.13954400	2.83538100	3.08450200	N	6.44808000	1.43290600	3.23878500
H	-1.74983500	2.02431400	1.88132400	C	7.23299300	0.59466000	4.13230900

### 9-R

B3LYP-D3 SCF energy: -4539.841021 a.u.

B3LYP-D3 enthalpy: -4537.933325 a.u.

B3LYP-D3 free energy: -4538.188356 a.u.

M06 SCF energy in solution: -4538.815303 a.u.

### Cartesian coordinates

ATOM	X	Y	Z				
C	-0.25239300	-4.39324400	-0.93435500	N	3.36048300	-3.67629000	-4.71929300
C	-0.58840500	-3.17013100	-0.31924800	N	-5.40257200	2.53441400	-3.97763500
C	-1.37176000	-2.24329300	-1.03857700	N	-4.68639600	-1.94227800	4.83728900
C	-1.79066900	-2.54618300	-2.34299600	C	2.82434600	-4.99862600	-5.00303100
C	-1.43213900	-3.75533600	-2.93519100	H	2.73370700	-5.12369500	-6.08979500
C	-0.66203500	-4.68266500	-2.23856300	H	3.43424900	-5.83584200	-4.62321700
C	-0.16743600	-2.98629400	1.10648500	H	1.82424100	-5.08195600	-4.56649500
C	0.85171500	-2.10934800	1.53098100	C	4.69248200	-3.41337600	-5.24306000
C	-0.80101300	-3.80268700	2.07506600	H	4.93734400	-2.35493300	-5.10843800
C	1.21915200	-2.05667900	2.88627500	H	5.48897800	-4.00927500	-4.76218700
C	-0.44528600	-3.72554500	3.42428800	H	4.71126500	-3.63428000	-6.31721600
C	0.57201900	-2.85967800	3.81792300	C	-5.74426700	3.87718400	-3.53282200
P	-1.74399700	-0.59894100	-0.28452900	H	-6.00146000	4.48989000	-4.40574400
P	1.62663500	-0.90520600	0.36990900	H	-6.59173700	3.92923600	-2.82707100
C	-2.64937700	-0.98285100	1.24722300	H	-4.87326300	4.32804700	-3.04669900
C	-2.32118700	-0.30810100	2.41951900	C	-6.40660900	1.84819100	-4.77608400
C	-3.66119400	-1.94938400	1.27039500	H	-7.32834300	1.58495700	-4.22713700
C	-2.96312200	-0.58752900	3.63098500	H	-6.69293800	2.48608900	-5.62114100
C	-4.34630900	-2.24381400	2.44933100	H	-5.97965000	0.92404900	-5.17882700
C	-3.98589900	-1.56220200	3.64397100	C	-3.98543600	-2.86860900	5.71162000
C	-2.94296600	0.20565800	-1.40908100	H	-3.17423700	-2.40615400	6.30362600
C	-4.26244600	0.46832900	-1.04760400	H	-4.69870100	-3.31768500	6.41330500
C	-2.46510200	0.71061000	-2.62666400	H	-3.54409200	-3.67334500	5.11375200
C	-5.11277700	1.21678700	-1.87374600	C	-5.50677800	-0.95225200	5.52091200
C	-3.27379300	1.46721800	-3.47474100	H	-5.96593500	-0.28823100	4.78333900
C	-4.61443100	1.73009300	-3.09171700	H	-6.31191200	-1.46539600	6.06258800
C	2.18513000	-1.80774800	-1.10710600	H	-4.96368100	-0.32673100	6.24912600
C	1.91643200	-1.22826100	-2.35201900	C	6.90855500	-0.66167900	1.11358200
C	2.88974400	-3.01022900	-1.05047700	H	7.66560700	-0.03479600	1.58704400
C	2.30260700	-1.84131600	-3.54137500	C	7.12142000	-0.54534800	-0.40790700
C	3.35739400	-3.62511200	-2.21967800	H	6.44312100	-1.20112800	-0.96635900
C	3.02090200	-3.06148400	-3.47243100	H	6.95645400	0.48115200	-0.75346900
C	3.11778800	-0.27175400	1.22266100	H	8.14607200	-0.83406200	-0.66793400
C	4.40676600	-0.70249000	0.90804300	C	7.13346800	-2.10853600	1.59345700
C	2.95911200	0.72376600	2.19432300	H	8.13603900	-2.45530000	1.31784900
C	5.53333200	-0.15623800	1.53830000	H	7.03087600	-2.18705300	2.68106500
C	4.05012100	1.27610800	2.86326100	H	6.40589600	-2.78952300	1.13684700
C	5.35597100	0.83082100	2.53491000	C	3.80498800	2.37034300	3.89365600
H	-2.40669600	-1.84636900	-2.89480300	H	4.76638000	2.57102500	4.37396600
H	-1.75895800	-3.97788900	-3.94678500	C	3.33034100	3.66761400	3.20877700
				H	2.36005200	3.52738300	2.71691200
				H	3.21074000	4.47268100	3.94303800

H	4.05273200	4.00139400	2.45448300	H	-4.47590300	-4.65845600	1.09029900
C	2.80579800	1.93134200	4.97950200	H	-6.18796700	-5.02163700	1.39774100
H	1.80384300	1.75923400	4.56705700	C	-6.85027400	-2.52671200	2.48876200
H	3.13114200	1.00647200	5.46873700	H	-6.97038700	-1.88573800	1.60632300
H	2.71406300	2.70829800	5.74718000	H	-7.67269100	-3.25155900	2.49246200
C	-2.69295500	2.00476100	-4.77523700	H	-6.94165100	-1.90437300	3.38115600
H	-3.48412000	2.58904700	-5.25214800	C	-2.55066400	0.20499900	4.86854500
C	-2.29770100	0.86082800	-5.72694100	H	-2.95639700	-0.29661300	5.74897700
H	-1.50298900	0.23748200	-5.30048600	C	-1.02392900	0.26700000	5.06067100
H	-3.15381300	0.21090900	-5.93997600	H	-0.53092100	0.83565900	4.26299300
H	-1.92990400	1.26148500	-6.67878500	H	-0.78464600	0.76266400	6.00843900
C	-1.50096200	2.94562100	-4.51563300	H	-0.58256100	-0.73323900	5.06941600
H	-1.13884100	3.37505500	-5.45697900	C	-3.14573700	1.62695000	4.81695700
H	-1.78185600	3.76555700	-3.84548800	H	-2.75654500	2.18037200	3.95419300
H	-0.66051100	2.40992900	-4.05583700	H	-4.23657000	1.60284200	4.73130900
C	-6.54383100	1.44647200	-1.39929400	H	-2.88705100	2.18808100	5.72286200
H	-7.07948700	2.00342400	-2.16891000	Rh	0.22557700	0.80569800	-0.23980600
C	-7.29189900	0.11358100	-1.20411900	C	2.90447600	6.48547500	-0.39983600
H	-6.83367300	-0.49345000	-0.41417400	C	2.48213200	5.15683900	-0.37333500
H	-8.33312000	0.29960900	-0.91742200	C	1.68794100	4.63127500	-1.40350500
H	-7.29079800	-0.47924800	-2.12547100	C	1.31881700	5.47668700	-2.46610500
C	-6.57321400	2.29455400	-0.11314600	C	1.72341900	6.80645700	-2.50343100
H	-6.07421500	1.77848000	0.71568600	C	2.51480500	7.29142800	-1.46262800
H	-6.06817500	3.25523900	-0.26228000	H	3.51962200	6.90226500	0.39034400
H	-7.60723400	2.49384200	0.19079100	H	2.77419600	4.53106700	0.46088500
H	-0.38559900	-5.62349400	-2.70142600	H	0.69340300	5.08645200	-3.26581500
H	-0.94458600	-4.33659000	4.16584200	H	1.44655800	7.46817200	-3.31711400
O	-1.75529500	-4.65174800	1.60302300	F	2.91049400	8.57589800	-1.49081700
O	0.49589300	-5.25706500	-0.18679700	C	1.18903500	3.22793600	-1.38484500
C	-2.32770800	-5.59279100	2.50267300	C	1.81269700	2.17159200	-0.51759300
H	-2.93722600	-5.09434300	3.26705000	C	-0.60936000	4.11695200	0.99214500
H	-2.97042900	-6.23225700	1.89651100	C	-0.38435500	5.49779500	0.94476000
H	-1.55607700	-6.20520700	2.98606600	C	-0.18570600	6.20734300	2.13185700
C	0.22964600	-6.64994000	-0.33476100	C	-0.22939500	5.55114300	3.36300100
H	0.63933600	-7.05157700	-1.26854800	C	-0.48451400	4.17853300	3.40921000
H	0.72689100	-7.14028900	0.50450800	C	-0.67451600	3.46183800	2.22689500
H	-0.84886100	-6.84206400	-0.29205200	H	-0.35276000	6.01805800	-0.00658500
C	4.23474000	-4.86616400	-2.09026700	H	0.00376400	7.27593900	2.08799600
H	4.63901600	-5.10133500	-3.07634000	H	-0.07558800	6.10784900	4.28282700
C	5.44135100	-4.60753200	-1.16735400	H	-0.53602300	3.65949700	4.36212500
H	5.12944800	-4.44191300	-0.12976100	H	-0.88359300	2.40099100	2.26706400
H	6.11529200	-5.47149000	-1.17263000	Se	-0.87784700	3.15272700	-0.69957000
H	6.00981500	-3.72899900	-1.49270800	H	0.22437700	1.09695600	1.24388700
C	3.42547300	-6.08269800	-1.60843000	H	2.16895700	2.55609000	0.43653000
H	2.97159300	-5.88614400	-0.63208600	H	1.01887000	2.87225800	-2.40533600
H	2.61701900	-6.31524700	-2.30938600	H	2.64323600	1.67125700	-1.03182000
H	4.06890700	-6.96575400	-1.52218800				
C	1.90241000	-1.24163000	-4.88457500				
H	2.69810900	-1.46930100	-5.59994600				
C	0.61714900	-1.92172700	-5.39677100				
H	-0.20640900	-1.76617600	-4.69062000				
H	0.32191300	-1.50989900	-6.36887500				
H	0.76543200	-2.99932800	-5.50937200				
C	1.72361800	0.28460100	-4.84906200				
H	0.84272400	0.57930400	-4.26466800				
H	2.59851400	0.78846100	-4.42169700				
H	1.56963900	0.66696100	-5.86353700				
C	-5.49045700	-3.25422200	2.44374700				
H	-5.40932300	-3.84716000	3.36179600				
C	-5.46379100	-4.21459800	1.24335700				
H	-5.74461200	-3.70409100	0.31390800				

### 10-ts-R

B3LYP-D3 SCF energy: -4539.831862 a.u.

B3LYP-D3 enthalpy: -4537.925575 a.u.

B3LYP-D3 free energy: -4538.177978 a.u.

M06 SCF energy in solution: -4538.807230 a.u

Imaginary frequency: -865.03 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z
C	1.08731600	-1.19876500	3.97690600
C	1.28006800	-1.17881200	2.57509100
C	1.88364000	-0.03949500	1.99958100
C	2.29256600	1.02596100	2.81857700
C	2.09070100	0.97963400	4.19352300

C	1.48037300	-0.12530900	4.77910600	C	7.06082800	4.87514200	0.21360400
C	0.89097400	-2.42274800	1.83333500	H	7.94624400	4.35061000	-0.18408200
C	-0.21760700	-2.52406600	0.96606200	H	7.33341900	5.93013900	0.34469600
C	1.62695700	-3.59390500	2.12332200	H	6.83617500	4.45996100	1.20064800
C	-0.57081000	-3.76864300	0.42244800	C	3.86058500	-6.14584200	-1.82520400
C	1.28258400	-4.82420300	1.55762700	H	3.12197200	-6.35653200	-2.61838900
C	0.17752000	-4.90497500	0.71504600	H	4.56155700	-6.98962400	-1.79391700
P	2.03890800	0.13931000	0.16862500	H	3.32725000	-6.10963300	-0.86993600
P	-1.09821800	-0.99702500	0.41605700	C	5.42905400	-4.82146100	-3.19696300
C	2.83630500	-1.38530000	-0.44618900	H	6.07078100	-3.93664900	-3.13225300
C	2.28227100	-2.00245600	-1.56952300	H	6.07513900	-5.70560500	-3.25792600
C	3.99040800	-1.92780700	0.12835600	H	4.85696000	-4.75763000	-4.14009300
C	2.83587600	-3.15751800	-2.12620000	C	-6.44995500	-1.30824500	0.22728000
C	4.60114200	-3.05857900	-0.42275300	H	-7.19822100	-1.24513400	-0.56750400
C	3.99824800	-3.70045300	-1.53469000	C	-6.48406300	0.00608400	1.02229800
C	3.23275300	1.50558900	-0.10251500	H	-5.83544000	-0.02557300	1.90597800
C	4.52602100	1.28220900	-0.57372500	H	-6.16902100	0.85178700	0.40469500
C	2.82346400	2.82513900	0.14300500	H	-7.50297000	0.19754900	1.37738000
C	5.41863800	2.34118400	-0.79476600	C	-6.83609100	-2.49937400	1.12784700
C	3.69641400	3.90203200	-0.01495200	H	-7.81489700	-2.33179200	1.59247800
C	5.01361400	3.65705700	-0.48463600	H	-6.88676400	-3.42977300	0.55314300
C	-1.59287500	-0.12759000	1.94632300	H	-6.09836600	-2.63370400	1.92853700
C	-1.41936100	1.25397100	2.03880800	C	-3.66752800	-3.30064600	-3.59816400
C	-2.22415400	-0.80659800	2.99242700	H	-4.65753900	-3.36502800	-4.05146800
C	-1.84780400	1.96810900	3.15963700	C	-2.76184400	-2.58002800	-4.61235600
C	-2.71745300	-0.12184600	4.10780200	H	-1.72393900	-2.51634600	-4.26636200
C	-2.49776800	1.27425600	4.20820700	H	-2.75787100	-3.12392600	-5.56381100
C	-2.67486600	-1.54592900	-0.34831000	H	-3.11055400	-1.55954700	-4.80141800
C	-3.92036000	-1.24899100	0.21010600	C	-3.17541600	-4.74036100	-3.34846600
C	-2.63219600	-2.18284300	-1.59499100	H	-2.17272400	-4.73823800	-2.90465000
C	-5.10983200	-1.58882200	-0.44192500	H	-3.84461600	-5.27508400	-2.66603900
C	-3.79713800	-2.55112300	-2.27573500	H	-3.12563400	-5.30142800	-4.28893300
C	-5.04992000	-2.25279700	-1.69013000	C	3.26346700	5.30412800	0.39431500
H	2.78095000	1.89091900	2.39049100	H	3.96912200	6.00153000	-0.06325500
H	2.41423000	1.81013000	4.81447400	C	3.39327200	5.45478700	1.92373700
H	-1.43825400	-3.85901100	-0.21857200	H	2.72370100	4.75595500	2.44165600
H	-0.10662500	-5.86281600	0.28841300	H	4.41775900	5.25118100	2.25363200
H	1.38592900	-1.57901000	-2.01852100	H	3.12917300	6.47149900	2.23745800
H	4.41529900	-1.46680000	1.01514000	C	1.84779300	5.67687600	-0.07023700
H	4.85322700	0.27177000	-0.78594300	H	1.65259400	6.73519400	0.13604300
H	1.81215600	3.01165100	0.49165400	H	1.71499000	5.51223600	-1.14469800
H	-0.91394500	1.77244400	1.22981600	H	1.07855300	5.10244200	0.45926100
H	-2.35535200	-1.88257000	2.92526700	C	6.80777800	2.01464800	-1.33298200
H	-3.97133700	-0.73917000	1.16268400	H	7.29099000	2.95027500	-1.62035800
H	-1.67039000	-2.39330200	-2.05360900	C	7.67241800	1.35302900	-0.24216700
N	-6.29725700	-2.57430300	-2.31792900	H	7.23067700	0.40398900	0.08032300
N	-2.90220800	2.03955400	5.34782200	H	8.67970700	1.14428000	-0.62069500
N	5.87486300	4.79190900	-0.62469300	H	7.76474100	1.99626700	0.63899300
N	4.60725800	-4.91000400	-2.00042400	C	6.75124700	1.13500700	-2.59635400
C	-2.29787200	1.73099400	6.63350800	H	6.35433700	0.13578300	-2.38180700
H	-2.31458700	2.62936400	7.26401500	H	6.12073100	1.58947100	-3.36860600
H	-2.79356700	0.92217000	7.19754600	H	7.75814100	1.00565100	-3.00885300
H	-1.25268900	1.44559800	6.47782400	H	1.32025100	-0.15315600	5.85057200
C	-4.28367000	2.49144400	5.38416100	H	1.86295100	-5.71164500	1.78232800
H	-4.57404100	2.85608500	4.39360700	O	2.67788600	-3.44891100	2.98192300
H	-5.00613800	1.71031100	5.68300100	O	0.49690300	-2.31781700	4.48651800
H	-4.37707000	3.32288000	6.09349900	C	3.02507400	-4.56673300	3.79521900
C	6.00365900	5.34850800	-1.96247300	H	3.54207100	-5.34653300	3.22575200
H	6.41217100	6.36400900	-1.89457200	H	3.70562400	-4.18120500	4.55690300
H	6.65972400	4.76528000	-2.63357100	H	2.13329800	-4.99043900	4.27257700
H	5.01479100	5.41081500	-2.42885700	C	0.78655300	-2.66637700	5.83671000

H	0.29248200	-1.99849500	6.55058500
H	0.39432600	-3.67566600	5.97434400
H	1.86850600	-2.65916800	6.01693500
C	-3.50128300	-0.90596600	5.15659000
H	-3.94154900	-0.19387500	5.85677200
C	-4.67177900	-1.68489300	4.52652900
H	-4.32259100	-2.46170800	3.83681200
H	-5.26226600	-2.17807300	5.30690300
H	-5.33657400	-1.01646700	3.96921700
C	-2.58148200	-1.84286300	5.95818200
H	-2.06497600	-2.54594700	5.29617600
H	-1.81963500	-1.26828800	6.49493800
H	-3.15680000	-2.41676800	6.69370400
C	-1.61911900	3.47274700	3.21097900
H	-1.93761100	3.80835100	4.20152900
C	-0.13343100	3.83294900	3.04084700
H	0.24303100	3.52515200	2.05821000
H	0.01353600	4.91572000	3.12731600
H	0.48423400	3.33638500	3.79540100
C	-2.47924500	4.19735500	2.15818500
H	-2.20354600	3.89816600	1.13951200
H	-3.54390400	3.97571300	2.29587100
H	-2.34974500	5.28371000	2.23296200
C	5.89013700	-3.59435200	0.18624100
H	6.28476600	-4.33751000	-0.51080200
C	5.60553900	-4.31303400	1.51546800
H	5.15149300	-3.62782600	2.23886600
H	4.91140100	-5.14643400	1.35859400
H	6.53025000	-4.71419900	1.94640800
C	6.94988000	-2.49436200	0.36603000
H	6.64578000	-1.74865600	1.11053400
H	7.89456500	-2.93054300	0.70976300
H	7.14235500	-1.96999900	-0.57692700
C	2.14779600	-3.77716000	-3.33821100
H	2.77999300	-4.57938000	-3.72164400
C	0.79469900	-4.39677600	-2.94316400
H	0.11906800	-3.63020700	-2.54763000
H	0.31119200	-4.86023800	-3.81072400
H	0.91453000	-5.15479200	-2.16300000
C	1.96911900	-2.75982800	-4.48159100
H	1.27964500	-1.95316200	-4.20300700
H	2.92540200	-2.30409600	-4.76054100
H	1.55290200	-3.25416100	-5.36656300
Rh	0.12498400	0.40595900	-1.06558800
Se	-1.59875300	0.63420500	-2.99690200
C	-3.25181000	1.46502000	-2.38111400
C	-4.33887000	1.49280100	-3.26033200
C	-3.34383600	2.04327200	-1.11331500
C	-5.52216200	2.12302300	-2.86948700
H	-4.26328900	1.03322600	-4.24122700
C	-4.52262300	2.68757100	-0.73898900
H	-2.50459700	1.99331700	-0.43126300
C	-5.60994800	2.73105000	-1.61506200
H	-6.36781700	2.14951700	-3.55083400
H	-4.58870300	3.14929700	0.24119300
H	-6.52670600	3.23195200	-1.31783200
H	0.27932100	1.94605700	-0.93339100
C	-1.60490800	5.35399400	-1.41141600
C	-0.87785100	4.21018400	-1.73638100
C	-1.02862500	3.57827900	-2.97936500
C	-1.94285700	4.12869400	-3.89529100

C	-2.68855100	5.26074400	-3.58456600
C	-2.50975500	5.85617100	-2.33850200
H	-1.48328800	5.84936100	-0.45455100
H	-0.18297600	3.81927600	-1.00442400
H	-2.08213900	3.65085800	-4.86180300
H	-3.39951000	5.68677800	-4.28398200
F	-3.22801100	6.94961700	-2.02728200
C	-0.31896100	2.31671400	-3.33690500
H	-0.14385000	2.26541900	-4.41424100
C	0.88051000	1.88060000	-2.51302100
H	1.52531900	2.71558000	-2.22618100
H	1.50290800	1.15423600	-3.04957200
C	-6.66948400	-3.97350400	-2.45475600
H	-6.33319400	-4.52610000	-1.57253100
H	-7.76298900	-4.05208100	-2.50648500
H	-6.25834500	-4.47679000	-3.34736500
C	-6.71601800	-1.69603200	-3.39811400
H	-6.53770700	-0.65555600	-3.10756100
H	-6.19485400	-1.87490900	-4.35717800
H	-7.79099700	-1.82483600	-3.57480900

### 11-R

B3LYP-D3 SCF energy: -4539.874368 a.u.

B3LYP-D3 enthalpy: -4537.961762 a.u.

B3LYP-D3 free energy: -4538.216709 a.u.

M06 SCF energy in solution: -4538.849377 a.u.

### Cartesian coordinates

ATOM	X	Y	Z
C	2.36130100	-3.63413600	1.22534200
C	1.48978700	-2.52056200	1.24827900
C	0.46179100	-2.44501300	0.28274900
C	0.30731100	-3.48510000	-0.64788700
C	1.16455600	-4.58157600	-0.63502700
C	2.19798300	-4.66170400	0.29281800
C	1.74119700	-1.50756400	2.32239100
C	2.25804700	-0.22668200	2.05173800
C	1.55609800	-1.88902500	3.66999800
C	2.61440300	0.63835500	3.09605600
C	1.89247800	-1.01508200	4.70975700
C	2.43753500	0.23358500	4.41550500
P	-0.63550100	-0.94845700	0.17667100
P	2.27551600	0.35158700	0.31392700
C	-1.31996300	-0.80614100	1.86698800
C	-1.35911100	0.43344600	2.50253200
C	-1.77282200	-1.94321700	2.54693600
C	-1.81817500	0.56383800	3.81852600
C	-2.29812900	-1.84830800	3.83497700
C	-2.31488700	-0.58194400	4.47880200
C	-2.01353400	-1.51057600	-0.90297500
C	-3.25045900	-1.90984200	-0.39455200
C	-1.79753800	-1.59131200	-2.28578100
C	-4.26630800	-2.39445500	-1.22824500
C	-2.76228600	-2.12603100	-3.14542600
C	-4.01053400	-2.54020700	-2.61144300
C	3.36030800	-0.75904000	-0.62668600
C	2.96709200	-1.13232500	-1.91508700
C	4.58400600	-1.19586500	-0.12039800
C	3.76816200	-1.96176500	-2.69922100
C	5.43486600	-1.99665100	-0.89184100
C	5.00495700	-2.41339200	-2.17327800

C	3.01154700	2.01835800	0.26043400	H	8.06841700	3.36459700	-1.10152600
C	4.19220000	2.30815600	-0.42628800	H	7.20530100	3.45827300	0.44663900
C	2.25282200	3.07516700	0.79317300	H	6.99254600	2.05005900	-0.60598800
C	4.63662100	3.62657000	-0.57664800	C	1.79103400	5.50702700	1.24513400
C	2.64957200	4.40517600	0.64025600	H	2.15996200	6.45228700	0.83805100
C	3.85418400	4.68536500	-0.05179600	C	0.30318900	5.36646400	0.87196700
H	-0.48796800	-3.45298000	-1.38051300	H	-0.15400900	4.47471700	1.31881200
H	1.02971200	-5.37819300	-1.36068900	H	-0.25890800	6.23412100	1.23611100
H	3.02425400	1.61848800	2.88212900	H	0.16724800	5.29927700	-0.21303700
H	2.71967500	0.89783500	5.22746200	C	1.97073300	5.54713000	2.77566800
H	-0.99192200	1.30360800	1.96753300	H	1.63736500	4.60842600	3.23543400
H	-1.70575000	-2.90940200	2.06074100	H	3.02062700	5.70139600	3.04836700
H	-3.43879100	-1.83920100	0.67015100	H	1.38262900	6.36268700	3.21228300
H	-0.83961600	-1.27066100	-2.68954700	C	-2.43830000	-2.29124300	-4.62405000
H	2.00803300	-0.78276000	-2.28358600	H	-3.33290600	-2.70287300	-5.09763100
H	4.88098100	-0.90851400	0.88422100	C	-1.29381700	-3.30328000	-4.81951800
H	4.77730700	1.49608000	-0.84515000	H	-0.36280600	-2.95059600	-4.36173100
H	1.34359800	2.85075500	1.34446100	H	-1.54290200	-4.27169000	-4.37096400
N	4.22329500	6.06264900	-0.18682800	H	-1.09931000	-3.46250900	-5.88637200
C	5.29183300	6.54782700	0.67386200	C	-2.11234300	-0.94838200	-5.29925100
H	5.15479400	6.14804400	1.68346700	H	-1.94529400	-1.09224900	-6.37256600
H	6.30883300	6.27841600	0.33720800	H	-2.93424400	-0.23426600	-5.17569300
H	5.23870300	7.64174100	0.73240500	H	-1.20392000	-0.49514400	-4.88344100
C	4.16035900	6.64614100	-1.51853700	C	-5.60236200	-2.76159100	-0.59174300
H	3.25292700	6.29854900	-2.02251400	H	-6.32374600	-2.94172100	-1.39098100
H	4.10036700	7.73767100	-1.42774900	C	-5.47835200	-4.05407100	0.23893600
H	5.02160000	6.41227800	-2.16839800	H	-4.76375600	-3.91969000	1.06043000
N	5.76569400	-3.30680300	-2.99579100	H	-6.44526300	-4.32759500	0.67627500
N	-4.96636200	-3.08826300	-3.52237200	H	-5.13005700	-4.89185100	-0.37371700
N	-2.83674800	-0.54792700	5.81467700	C	-6.16419500	-1.61491500	0.27060600
C	6.00922200	-4.65249300	-2.50041100	H	-5.55761900	-1.45409200	1.16992900
H	6.15319300	-5.32913700	-3.35269200	H	-6.19699900	-0.67174500	-0.28559200
H	6.89210200	-4.75260100	-1.84572400	H	-7.18028700	-1.85560400	0.60218900
H	5.13279500	-4.99346000	-1.94053100	H	2.86951300	-5.51232400	0.28726000
C	6.84347800	-2.72096700	-3.77782600	H	1.74704100	-1.30314100	5.74361100
H	6.49956500	-1.78553400	-4.23099300	O	1.05370400	-3.13808800	3.87139900
H	7.75565600	-2.50001200	-3.19448400	O	3.36106000	-3.62613100	2.15074200
H	7.12168600	-3.40877000	-4.58570200	C	0.99469800	-3.63819500	5.20085200
C	-5.97163700	-2.17632500	-4.04372800	H	0.26855400	-3.08118200	5.80670900
H	-6.42181500	-2.60741300	-4.94577800	H	0.66560900	-4.67461500	5.11615100
H	-6.78947800	-1.95688900	-3.33215900	H	1.97919300	-3.60573600	5.68452000
H	-5.50362400	-1.22571100	-4.31675100	C	3.90865400	-4.87525300	2.55792800
C	-5.39022700	-4.46878700	-3.34635900	H	4.53672500	-5.32201600	1.77864500
H	-6.23127800	-4.60907400	-2.64644300	H	4.53135500	-4.65760400	3.42749100
H	-5.69904500	-4.87455600	-4.31808000	H	3.11287800	-5.57724200	2.83629600
H	-4.54561400	-5.06337000	-2.98595200	C	6.79384600	-2.37471200	-0.31205800
C	-1.85318000	-0.57946200	6.88509000	H	7.37585900	-2.86896100	-1.09170500
H	-1.33200200	0.38158200	7.04767900	C	7.59321300	-1.12766700	0.11311100
H	-2.34541000	-0.85808600	7.82483500	H	7.11322700	-0.59813300	0.94396600
H	-1.09359700	-1.33596100	6.66094800	H	8.59805400	-1.41515100	0.44250400
C	-4.01466700	0.26500900	6.08255300	H	7.69604600	-0.42309300	-0.72006600
H	-4.67610200	0.24216100	5.21166000	C	6.64110600	-3.36449100	0.85729300
H	-4.55948400	-0.16223100	6.93447800	H	6.01008000	-2.94527600	1.64872100
H	-3.80344600	1.32118300	6.31936500	H	6.17288400	-4.29417400	0.51704600
C	5.95604600	3.85545200	-1.30689500	H	7.61820500	-3.61217100	1.28777300
H	6.18062200	4.92242100	-1.29067000	C	3.28717600	-2.42388500	-4.07006400
C	5.85539200	3.42805500	-2.78377700	H	4.17179800	-2.58137800	-4.69396200
H	5.65320000	2.35413400	-2.87432000	C	2.57169000	-3.78309200	-3.94257600
H	5.05030000	3.96575600	-3.29673500	H	1.69730900	-3.69513300	-3.28836700
H	6.79495500	3.63723500	-3.30781300	H	2.23496100	-4.13865500	-4.92359600
C	7.12164600	3.13875000	-0.59798100	H	3.23959200	-4.53625400	-3.51402300

C	2.38408300	-1.40248800	-4.78035600
H	1.41508000	-1.28931000	-4.27831800
H	2.85356700	-0.41329400	-4.83007300
H	2.17703200	-1.73515500	-5.80330300
C	-2.88380000	-3.07996200	4.51914900
H	-2.60056500	-3.03771500	5.57656600
C	-2.37782200	-4.41031300	3.93798600
H	-2.80377800	-4.60505200	2.94549500
H	-1.28846400	-4.42662900	3.83881200
H	-2.68333000	-5.23918700	4.58552000
C	-4.42489200	-3.03850400	4.45779800
H	-4.76671400	-3.04366000	3.41475800
H	-4.85406100	-3.91554400	4.95634400
H	-4.81793800	-2.14314900	4.94456400
C	-1.76568500	1.94294500	4.47128900
H	-1.97129400	1.82587100	5.53668100
C	-0.37201600	2.58672400	4.35928400
H	-0.10843300	2.80079200	3.31727800
H	-0.35156800	3.53797300	4.90340200
H	0.40237200	1.93220900	4.76755400
C	-2.83702200	2.87627000	3.87962900
H	-2.66488700	3.04158200	2.81086700
H	-3.84070000	2.45514400	3.98760500
H	-2.81784300	3.85111300	4.38102400
Rh	0.28278000	0.94937100	-0.50090400
C	-3.73199700	1.62899200	0.39271900
C	-3.08172700	2.75545700	-0.11556400
C	-3.56107600	4.04000300	0.15969500
C	-4.70346000	4.19356300	0.94875800
C	-5.36568800	3.07067000	1.44823500
C	-4.87671100	1.79220500	1.17326900
H	-3.36252200	0.63706300	0.17188100
H	-3.05321800	4.91030600	-0.24381700
H	-5.07798000	5.19024000	1.16334500
H	-6.25819700	3.19246200	2.05522500
H	-5.38333200	0.91640400	1.56616400
Se	-1.52780300	2.60031900	-1.29797300
C	-2.40234900	1.85407200	-3.04892900
H	-2.22952600	0.78441900	-2.94711600
C	-1.57127900	2.42305200	-4.19364300
H	-1.93388200	2.01133500	-5.14175100
H	-1.63147700	3.51363100	-4.24797100
H	-0.51640900	2.14541700	-4.08716700
C	-3.86869300	2.13038600	-3.07046200
C	-4.75836700	1.10965600	-2.69951200
C	-4.39220600	3.38964200	-3.40401100
C	-6.13472400	1.32474300	-2.67797700
H	-4.36877400	0.13652500	-2.42001600
C	-5.76479500	3.62345400	-3.38132900
H	-3.72432300	4.20162600	-3.67495100
C	-6.61659500	2.58391200	-3.01700900
H	-6.83020600	0.53915900	-2.40275800
H	-6.18382900	4.59075400	-3.63683100
F	-7.94331900	2.80531200	-2.99252500

## 12-R

B3LYP-D3 SCF energy: -650.391938 a.u.

B3LYP-D3 enthalpy: -650.145789 a.u.

B3LYP-D3 free energy: -650.206444 a.u.

M06 SCF energy in solution: -650.183171 a.u.

## Cartesian coordinates

ATOM	X	Y	Z
C	2.31358300	-1.42413500	-0.69553200
C	1.58365900	-0.73039400	0.27618200
C	0.64142400	-1.40799800	1.05844300
C	0.42982700	-2.77457700	0.86573300
C	1.15782400	-3.46771500	-0.10373900
C	2.10005400	-2.79206800	-0.88269400
H	3.04367400	-0.89558400	-1.30096900
H	0.06452300	-0.86392800	1.79878600
H	-0.30810400	-3.29487500	1.47049100
H	0.99149200	-4.53137800	-0.25228300
H	2.66916600	-3.32798600	-1.63793000
Se	1.84081500	1.20440400	0.50747700
C	0.35872100	1.78604700	-0.81501700
H	0.73991500	1.46949200	-1.78876200
C	0.28219400	3.31202600	-0.76322200
H	-0.46907300	3.66637200	-1.47896900
H	-0.00240600	3.67426700	0.22975000
H	1.24563100	3.76232300	-1.02421200
C	-0.92635500	1.06644800	-0.52219700
C	-1.33140000	0.00218900	-1.33932500
C	-1.72153800	1.39252800	0.58844100
C	-2.49855000	-0.71509200	-1.07426700
H	-0.71460900	-0.28397200	-2.18681500
C	-2.89103400	0.69033000	0.86856800
H	-1.41135700	2.18987000	1.25687700
C	-3.26192100	-0.35618700	0.02834800
H	-2.81413200	-1.54349200	-1.69944400
H	-3.51271000	0.93396800	1.72379900
F	-4.39207200	-1.04369200	0.29967900

## 13

B3LYP-D3 SCF energy: -4539.852673 a.u.

B3LYP-D3 enthalpy: -4537.943276 a.u.

B3LYP-D3 free energy: -4538.194582 a.u.

M06 SCF energy in solution: -4538.824617 a.u.

## Cartesian coordinates

ATOM	X	Y	Z
C	-0.52355200	0.87401400	4.01918000
C	-0.06297600	0.23304300	2.84977200
C	0.81415600	0.93040500	1.99368000
C	1.20816600	2.23921800	2.31950000
C	0.74302400	2.84863600	3.48160900
C	-0.12296200	2.17382600	4.33586000
C	-0.50885500	-1.17317700	2.62542400
C	-1.39182800	-1.54582400	1.59365300
C	-0.07907200	-2.15859500	3.54755000
C	-1.82942100	-2.87791100	1.50089600
C	-0.48868300	-3.48750100	3.41867700
C	-1.37225300	-3.83362700	2.40063200
P	1.47050500	0.14607900	0.44869600
P	-1.89552400	-0.32498600	0.28915200
C	2.18742700	-1.43442100	0.99229200
C	2.02765500	-2.60254200	0.25310500
C	2.92387900	-1.46883300	2.18466400
C	2.53120300	-3.82588000	0.70920500
C	3.51351200	-2.65012900	2.63206000
C	3.29153800	-3.84773100	1.89932800
C	2.85140600	1.25185000	-0.01967200

C	4.16680100	0.94741800	0.31927100	C	4.83146700	-5.78969200	1.65638400
C	2.57403300	2.46127700	-0.67357300	H	5.43755900	-5.08822300	1.07670300
C	5.21447400	1.83324300	0.03921200	H	5.49913000	-6.33498100	2.33606900
C	3.59290400	3.36465800	-0.98196500	H	4.39860300	-6.52277100	0.95623200
C	4.93036200	3.03861300	-0.63601800	C	-7.08793400	-0.55355300	-0.97359000
C	-2.53575300	1.15060400	1.14851300	H	-7.75556100	-1.00828100	-1.70626100
C	-2.16101800	2.41842200	0.69010800	C	-7.09815600	0.96386100	-1.23592800
C	-3.42486300	1.04245100	2.22120500	H	-6.51119900	1.51183000	-0.48927300
C	-2.63666500	3.57932400	1.30415600	H	-6.68885400	1.19783100	-2.22506100
C	-3.95776100	2.18174600	2.83565600	H	-8.12373100	1.34687100	-1.19130800
C	-3.52535200	3.45615400	2.40097200	C	-7.64896600	-0.87840100	0.42435500
C	-3.34137000	-1.11271900	-0.52361200	H	-8.65899300	-0.46834700	0.53906300
C	-4.63129800	-0.59191200	-0.43643700	H	-7.69764000	-1.95984300	0.59061300
C	-3.12404800	-2.24008300	-1.33063900	H	-7.01847300	-0.44652000	1.20843500
C	-5.70074400	-1.16362200	-1.14470500	C	-3.86892700	-4.05348200	-2.91994300
C	-4.16070400	-2.84885800	-2.03526200	H	-4.82158800	-4.56529600	-3.08070300
C	-5.46385100	-2.29100500	-1.95975000	C	-3.36269400	-3.58518600	-4.29902100
H	1.89371500	2.78061300	1.68156300	H	-2.42771400	-3.01917100	-4.20594500
H	1.05812500	3.85966800	3.72052500	H	-3.17065200	-4.44256500	-4.95461600
H	-2.53689700	-3.17747400	0.74150600	H	-4.09742000	-2.94090200	-4.79218800
H	-1.71382800	-4.86095800	2.31276300	C	-2.88654400	-5.04917000	-2.28027000
H	1.49757600	-2.57478900	-0.68999900	H	-1.87589600	-4.63641900	-2.17967900
H	3.03227400	-0.56024500	2.76389600	H	-3.22186600	-5.35773800	-1.28346200
H	4.39371800	0.00830000	0.80796600	H	-2.80606400	-5.94730100	-2.90273300
H	1.54905400	2.70101200	-0.94383500	C	3.28485700	4.65748100	-1.72700600
H	-1.46211700	2.49660000	-0.13861400	H	4.01194200	5.40533100	-1.39713500
H	-3.71121500	0.05807000	2.57965200	C	1.87793800	5.20475500	-1.44689500
H	-4.82019400	0.27529000	0.18522800	H	1.09927300	4.56052200	-1.86736500
H	-2.11870000	-2.63971100	-1.42486000	H	1.68820500	5.31223700	-0.37249200
N	-6.48359800	-2.91778800	-2.74724000	H	1.76040300	6.18836700	-1.91476600
C	-7.49022700	-3.69782000	-2.04246200	C	3.49898100	4.44168200	-3.23853900
H	-7.01022500	-4.27778800	-1.24792900	H	3.18970700	5.32639800	-3.80743800
H	-8.29779800	-3.09781000	-1.58793600	H	4.55096700	4.23888400	-3.45664600
H	-7.95446100	-4.40240000	-2.74348300	H	2.90690700	3.58962700	-3.58749800
C	-6.95542800	-2.20293700	-3.92427500	C	6.61466200	1.44528700	0.50263000
H	-6.11098800	-1.71110600	-4.41582800	H	7.29883400	2.25778700	0.25593400
H	-7.38998300	-2.92022800	-4.63153500	C	6.66376400	1.26928900	2.03294500
H	-7.72067400	-1.43388600	-3.71703200	H	6.02485500	0.44213700	2.36341200
N	-3.93353400	4.67098500	3.03874800	H	7.68645900	1.04801700	2.35889400
N	5.94241600	3.98160000	-1.01006300	H	6.32910300	2.17738900	2.54681600
N	3.85434100	-5.04915500	2.44408300	C	7.11534100	0.17997100	-0.21885200
C	-3.54985100	4.87728800	4.42635800	H	6.48406000	-0.68636100	0.01229100
H	-3.48753700	5.95476000	4.62589500	H	7.10967700	0.31621200	-1.30558200
H	-4.24217400	4.44234300	5.16752600	H	8.13862000	-0.05888900	0.09267200
H	-2.55884900	4.44328000	4.59265400	H	-0.48698200	2.65261000	5.23808600
C	-5.22086500	5.22541900	2.64846700	H	-0.13839400	-4.24653400	4.10675000
H	-5.33405900	5.15721600	1.56158600	O	0.73943900	-1.72761200	4.54670500
H	-6.08826400	4.72194100	3.11172000	O	-1.38560500	0.16091200	4.79875300
H	-5.26015600	6.28495200	2.92914600	C	1.04066700	-2.62710400	5.60779300
C	6.93390700	3.56235100	-1.99104600	H	1.68269100	-3.44773500	5.26559000
H	7.33009200	4.44945500	-2.50133200	H	1.58143300	-2.04131600	6.35187000
H	7.79222900	3.00868100	-1.57316800	H	0.12612400	-3.03404800	6.05666200
H	6.45533000	2.92491200	-2.73999100	C	-1.26446000	0.30553600	6.21201900
C	6.43436000	4.85708100	0.04287700	H	-1.66978100	1.26021700	6.56613900
H	7.13624000	4.37184600	0.74497400	H	-1.85159200	-0.50552400	6.64685300
H	6.95170300	5.71159600	-0.40985800	H	-0.21625000	0.21256900	6.51874700
H	5.58892800	5.24104700	0.62337300	C	-5.00174000	2.00733500	3.93444900
C	2.94405200	-5.87439100	3.22158300	H	-5.40177500	2.99199800	4.18099400
H	2.22702300	-6.45249200	2.61038700	C	-6.18982000	1.15589700	3.45039600
H	3.52145600	-6.58497200	3.82529500	H	-5.88946400	0.12245200	3.24330100
H	2.36547800	-5.24056900	3.90209000	H	-6.97169000	1.12303800	4.21739400

H	-6.62720200	1.57132700	2.53580700
C	-4.38851000	1.41859500	5.21630300
H	-3.93919700	0.43940600	5.02397500
H	-3.60243300	2.07294700	5.60628800
H	-5.15482800	1.30454100	5.99155200
C	-2.16610300	4.95526800	0.84673800
H	-2.94498000	5.67139900	1.11971000
C	-0.88993000	5.36178900	1.60823400
H	-0.07123100	4.66886200	1.38437800
H	-0.57468600	6.37169000	1.32093700
H	-1.05894500	5.34727500	2.68942500
C	-1.93883400	5.05171100	-0.66753200
H	-1.08026400	4.45434100	-0.98973900
H	-2.81941000	4.71920500	-1.23039400
H	-1.72628600	6.08948300	-0.94788100
C	4.41431000	-2.64212100	3.86553300
H	4.15782800	-3.52045700	4.46951100
C	4.25994200	-1.38885300	4.74335400
H	4.69132900	-0.50469200	4.25758700
H	3.21431300	-1.16355100	4.96904700
H	4.79801400	-1.52995400	5.68684700
C	5.89365900	-2.78952200	3.44995600
H	6.19505800	-1.95544400	2.80442600
H	6.54099200	-2.78067400	4.33468800
H	6.06673400	-3.72241700	2.91113200
C	2.23719200	-5.07045900	-0.12342300
H	2.49787700	-5.94884700	0.46974600
C	0.74106200	-5.19728700	-0.47159300
H	0.42328800	-4.41720500	-1.17187600
H	0.55069900	-6.16128900	-0.95694600
H	0.11542200	-5.12667500	0.42357800
C	3.09199000	-5.08213200	-1.40597400
H	2.85882100	-4.21891200	-2.03781100
H	4.16151300	-5.05153700	-1.17296600
H	2.89401200	-5.98653100	-1.99248500
Rh	-0.09609800	0.03502800	-1.26069700
C	-0.67957000	4.38878700	-3.88298400
C	-1.09180100	3.10703100	-3.53670900
C	-0.48514800	1.97320700	-4.11013000
C	0.54462700	2.16126400	-5.05239800
C	0.95858200	3.43727100	-5.41667000
C	0.34796400	4.53177400	-4.81242700
H	-1.12681500	5.27143300	-3.44063900
H	-1.89492300	2.99247500	-2.81623600
H	1.03009800	1.29365900	-5.48710500
H	1.75724000	3.59799900	-6.13204800
F	0.78194900	5.76741800	-5.11266900
C	-0.90470100	0.60918900	-3.79482100
C	-1.91616800	0.22762400	-2.96147000
C	1.73151600	-2.00374400	-3.62832100
C	2.81922000	-2.54966100	-4.33155300
C	2.70297700	-3.77918900	-4.97861300
C	1.50334900	-4.49517200	-4.93172800
C	0.41869400	-3.96007300	-4.23874500
C	0.52670000	-2.72197200	-3.59611000
H	3.76401200	-2.01364600	-4.36369900
H	3.55804700	-4.18321800	-5.51404700
H	1.41745300	-5.45702000	-5.42851200
H	-0.52009600	-4.50378300	-4.19404800
H	-0.33204700	-2.32406400	-3.06554400
Se	2.04393400	-0.29042200	-2.72811600

H	-0.01041600	-1.46954800	-1.13548900
H	-2.26222300	-0.79607100	-2.98040700
H	-2.58454900	0.93950100	-2.48494700
H	-0.39709500	-0.17380100	-4.35143700

#### 14-ts-S

B3LYP-D3 SCF energy: -4539.840613 a.u.

B3LYP-D3 enthalpy: -4537.933647 a.u.

B3LYP-D3 free energy: -4538.184222 a.u.

M06 SCF energy in solution: -4538.809519 a.u.

Imaginary frequency: -128.70 cm<sup>-1</sup>

#### Cartesian coordinates

ATOM	X	Y	Z	
C	0.85708700	-1.27978300	-4.01995700	
C	0.26147700	-1.24643300	-2.74292900	
C	-0.67134100	-0.22763900	-2.45928800	
C	-0.98218700	0.73053700	-3.43593600	
C	-0.37344400	0.68125200	-4.68790000	
C	0.54722000	-0.31928100	-4.98655000	
C	0.59466600	-2.36111000	-1.80109100	
C	1.37803700	-2.21315600	-0.63782100	
C	0.13683600	-3.65665600	-2.14827100	
C	1.68879300	-3.33805200	0.14486900	
C	0.41984700	-4.76063100	-1.34058400	
C	1.20591300	-4.59332600	-0.20395400	
P	-1.42840700	-0.12331600	-0.78218100	
P	1.88781800	-0.53949200	-0.02957200	
C	-2.27792600	-1.71778200	-0.55387300	
C	-2.23994200	-2.36331400	0.67888900	
C	-2.97708100	-2.30346900	-1.61679500	
C	-2.83387000	-3.61789600	0.86160200	
C	-3.63744000	-3.52144600	-1.46035600	
C	-3.54544000	-4.19615600	-0.21235700	
C	-2.74439600	1.13954100	-0.91837600	
C	-4.09481600	0.80587400	-0.96082400	
C	-2.37995400	2.49453900	-0.88271100	
C	-5.09178000	1.79159200	-0.97701800	
C	-3.34019200	3.50581800	-0.87577500	
C	-4.71437100	3.14793500	-0.90250100	
C	2.65810500	0.33219000	-1.43224100	
C	2.30720700	1.66264400	-1.68005400	
C	3.62209900	-0.28336100	-2.23545300	
C	2.88427000	2.38230900	-2.72836000	
C	4.25501800	0.41602900	-3.26933800	
C	3.85193500	1.74446500	-3.54247200	
C	3.21933700	-0.84455700	1.19536700	
C	4.55488700	-0.51366000	0.96517500	
C	2.86818500	-1.38726900	2.43922200	
C	5.53643000	-0.70789700	1.94864500	
C	3.81590300	-1.62646700	3.43254500	
C	5.16873900	-1.27438900	3.18973500	
H	-1.70842800	1.50650200	-3.22626700	
H	-0.62115200	1.42715000	-5.43728500	
H	2.31432400	-3.24424800	1.02169400	
H	1.44863500	-5.45418500	0.41244700	
H	-1.72576400	-1.89644800	1.51084100	
H	-2.99576500	-1.79640900	-2.57397900	
H	-4.38875600	-0.23699300	-0.97938000	
H	-1.32627400	2.76185600	-0.83877800	
H	1.54470300	2.13525800	-1.06540400	



H	3.88723200	-1.32017200	-2.05061800	C	-1.59863400	5.28795700	-1.45844800
H	4.84601500	-0.08709400	0.01263800	H	-0.74618400	4.82982500	-0.94621800
H	1.82947900	-1.63145800	2.63672500	H	-1.59338700	4.94383900	-2.49870700
N	6.10333700	-1.51007500	4.24927500	H	-1.42613800	6.36998900	-1.45478600
C	7.12404700	-2.52819200	4.05113100	C	-2.86425800	5.36393300	0.73250300
H	6.69465300	-3.36974900	3.49921200	H	-2.56123600	6.41182200	0.84313500
H	8.01932900	-2.18246800	3.50639100	H	-3.83929700	5.23540800	1.21160300
H	7.45562500	-2.89846700	5.02949800	H	-2.13798400	4.74301100	1.26856500
C	6.51248600	-0.35789800	5.03801700	C	-6.54326800	1.33330700	-1.06947200
H	5.64580300	0.28206800	5.22847400	H	-7.18074900	2.21483800	-1.14968500
H	6.90167000	-0.70029000	6.00480800	C	-6.78543400	0.49009600	-2.33650000
H	7.29364900	0.26247200	4.56267600	H	-6.20794100	-0.44169500	-2.31858900
N	4.36973700	2.49796700	-4.64327300	H	-7.84479000	0.22140800	-2.41747500
N	-5.66227800	4.22041500	-0.83330800	H	-6.50208000	1.04250100	-3.23926200
N	-4.18536100	-5.47736100	-0.12455800	C	-6.96602700	0.56530800	0.19743600
C	4.10098200	2.01514700	-5.98836300	H	-6.37329400	-0.34878300	0.32240900
H	4.10853900	2.86424600	-6.68382900	H	-6.82914900	1.17827500	1.09494300
H	4.82329100	1.27099500	-6.36568500	H	-8.02129900	0.27531500	0.13717300
H	3.10403600	1.56398300	-6.01376200	H	1.01899300	-0.35593200	-5.96225500
C	5.64594800	3.16809900	-4.44874200	H	0.04559300	-5.74468100	-1.59338000
H	5.66427200	3.63868600	-3.46022400	O	-0.58056600	-3.74631800	-3.30275800
H	6.52313100	2.50051000	-4.52276100	O	1.74890700	-2.28882000	-4.24308500
H	5.76098800	3.95605300	-5.20296800	C	-0.92780500	-5.03981500	-3.78238900
C	-6.52140200	4.29467700	0.33933300	H	-1.66047300	-5.52542300	-3.12582400
H	-6.84830100	5.33299300	0.47868900	H	-1.37849700	-4.88380800	-4.76311400
H	-7.42665600	3.66511400	0.29102600	H	-0.04190100	-5.67886800	-3.88558000
H	-5.95137900	3.99687500	1.22434600	C	1.76135500	-2.87485400	-5.54249800
C	-6.27444100	4.62943100	-2.08832600	H	2.24694000	-2.22900900	-6.28310100
H	-7.06426800	3.94703900	-2.45076500	H	2.34014000	-3.79589200	-5.44989700
H	-6.72150600	5.62345900	-1.96603000	H	0.74093600	-3.10750900	-5.86855100
H	-5.50515100	4.69611800	-2.86470300	C	5.37303700	-0.27120600	-4.04715700
C	-3.31625200	-6.62979300	-0.29820300	H	5.84267600	0.47197900	-4.69353800
H	-2.68492300	-6.85495600	0.58097400	C	6.47157900	-0.79717600	-3.10469300
H	-3.92499200	-7.51700400	-0.51091100	H	6.10244000	-1.60943900	-2.46823300
H	-2.65060400	-6.46138800	-1.15170600	H	7.31339700	-1.19185800	-3.68456500
C	-5.26383200	-5.66099200	0.83713300	H	6.84958800	-0.00176700	-2.45269800
H	-5.83250800	-4.73135700	0.92697400	C	4.83365800	-1.39789100	-4.94477800
H	-5.94344000	-6.44091400	0.46957600	H	4.32126600	-2.16125600	-4.35121800
H	-4.93571300	-5.95619900	1.84762900	H	4.11457900	-1.00565700	-5.67088900
C	6.97435200	-0.31739000	1.62203200	H	5.65187900	-1.87524900	-5.49612800
H	7.55481700	-0.34975200	2.54537100	C	2.43669500	3.80899900	-3.01924500
C	7.08281100	1.11896300	1.07668600	H	3.20572500	4.26659600	-3.64570100
H	6.59788100	1.22358000	0.09890400	C	1.12881300	3.80084000	-3.83264400
H	6.62077300	1.83921500	1.76091600	H	0.32201100	3.31889000	-3.26884400
H	8.13593100	1.39390700	0.95025000	H	0.81614200	4.82375100	-4.07307400
C	7.60073100	-1.32709900	0.64068800	H	1.25605800	3.24789000	-4.76883600
H	8.64459600	-1.06608200	0.43151600	C	2.28236900	4.65908500	-1.74931000
H	7.57690400	-2.34412500	1.04578800	H	1.44000100	4.31730300	-1.13937700
H	7.05757100	-1.33178100	-0.31034600	H	3.18619100	4.63131500	-1.12981700
C	3.37172800	-2.21998400	4.76312800	H	2.08002200	5.70237500	-2.01692900
H	4.27969700	-2.54785700	5.27653700	C	-4.47482100	-4.09673200	-2.60038000
C	2.70108200	-1.14614300	5.64267400	H	-4.27119100	-5.17280100	-2.65024800
H	1.77932400	-0.77259600	5.18013200	C	-4.16206400	-3.48013900	-3.97385500
H	2.43659900	-1.55911100	6.62320900	H	-4.53519300	-2.45076800	-4.04399300
H	3.36469400	-0.29005800	5.80396400	H	-3.08949900	-3.45671700	-4.18525100
C	2.44660400	-3.43792300	4.59088300	H	-4.65993300	-4.05656300	-4.76093700
H	1.48027800	-3.16735800	4.14632300	C	-5.97941200	-3.92986600	-2.30044800
H	2.90510500	-4.20091800	3.95177400	H	-6.23375800	-2.86718700	-2.20174000
H	2.23875200	-3.89365200	5.56574500	H	-6.58044200	-4.34470000	-3.11811600
C	-2.92570700	4.96665300	-0.75597100	H	-6.26271700	-4.43925100	-1.37781000
H	-3.71261500	5.56697500	-1.22080100	C	-2.68948700	-4.28357500	2.22668000

H	-3.01725600	-5.32100200	2.14066800	P	1.86564600	-0.54724700	0.23675300
C	-1.22478200	-4.32180700	2.70461000	C	-2.23713200	-1.88195100	-0.38522400
H	-0.84088500	-3.31789800	2.91581500	C	-2.27886200	-2.22721400	0.96265500
H	-1.14817800	-4.89988400	3.63276600	C	-2.86970200	-2.70040000	-1.32798800
H	-0.57400400	-4.77927000	1.95310200	C	-2.88714300	-3.41364400	1.39026600
C	-3.58628400	-3.58212700	3.26550700	C	-3.52379500	-3.86940600	-0.94144800
H	-3.29717900	-2.53286200	3.38612800	C	-3.51084900	-4.24175700	0.43044800
H	-4.63879800	-3.61049200	2.96425400	C	-2.69120700	0.81212100	-1.36865300
H	-3.49643800	-4.06591000	4.24477800	C	-4.02374300	0.54174800	-1.07209600
Rh	0.08312500	0.55681900	0.94572700	C	-2.33845800	2.10457000	-1.79096600
C	0.74711200	5.65976500	1.41466300	C	-5.01673600	1.52431200	-1.19853800
C	0.83978500	4.30280300	1.70649400	C	-3.29234600	3.11396800	-1.91858000
C	0.25621400	3.76913600	2.87088000	C	-4.64730300	2.82314200	-1.60191100
C	-0.42636500	4.64325400	3.73970300	C	2.81251500	-0.06591900	-1.24386900
C	-0.52560700	6.00102200	3.46414500	C	2.52616600	1.14779900	-1.87794900
C	0.05825100	6.48705000	2.29632800	C	3.83484400	-0.87650800	-1.74288600
H	1.18602600	6.08198900	0.51816300	C	3.22089200	1.54939300	-3.01996900
H	1.37835200	3.65698800	1.02106000	C	4.58959100	-0.48576800	-2.85540500
H	-0.89676100	4.24281400	4.63370900	C	4.24750600	0.71206000	-3.52370100
H	-1.05337000	6.68274500	4.12189700	C	3.02956600	-0.53329900	1.65262500
F	-0.06338000	7.79120700	2.00198300	C	4.39047900	-0.26481000	1.51429700
C	0.33577000	2.34140000	3.20021100	C	2.50929100	-0.73643400	2.93950300
C	1.25469700	1.42698500	2.55080000	C	5.23539700	-0.18051200	2.63236900
C	-2.04993000	0.19041500	3.91170000	C	3.31624000	-0.68060600	4.07340100
C	-3.25151900	0.20759100	4.63327900	C	4.69313200	-0.37250800	3.92120800
C	-3.42987600	-0.65375600	5.71806600	H	-1.49955700	0.58291900	-3.71791300
C	-2.41189600	-1.52989500	6.10101000	H	-0.20456500	0.00985700	-5.73876700
C	-1.21442600	-1.54673800	5.38436300	H	2.12266500	-2.91961500	1.92818000
C	-1.03479000	-0.69696700	4.29071000	H	1.30419300	-5.22707200	1.75448300
H	-4.04686700	0.89132200	4.35014900	H	-1.81157300	-1.57538300	1.69220400
H	-4.36793700	-0.63503600	6.26581000	H	-2.83526700	-2.41861600	-2.37363000
H	-2.55354400	-2.19683900	6.94622300	H	-4.30410200	-0.44742000	-0.72920500
H	-0.41521900	-2.22702100	5.66513000	H	-1.29478100	2.32908300	-1.99491600
H	-0.10633500	-0.73185000	3.73533500	H	1.72604600	1.77348900	-1.49145900
Se	-1.88173900	1.46643200	2.42706600	H	4.05155100	-1.82282900	-1.25620100
H	-0.06537500	-0.77491700	1.64554400	H	4.81104900	-0.11185400	0.52706800
H	1.62788700	0.64727800	3.20814400	H	1.44831700	-0.93139100	3.05487200
H	2.08139400	1.90439800	2.01906300	N	5.46704000	-0.26427200	5.12327400
H	0.03234900	2.09242900	4.21442000	C	6.38108000	-1.35683400	5.42231700

### 15-S

B3LYP-D3 SCF energy: -4539.842729 a.u.

B3LYP-D3 enthalpy: -4537.934549 a.u.

B3LYP-D3 free energy: -4538.184297 a.u.

M06 SCF energy in solution: -4538.816130 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z
C	1.19167800	-2.19494600	-3.56754600
C	0.48073100	-1.87337000	-2.39386600
C	-0.49314000	-0.85354300	-2.45573400
C	-0.73552900	-0.18357300	-3.66365300
C	-0.01189100	-0.51444300	-4.80747800
C	0.95554500	-1.51427500	-4.76527300
C	0.71886000	-2.73249100	-1.18800100
C	1.37943600	-2.31420700	-0.01325700
C	0.28602300	-4.07991000	-1.27237600
C	1.59353300	-3.22442600	1.03544100
C	0.47367200	-4.96611100	-0.20879900
C	1.13743000	-4.53316100	0.93552000
P	-1.37267600	-0.36909100	-0.91380300

P	1.86564600	-0.54724700	0.23675300
C	-2.23713200	-1.88195100	-0.38522400
C	-2.27886200	-2.22721400	0.96265500
C	-2.86970200	-2.70040000	-1.32798800
C	-2.88714300	-3.41364400	1.39026600
C	-3.52379500	-3.86940600	-0.94144800
C	-3.51084900	-4.24175700	0.43044800
C	-2.69120700	0.81212100	-1.36865300
C	-4.02374300	0.54174800	-1.07209600
C	-2.33845800	2.10457000	-1.79096600
C	-5.01673600	1.52431200	-1.19853800
C	-3.29234600	3.11396800	-1.91858000
C	-4.64730300	2.82314200	-1.60191100
C	2.81251500	-0.06591900	-1.24386900
C	2.52616600	1.14779900	-1.87794900
C	3.83484400	-0.87650800	-1.74288600
C	3.22089200	1.54939300	-3.01996900
C	4.58959100	-0.48576800	-2.85540500
C	4.24750600	0.71206000	-3.52370100
C	3.02956600	-0.53329900	1.65262500
C	4.39047900	-0.26481000	1.51429700
C	2.50929100	-0.73643400	2.93950300
C	5.23539700	-0.18051200	2.63236900
C	3.31624000	-0.68060600	4.07340100
C	4.69313200	-0.37250800	3.92120800
H	-1.49955700	0.58291900	-3.71791300
H	-0.20456500	0.00985700	-5.73876700
H	2.12266500	-2.91961500	1.92818000
H	1.30419300	-5.22707200	1.75448300
H	-1.81157300	-1.57538300	1.69220400
H	-2.83526700	-2.41861600	-2.37363000
H	-4.30410200	-0.44742000	-0.72920500
H	-1.29478100	2.32908300	-1.99491600
H	1.72604600	1.77348900	-1.49145900
H	4.05155100	-1.82282900	-1.25620100
H	4.81104900	-0.11185400	0.52706800
H	1.44831700	-0.93139100	3.05487200
N	5.46704000	-0.26427200	5.12327400
C	6.38108000	-1.35683400	5.42231700
H	5.88750900	-2.31150500	5.21384600
H	7.32616800	-1.32971000	4.85197500
H	6.63520100	-1.33172000	6.48911800
C	5.92880700	1.06131400	5.50951200
H	5.15173900	1.79770900	5.28466400
H	6.11148100	1.07785300	6.59134100
H	6.85803300	1.38820100	5.01039500
N	4.88836600	1.13546800	-4.73161300
N	-5.57998000	3.90658300	-1.70069100
N	-4.12410900	-5.49686800	0.76048000
C	4.75624600	0.28893600	-5.90680700
H	4.85362900	0.90762700	-6.80815900
H	5.50134300	-0.52185000	-5.97902900
H	3.75991100	-0.16424900	-5.91167600
C	6.15347700	1.84190500	-4.59945400
H	6.08566700	2.56346600	-3.77881800
H	7.01884200	1.18433100	-4.40143900
H	6.35869300	2.39542700	-5.52384100
C	-6.25015000	4.35386100	-0.48889200
H	-6.51976900	5.41249600	-0.59682700
H	-7.17258200	3.80156300	-0.24004000
H	-5.56400600	4.26396600	0.35861400

C	-6.38395600	3.95974900	-2.91223500	H	2.76934700	-3.62478800	-5.41051100
H	-7.21896500	3.23596100	-2.93033700	H	2.82952400	-4.93068300	-4.20737600
H	-6.80949300	4.96470900	-3.02164500	H	1.25404300	-4.43129200	-4.89770800
H	-5.74910700	3.76259100	-3.78209300	C	5.77066700	-1.35144100	-3.28402800
C	-3.21148500	-6.61748200	0.91933500	H	6.32329000	-0.81322300	-4.05586000
H	-2.64855700	-6.61033600	1.87086400	C	6.74866200	-1.58019100	-2.11634200
H	-3.77550500	-7.55682800	0.86979100	H	6.29725700	-2.19149900	-1.32670300
H	-2.48251100	-6.61454700	0.10192000	H	7.64318100	-2.10687000	-2.46725500
C	-5.27654600	-5.51543800	1.64986600	H	7.06462600	-0.63057900	-1.67018400
H	-5.88369500	-4.62250400	1.47777400	C	5.31275900	-2.69109100	-3.88514500
H	-5.89335300	-6.39386200	1.41934100	H	4.71385200	-3.26001300	-3.16702900
H	-5.02929900	-5.55641500	2.72386200	H	4.69606400	-2.52812000	-4.77401600
C	6.71931800	0.08150500	2.39634600	H	6.17859300	-3.29753700	-4.17487900
H	7.19863000	0.24117700	3.36262600	C	2.85091700	2.83674800	-3.74667600
C	6.96232000	1.34924700	1.55660200	H	3.74470200	3.18163900	-4.27248900
H	6.57128200	1.24385300	0.53769200	C	1.77507800	2.55684800	-4.81335800
H	6.48397900	2.22363500	2.01162000	H	0.85388600	2.19207400	-4.34523300
H	8.03670300	1.54945200	1.47691200	H	1.53979500	3.46990900	-5.37279900
C	7.38880700	-1.14793900	1.75235700	H	2.11645400	1.79576000	-5.52155400
H	8.46267600	-0.97462300	1.61714100	C	2.39125400	3.95756800	-2.80503000
H	7.26171600	-2.03991300	2.37539300	H	1.41683400	3.73344700	-2.35756000
H	6.95633700	-1.36045100	0.76904800	H	3.10788800	4.12943900	-1.99347900
C	2.70657700	-0.89088300	5.45414000	H	2.27533200	4.89207700	-3.36528900
H	3.51639500	-1.21869200	6.11187200	C	-4.27159200	-4.71148600	-1.97199100
C	2.17833600	0.44371200	6.01668200	H	-4.06951100	-5.76484100	-1.74630900
H	1.37709700	0.84625600	5.38395900	C	-3.84981400	-4.43626200	-3.42476500
H	1.77302300	0.30612600	7.02612800	H	-4.21540100	-3.46131300	-3.76983900
H	2.97323700	1.19362900	6.06933300	H	-2.76362800	-4.44366100	-3.55040500
C	1.60351700	-1.96211100	5.47604100	H	-4.28250700	-5.19430400	-4.08647600
H	0.70312000	-1.64398400	4.93661300	C	-5.79366800	-4.49799200	-1.83403900
H	1.94392900	-2.90238300	5.02770200	H	-6.04878500	-3.44590000	-2.01344300
H	1.30356800	-2.16857100	6.50960900	H	-6.33426700	-5.10564500	-2.56919600
C	-2.88093900	4.52978400	-2.30768300	H	-6.14806100	-4.77404200	-0.83902100
H	-3.69674100	4.95584700	-2.89990600	C	-2.87313500	-3.73274100	2.88177000
C	-1.59753900	4.59198200	-3.14945400	H	-3.11918700	-4.78872100	3.01061600
H	-0.71199500	4.33920300	-2.55571100	C	-1.49124500	-3.51274100	3.52641700
H	-1.63569600	3.91372600	-4.00976400	H	-1.22951800	-2.44951600	3.56938400
H	-1.44749300	5.61024600	-3.52407200	H	-1.49543600	-3.88443000	4.55744000
C	-2.73009700	5.39918900	-1.04236200	H	-0.70388000	-4.03111300	2.97105900
H	-2.41998900	6.41677900	-1.30741800	C	-3.94229500	-2.89418200	3.60936200
H	-3.67271200	5.46046700	-0.49340300	H	-3.73585300	-1.82567100	3.49028600
H	-1.97019300	4.98009800	-0.37469600	H	-4.94428800	-3.08986200	3.21457900
C	-6.44963900	1.13332600	-0.85339100	H	-3.94735100	-3.11631200	4.68303100
H	-7.11199300	1.94860300	-1.14898200	Rh	0.03299500	0.78923300	0.66758200
C	-6.91105300	-0.11738700	-1.62641000	C	0.81744200	5.80207400	-0.24329200
H	-6.34527200	-1.01039600	-1.33611300	C	0.77228900	4.57814000	0.42256700
H	-7.96880200	-0.31794000	-1.42205700	C	0.12137600	4.44973900	1.65977800
H	-6.79119000	0.02013700	-2.70652000	C	-0.48966200	5.58741000	2.21430100
C	-6.60252600	0.92928000	0.66744500	C	-0.45612800	6.81623400	1.56294900
H	-5.94998700	0.12200200	1.02195600	C	0.19548200	6.90146900	0.33566100
H	-6.33755600	1.84087100	1.21502700	H	1.31505600	5.91293100	-1.19932100
H	-7.63554900	0.66625500	0.92267700	H	1.25952700	3.72099500	-0.02986100
H	1.51708400	-1.76977800	-5.65701500	H	-1.00796200	5.50394700	3.16626900
H	0.11744500	-5.98687000	-0.26751600	H	-0.92591900	7.69927600	1.98217900
O	-0.31109900	-4.44253900	-2.44185100	F	0.21558600	8.07894900	-0.31330300
O	2.11271300	-3.19680800	-3.46062800	C	0.01894000	3.13815200	2.36711900
C	-0.61732800	-5.81648700	-2.64689600	C	1.01826500	2.05537700	2.05770400
H	-1.41895700	-6.15117800	-1.97683000	C	-2.39745200	1.29581700	3.30205400
H	-0.96169200	-5.89466000	-3.67877200	C	-3.76136400	1.28974700	3.61130800
H	0.26892600	-6.44861400	-2.50939200	C	-4.20425800	0.65659900	4.77586200
C	2.24047700	-4.08529500	-4.56789600	C	-3.29166900	0.04000200	5.63365900

C	-1.93162700	0.04286100	5.31616500	H	-1.98819700	-4.95978600	-2.37253300
C	-1.48127900	0.66286700	4.14873000	H	2.01507100	-0.44447000	3.56320600
H	-4.47545700	1.77830000	2.95459300	H	0.82856700	-1.16656400	5.59325900
H	-5.26467100	0.65187600	5.01127300	H	-1.38969000	1.45550000	1.87732200
H	-3.63886300	-0.44681800	6.54005600	H	-3.96587400	-1.89333400	1.20336200
H	-1.21368400	-0.44040400	5.97261000	H	-4.72157700	-0.03005700	-0.17616900
H	-0.42612600	0.64870400	3.90653500	H	-1.55755700	-0.18229300	-3.06026600
Se	-1.85572200	2.27370000	1.68090700	H	1.04550500	-1.00838800	-2.13182100
H	-0.23118200	-0.22796000	1.75810100	H	2.73883200	-3.35841900	1.02057500
H	1.31082100	1.51074800	2.95458400	H	4.27870300	-1.35328000	0.10146400
H	1.92984300	2.44105800	1.58878100	H	2.10692100	1.55434700	2.38408900
H	-0.20226900	3.26648100	3.42927200	N	6.61727300	2.18462200	1.97558700

### 16-ts-S

B3LYP-D3 SCF energy: -4539.828075 a.u.

B3LYP-D3 enthalpy: -4537.921544 a.u.

B3LYP-D3 free energy: -4538.174812 a.u.

M06 SCF energy in solution: -4538.805302 a.u.

Imaginary frequency: -837.69 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z				
C	-0.61975400	-4.38808400	0.68122100	N	2.93335600	-5.00610500	-3.31895500
C	-0.84781700	-2.99906800	0.80543000	N	-5.77374600	0.61304500	-4.64739300
C	-1.50404300	-2.33436200	-0.25313700	N	-4.49648000	0.36420700	5.15032000
C	-1.91050800	-3.05004900	-1.38979600	C	2.23333600	-6.27878900	-3.25185600
C	-1.66838900	-4.41704400	-1.48769600	H	2.21167500	-6.73188700	-4.25122400
C	-1.02334600	-5.09234700	-0.45584100	H	2.67879200	-7.01690000	-2.56206200
C	-0.40214700	-2.36900000	2.09195500	H	1.20006300	-6.10223300	-2.93637600
C	0.70360300	-1.49915800	2.20409600	C	4.30251600	-5.05016000	-3.80579600
C	-1.06061800	-2.77592600	3.27765600	H	4.65888000	-4.02933800	-3.97919600
C	1.14644700	-1.08327400	3.46995100	H	5.01493300	-5.54631600	-3.12219200
C	-0.63682500	-2.32226800	4.53008000	H	4.32997900	-5.58648100	-4.76224900
C	0.47882600	-1.49390000	4.61813800	C	-6.18955200	1.99268100	-4.85418600
P	-1.78899900	-0.51428000	-0.19836400	H	-6.59456700	2.09968900	-5.86768000
P	1.43505400	-0.71460300	0.70024400	H	-6.95913800	2.34588100	-4.14467100
C	-2.62124300	-0.23400900	1.39944700	H	-5.32063000	2.65289400	-4.76405500
C	-2.20267500	0.81639700	2.21280400	C	-6.78159300	-0.39606100	-4.94058500
C	-3.66376800	-1.06231900	1.82927500	H	-7.70004800	-0.32325400	-4.33318700
C	-2.77061900	1.03816900	3.47168500	H	-7.07495100	-0.31290900	-5.99462400
C	-4.30940900	-0.83233000	3.04369200	H	-6.35413000	-1.39121100	-4.78590800
C	-3.84390500	0.21693800	3.88258700	C	-3.82099500	-0.25369600	6.28046100
C	-3.03401100	-0.17101900	-1.49755800	H	-2.94477100	0.31314100	6.64517800
C	-4.38147400	0.02348600	-1.20289200	H	-4.52543700	-0.35780000	7.11455200
C	-2.61069300	-0.06096400	-2.82971700	H	-3.47533400	-1.25367700	5.99710200
C	-5.31817100	0.30725900	-2.20691600	C	-5.18701900	1.61090700	5.44961700
C	-3.51033600	0.20767200	-3.86042000	H	-5.62849000	2.01110200	4.53259300
C	-4.88615000	0.37276900	-3.54796100	H	-6.00099200	1.40912900	6.15788200
C	1.86829500	-2.06201800	-0.45845000	H	-4.55146500	2.39669100	5.89134700
C	1.58954000	-1.89364400	-1.81628800	C	6.75742900	-0.42782600	0.46449500
C	2.53237300	-3.21772800	-0.03671500	H	7.58552500	0.24523700	0.68731000
C	1.95773400	-2.85403500	-2.76058600	C	6.74830600	-0.64799500	-1.05885000
C	2.93533900	-4.19576600	-0.95367700	H	5.96476100	-1.35320400	-1.36186800
C	2.62309600	-4.02313100	-2.32413700	H	6.57378400	0.29291000	-1.58982900
C	3.04386600	0.02264400	1.19490200	H	7.70909400	-1.05998200	-1.38816100
C	4.25776000	-0.45311700	0.70361100	C	7.03127700	-1.74411100	1.21772200
C	3.04649100	1.18169900	1.99003800	H	7.97693300	-2.18782900	0.88503400
C	5.46591100	0.20905100	0.96751100	H	7.09434100	-1.57406000	2.29820700
C	4.22539400	1.87201600	2.27369600	H	6.23537800	-2.47481700	1.03977900
C	5.44549500	1.39788400	1.72341700	C	4.21135800	3.12929000	3.13903900
H	-2.42688000	-2.54538700	-2.19646900	H	5.13875900	3.12283500	3.72070100
				C	4.23695100	4.40535600	2.27382700
				H	3.31775500	4.49102300	1.68364200

H	4.31325000	5.29503400	2.90994000	H	-5.94755800	-2.81077100	1.61739800
H	5.08971500	4.40054400	1.59073500	H	-4.71910700	-3.55153100	2.65006800
C	3.03613000	3.18273200	4.12781000	H	-6.43400100	-3.60755400	3.11259100
H	2.07770500	3.33820600	3.61805300	C	-6.81704000	-0.83777600	3.24969400
H	2.95847600	2.26304100	4.71941600	H	-6.93403800	-0.54501500	2.19846100
H	3.17070900	4.02106400	4.81985800	H	-7.69511500	-1.42947100	3.53361400
C	-3.02682600	0.28827000	-5.30323400	H	-6.80477200	0.06717200	3.86014600
H	-3.69723000	0.97391300	-5.82932600	C	-2.20550700	2.17262700	4.32116500
C	-3.16180500	-1.08864100	-5.98370600	H	-2.61694500	2.08785000	5.32824100
H	-2.53983000	-1.83476800	-5.47492400	C	-0.67360400	2.09259900	4.45959700
H	-4.19935500	-1.43477800	-5.96320600	H	-0.16837800	2.25082200	3.49926400
H	-2.84054700	-1.03557700	-7.03059700	H	-0.31496600	2.86710300	5.14681200
C	-1.59196000	0.82390900	-5.44187200	H	-0.35960900	1.11586900	4.83795300
H	-1.36321800	1.00567700	-6.49755600	C	-2.62881400	3.54027000	3.74975900
H	-1.45950400	1.76771500	-4.89868400	H	-2.22525200	3.67631300	2.73764400
H	-0.84566900	0.11130800	-5.07149400	H	-3.71834800	3.62964500	3.68919700
C	-6.76762700	0.52330200	-1.78340200	H	-2.25025700	4.35691500	4.37509300
H	-7.34203100	0.83026700	-2.65841900	Rh	0.00000900	0.91257500	-0.29560000
C	-7.38735400	-0.78488100	-1.25442600	Se	1.50975000	3.01531800	-0.22912300
H	-6.86064800	-1.13593900	-0.35821800	C	3.04649200	2.77307000	-1.41663400
H	-8.43882100	-0.63241200	-0.98564000	C	3.97261400	3.81647100	-1.51998400
H	-7.33735600	-1.58076600	-2.00535900	C	3.23225500	1.57896200	-2.11838100
C	-6.89636500	1.65348700	-0.74381300	C	5.08869000	3.66264100	-2.34590500
H	-6.39962800	1.39697600	0.19943500	H	3.82958600	4.73509300	-0.95981600
H	-6.45427200	2.58475800	-1.11491400	C	4.34988200	1.43687800	-2.94205900
H	-7.95244400	1.84124400	-0.51936100	H	2.52082000	0.76832200	-2.01543500
H	-0.83189700	-6.15658900	-0.53402600	C	5.27707700	2.47508400	-3.05756400
H	-1.15381300	-2.62232200	5.43299200	H	5.80830100	4.47185700	-2.43201000
O	-2.10809500	-3.63264100	3.11542400	H	4.49794300	0.50763400	-3.48366100
O	0.02694400	-4.98570200	1.72313700	H	6.14679500	2.35818500	-3.69769200
C	-2.67391600	-4.23245800	4.27424200	H	-0.29480200	1.15402000	-1.81086900
H	-3.20658400	-3.49498400	4.88856400	C	-1.36834900	6.88050800	-0.19484900
H	-3.38782500	-4.97236400	3.91008600	C	-1.06585300	5.52856300	-0.32587200
H	-1.90741200	-4.73204100	4.87985500	C	-0.33862800	5.05243000	-1.43007100
C	-0.31284100	-6.33539700	2.02856500	C	0.08824800	5.97278600	-2.39956500
H	0.13197300	-7.04246400	1.31916900	C	-0.20862400	7.32999000	-2.28639200
H	0.09875400	-6.52894400	3.02116000	C	-0.93523100	7.76229000	-1.18226100
H	-1.40154600	-6.46569000	2.04583600	H	-1.92825000	7.26192000	0.65226000
C	3.69849300	-5.41332800	-0.44183900	H	-1.39377200	4.83972700	0.44815400
H	4.02528700	-5.99835900	-1.30252700	H	0.65884500	5.62307300	-3.25633300
C	4.96941100	-5.00644100	0.32563400	H	0.10930800	8.04971400	-3.03299000
H	4.73191400	-4.45035000	1.23973000	F	-1.22754700	9.06883000	-1.06177800
H	5.53852100	-5.89569500	0.61948200	C	0.01374600	3.60771600	-1.57245000
H	5.61759700	-4.37679700	-0.29370600	C	-1.05335100	2.56450500	-1.27746400
C	2.79541800	-6.31625000	0.41614600	H	-1.73396600	2.42848100	-2.12288600
H	2.41331800	-5.77618000	1.28786300	H	-1.66840900	2.80538700	-0.40270100
H	1.93285200	-6.66182000	-0.16438800	H	0.48818100	3.41198700	-2.53692700
H	3.34853900	-7.19574000	0.76558500				
C	1.59380400	-2.64117500	-4.22372400	<b>17</b>			
H	2.12660800	-3.40199200	-4.79973200	B3LYP-D3 SCF energy: -4539.858340 a.u.			
C	0.08649000	-2.86837000	-4.44047100	B3LYP-D3 enthalpy: -4537.948910 a.u.			
H	-0.50637200	-2.15331600	-3.85869300	B3LYP-D3 free energy: -4538.203764 a.u.			
H	-0.17627000	-2.74806000	-5.49784400	M06 SCF energy in solution: -4538.828677 a.u.			
H	-0.20940000	-3.87354400	-4.12214700				
C	2.02229400	-1.25709500	-4.74060500	Cartesian coordinates			
H	1.49546200	-0.44237800	-4.22849400	ATOM X Y Z			
H	3.09776900	-1.09879600	-4.60111900	C 0.13853300 -0.96796700 4.02489800			
H	1.80300400	-1.16524900	-5.81036900	C -0.23457200 -0.31203400 2.83189800			
C	-5.52705000	-1.66462100	3.43663900	C -1.01981000 -1.00975400 1.89303600			
H	-5.44046200	-1.89749300	4.50407500	C -1.42979000 -2.32540600 2.16451300			
C	-5.65430900	-2.98546300	2.66039100	C -1.06962100 -2.94146100 3.35955700			

C	-0.28184700	-2.27326300	4.29117600	C	5.23267800	-4.82914400	3.27264300
C	0.16673400	1.11938700	2.68893000	H	5.43108900	-4.82856500	2.19568200
C	1.12188100	1.57528600	1.75899500	H	6.02544000	-4.23697500	3.76357200
C	-0.39263100	2.04479500	3.60440500	H	5.31564600	-5.86181600	3.63246500
C	1.52284000	2.92155900	1.77890700	C	-6.34079800	-3.93787700	-2.92719800
C	-0.02357000	3.39175700	3.57842100	H	-6.57047400	-4.81711600	-3.54244200
C	0.94798600	3.81488900	2.67586000	H	-7.29907100	-3.52106600	-2.57291700
P	-1.57153800	-0.18825600	0.32943100	H	-5.86480600	-3.18983700	-3.56764900
P	1.75942300	0.42893800	0.44504000	C	-5.91083500	-5.33353900	-0.94448900
C	-2.48162700	1.27589300	0.91446500	H	-6.73338000	-4.98503900	-0.29408300
C	-2.35795200	2.51692400	0.29887700	H	-6.27606900	-6.19827500	-1.51156100
C	-3.32397500	1.14148300	2.02679100	H	-5.09209800	-5.67122000	-0.30039100
C	-3.02327200	3.64426400	0.79399100	C	-3.93615200	5.46314500	3.35099600
C	-4.06047600	2.22271700	2.50872700	H	-3.24603200	6.16545200	2.84865200
C	-3.89826300	3.49226900	1.89212200	H	-4.65739800	6.05578600	3.92655800
C	-2.78417000	-1.37133800	-0.35219300	H	-3.34867300	4.86660500	4.05666700
C	-4.15476100	-1.22553400	-0.15865900	C	-5.63593800	5.24216200	1.59568700
C	-2.30176100	-2.49998900	-1.02994100	H	-6.09365700	4.50625600	0.92891000
C	-5.05785500	-2.19587100	-0.61206900	H	-6.42634400	5.66684700	2.22791500
C	-3.16961700	-3.47716900	-1.51653700	H	-5.23317000	6.05867900	0.97378900
C	-4.56559800	-3.31450900	-1.31846900	C	6.87955200	0.49447300	-1.02703000
C	2.42422600	-1.01417900	1.34579200	H	7.53695000	1.00524800	-1.73281200
C	2.13736500	-2.32063300	0.93589600	C	6.67463000	-0.93391700	-1.56917000
C	3.25663800	-0.80432600	2.44911500	H	6.08506700	-1.55129300	-0.88099300
C	2.64139000	-3.42058600	1.64050800	H	6.16047000	-0.91967800	-2.53694900
C	3.80741000	-1.87582900	3.15758300	H	7.64314600	-1.42815900	-1.70446100
C	3.45837400	-3.19187100	2.77617500	C	7.58069100	0.46825600	0.34346100
C	3.22097000	1.27162800	-0.27629300	H	8.53578700	-0.06560700	0.28021100
C	4.48510500	0.67684400	-0.28847200	H	7.77890000	1.48091500	0.70973400
C	3.05021400	2.48703500	-0.95511600	H	6.95845800	-0.04027600	1.08787800
C	5.56491100	1.26472400	-0.96244300	C	3.86785600	4.49123100	-2.23374200
C	4.11537100	3.14228500	-1.57221700	H	4.84146400	4.86127800	-2.56581100
C	5.39382200	2.52770200	-1.57431900	C	2.95620400	4.35275900	-3.46750700
H	-2.04741500	-2.86471800	1.45881800	H	1.95019900	4.01434100	-3.19250700
H	-1.40170800	-3.95483500	3.56241500	H	2.84797100	5.31810600	-3.97520200
H	2.29735200	3.27927800	1.11661200	H	3.36117400	3.63560700	-4.19056200
H	1.26474400	4.85390100	2.67568600	C	3.28652700	5.51156800	-1.23706600
H	-1.72884000	2.61530300	-0.57475600	H	2.28920500	5.21539600	-0.88620500
H	-3.39906900	0.17903300	2.51738200	H	3.93377100	5.62160500	-0.35978800
H	-4.53611400	-0.35140800	0.35519400	H	3.18801200	6.49411200	-1.71233500
H	-1.23231800	-2.61428900	-1.18083700	C	-2.62874500	-4.66591000	-2.30201100
H	1.48802700	-2.48057300	0.07900800	H	-3.28871500	-5.51684700	-2.10839800
H	3.48298600	0.21159800	2.75938500	C	-1.20222000	-5.06662400	-1.89730200
H	4.63427300	-0.27372600	0.21103000	H	-0.47032100	-4.29604800	-2.16065100
H	2.06495100	2.94156900	-0.99991000	H	-1.12262800	-5.25540000	-0.82032400
N	6.45755500	3.22928700	-2.21919400	H	-0.90421800	-5.97743700	-2.42788000
C	7.62643100	3.60999600	-1.44122100	C	-2.70394000	-4.35787300	-3.81139200
H	7.31818600	3.85288400	-0.42025300	H	-2.23334800	-5.15800500	-4.39543800
H	8.41710200	2.84273400	-1.38734000	H	-3.74304400	-4.25648200	-4.13586400
H	8.07160700	4.51043200	-1.88341700	H	-2.18352500	-3.42019300	-4.03192200
C	6.70430900	2.90572200	-3.61579000	C	-6.53572500	-1.99384000	-0.29454500
H	5.75107700	2.81877500	-4.14677400	H	-7.08912400	-2.86175100	-0.65491800
H	7.28031100	3.71434400	-4.08150300	C	-6.77097100	-1.91633600	1.22686900
H	7.26310400	1.96362800	-3.76288100	H	-6.27207400	-1.04589100	1.66892600
N	3.88313200	-4.34311000	3.51478400	H	-7.84181600	-1.82877000	1.44262900
N	-5.41630300	-4.32634000	-1.87081400	H	-6.39181800	-2.81185300	1.73198100
N	-4.65216500	4.58091800	2.44417100	C	-7.09916900	-0.75140300	-1.00926900
C	3.38152200	-4.48972300	4.87181100	H	-6.59903900	0.16342400	-0.66969800
H	3.41484800	-5.54934700	5.15474900	H	-6.96227000	-0.82289400	-2.09351200
H	3.93968600	-3.92318800	5.63760300	H	-8.17036200	-0.64381200	-0.80390800
H	2.33710500	-4.16277500	4.90324200	H	0.00137000	-2.76171500	5.21662600

H	-0.46850800	4.10385100	4.26208400
O	-1.28742500	1.53560400	4.49500500
O	0.92027800	-0.25592000	4.88408600
C	-1.76189600	2.37971400	5.53692700
H	-2.39545100	3.18235100	5.14116100
H	-2.36184500	1.74298700	6.18777100
H	-0.93244500	2.81132700	6.11083500
C	0.73599000	-0.47644500	6.27935100
H	1.14899200	-1.43879400	6.60480600
H	1.27985700	0.32461100	6.78283600
H	-0.32804800	-0.42775600	6.53963700
C	4.78701200	-1.57704400	4.28891800
H	5.16550200	-2.52467600	4.67434500
C	6.00645900	-0.79432400	3.76610500
H	5.72162200	0.18811900	3.37236700
H	6.73056900	-0.63222300	4.57251300
H	6.50950900	-1.34570900	2.96417600
C	4.11078600	-0.84421700	5.45997100
H	3.64584400	0.09263700	5.13585500
H	3.32634800	-1.46622400	5.90022500
H	4.84429500	-0.61422300	6.24116300
C	2.28564600	-4.84470800	1.22735000
H	3.01317300	-5.50399000	1.70594500
C	0.89756100	-5.23801100	1.76369900
H	0.11900000	-4.59915700	1.33216900
H	0.66876100	-6.27964100	1.50929900
H	0.85279500	-5.13046900	2.85206400
C	2.35607100	-5.06859400	-0.28821500
H	1.57817400	-4.51261900	-0.81911400
H	3.32898400	-4.76625400	-0.69390400
H	2.20633800	-6.12950300	-0.51909000
C	-5.04829900	2.02883600	3.65677400
H	-4.94451100	2.88821600	4.32937500
C	-4.80911200	0.74615400	4.47111300
H	-5.09596300	-0.14811700	3.90359900
H	-3.76187900	0.62875100	4.76469500
H	-5.42572200	0.76206700	5.37616200
C	-6.49807100	2.03506500	3.12805400
H	-6.64877800	1.21770900	2.41222100
H	-7.20597600	1.89412800	3.95318600
H	-6.73769800	2.97672000	2.63116500
C	-2.76947400	4.98238400	0.10639800
H	-3.22774000	5.76977800	0.70667500
C	-1.26587700	5.31286000	0.03058800
H	-0.72080800	4.60347900	-0.60289500
H	-1.12058600	6.31250200	-0.39454400
H	-0.80528800	5.28490900	1.02309400
C	-3.41946800	5.01683000	-1.29054100
H	-2.99682700	4.24697400	-1.94513200
H	-4.49909800	4.84524000	-1.22769800
H	-3.25519300	5.99009400	-1.76761100
Rh	0.10452600	0.15513000	-1.26252500
C	0.33884900	-3.11325100	-5.00625400
C	0.62531900	-1.87531600	-4.45106600
C	1.60021800	-1.74654400	-3.43741900
C	2.27483100	-2.90314000	-3.00196900
C	1.99408900	-4.15187700	-3.54929000
C	1.01893300	-4.23653500	-4.53649100
H	-0.41091900	-3.23080600	-5.77997400
H	0.07934800	-1.00497400	-4.79381200
H	3.02837000	-2.81870300	-2.22389100

H	2.49611100	-5.05098300	-3.21148500
F	0.69981200	-5.44066100	-5.03743800
C	1.98601700	-0.45302900	-2.86951600
H	2.83206700	-0.48009600	-2.18649400
C	1.48373900	0.76978700	-3.22023100
H	1.96825500	1.66903000	-2.86927000
H	0.77264800	0.89353400	-4.02468500
C	-1.41695800	1.91299700	-4.05347900
C	-1.60925500	1.78937900	-5.43713100
C	-1.32972500	2.86101900	-6.29022100
C	-0.84828900	4.06636800	-5.77668600
C	-0.65131900	4.19477800	-4.39939700
C	-0.93323700	3.12794400	-3.54538000
H	-1.98192600	0.85516400	-5.84833900
H	-1.48559100	2.74807600	-7.35981400
H	-0.62986100	4.89723500	-6.44115300
H	-0.27983300	5.12820200	-3.98470300
H	-0.76868700	3.23909100	-2.47952200
Se	-1.89300300	0.40060300	-2.89767900
H	-0.03872100	1.64992600	-1.05118900

### 18-ts-R

B3LYP-D3 SCF energy: -4539.839904 a.u.

B3LYP-D3 enthalpy: -4537.932006 a.u.

B3LYP-D3 free energy: -4538.183208 a.u.

M06 SCF energy in solution: -4538.813095 a.u.

Imaginary frequency: -920.82 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z
C	0.22922100	-1.10405600	4.04103300
C	-0.15545800	-0.40121400	2.87735800
C	-1.03974200	-1.02435200	1.97489900
C	-1.54699500	-2.30183400	2.26134200
C	-1.18234800	-2.95694900	3.43367800
C	-0.28725700	-2.37096200	4.32256200
C	0.33090500	1.00641600	2.74687600
C	1.25451600	1.44212000	1.77519200
C	-0.11344000	1.92969500	3.72671200
C	1.75275100	2.75495900	1.83221900
C	0.35295200	3.24599200	3.74003200
C	1.30314600	3.64112900	2.80378100
P	-1.56600300	-0.16672300	0.42310800
P	1.75984900	0.31545400	0.38740200
C	-2.27202400	1.40358000	1.01506500
C	-1.96075800	2.60702900	0.38947200
C	-3.10844600	1.40238700	2.13760700
C	-2.44126600	3.82541500	0.88200900
C	-3.65463000	2.58823100	2.62705100
C	-3.30235000	3.81475200	2.00269100
C	-2.92911500	-1.21225500	-0.19659700
C	-4.26874400	-0.92510700	0.04901400
C	-2.59320800	-2.37898200	-0.89649900
C	-5.28526600	-1.79114800	-0.37505600
C	-3.57547000	-3.26257600	-1.34202900
C	-4.93858700	-2.95526000	-1.09460900
C	2.39624200	-1.17998900	1.22884500
C	1.99641100	-2.46847300	0.85365500
C	3.31019000	-1.01937300	2.27405000
C	2.46945900	-3.59413400	1.54076800
C	3.83237100	-2.11861400	2.96065100

C	3.37013000	-3.41008500	2.62100600	C	7.57517600	0.09811900	-0.04469900
C	3.23173100	1.11530600	-0.36732300	H	8.50219000	-0.46983800	-0.18340600
C	4.46128400	0.46347600	-0.48308200	H	7.83565000	1.08744000	0.34574000
C	3.08078100	2.36349400	-0.98961200	H	6.97624700	-0.41428800	0.71583200
C	5.52632300	1.02783000	-1.20183200	C	3.89753000	4.36281800	-2.26938600
C	4.13275100	2.98921700	-1.65626400	H	4.85495100	4.69481300	-2.67938000
C	5.37808900	2.31774700	-1.76060800	C	2.87571100	4.28853600	-3.41998800
H	-2.24215100	-2.77983600	1.58378000	H	1.88872500	3.96807200	-3.06472000
H	-1.59127500	-3.93901900	3.65015800	H	2.75214000	5.27117600	-3.88950500
H	2.50946000	3.09151400	1.13965600	H	3.19277400	3.58285600	-4.19675400
H	1.69896200	4.65232700	2.83298700	C	3.45294900	5.38628200	-1.20765800
H	-1.31891700	2.59285600	-0.48219500	H	2.47837900	5.12609900	-0.77515300
H	-3.32223200	0.46439800	2.63533800	H	4.17974000	5.44838900	-0.39008700
H	-4.53718000	-0.01671600	0.57478500	H	3.35831900	6.38237500	-1.65472900
H	-1.54840900	-2.59050400	-1.10328300	C	-3.18674500	-4.49872400	-2.14351700
H	1.28044700	-2.58759800	0.04478700	H	-3.94441400	-5.26494500	-1.95539800
H	3.62325600	-0.01869000	2.55738000	C	-1.81686100	-5.07360800	-1.75018400
H	4.59473500	-0.51128400	-0.02713000	H	-0.99643200	-4.40361100	-2.02806200
H	2.11655900	2.86288300	-0.95855000	H	-1.74893100	-5.26179500	-0.67206600
N	6.42991100	2.99322100	-2.45237900	H	-1.64411200	-6.02001700	-2.27437800
C	7.65605500	3.30643200	-1.73413500	C	-3.22935400	-4.16604100	-3.64877300
H	7.41489200	3.54591700	-0.69444900	H	-2.86673500	-5.01083300	-4.24683200
H	8.41149700	2.50269500	-1.73421700	H	-4.24911900	-3.92873300	-3.96509000
H	8.11823800	4.19279400	-2.18694700	H	-2.59561600	-3.29864800	-3.86182900
C	6.58304900	2.68982900	-3.86671600	C	-6.72386900	-1.42330400	-0.02713200
H	5.59846600	2.66245600	-4.34490500	H	-7.37438500	-2.24270000	-0.33598200
H	7.17172800	3.48032200	-4.34730900	C	-6.91146300	-1.25545200	1.49349600
H	7.08493800	1.72554200	-4.06564000	H	-6.32986900	-0.41158100	1.88339800
N	3.75755900	-4.57938600	3.35242500	H	-7.96497600	-1.06435500	1.72692200
N	-5.90985800	-3.87011300	-1.61734300	H	-6.59883200	-2.15635300	2.03326800
N	-3.83797800	5.01055300	2.58774600	C	-7.17216900	-0.15855100	-0.78369400
C	3.33223700	-4.66960200	4.74017100	H	-6.56251300	0.70774400	-0.50026800
H	3.30346600	-5.72485500	5.03965700	H	-7.07864400	-0.29109500	-1.86674200
H	3.97848000	-4.13706500	5.45974900	H	-8.21800000	0.07636000	-0.55465300
H	2.31958300	-4.26334900	4.82976700	H	0.00138200	-2.89256800	5.22786700
C	5.05312300	-5.16268000	3.04040100	H	0.00040600	3.95359800	4.47978900
H	5.18756800	-5.18961900	1.95394100	O	-0.99957100	1.44930500	4.64201800
H	5.91296400	-4.62213400	3.47474100	O	1.11392600	-0.47066400	4.86138800
H	5.08483800	-6.19409100	3.41195000	C	-1.33669600	2.26879300	5.75479200
C	-6.81801800	-3.38552500	-2.64730500	H	-1.92560800	3.14097200	5.44533600
H	-7.16280700	-4.23592900	-3.24929300	H	-1.94551900	1.64544700	6.41067300
H	-7.71267600	-2.86354700	-2.26685800	H	-0.43980200	2.59948100	6.29336800
H	-6.28211700	-2.69722900	-3.30723700	C	1.02473700	-0.73404400	6.25766700
C	-6.48037300	-4.81950300	-0.67411600	H	1.40462300	-1.73029400	6.51572600
H	-7.24123200	-4.38664200	0.00037600	H	1.65163700	0.01524400	6.74399200
H	-6.95256500	-5.64016500	-1.22770200	H	-0.01131300	-0.63762400	6.60402200
H	-5.68283300	-5.24269400	-0.05441700	C	4.90120200	-1.87394900	4.02209700
C	-2.94309500	5.73605600	3.47411300	H	5.23941200	-2.84010100	4.39890300
H	-2.16183900	6.31788200	2.95097900	C	6.13356100	-1.18311000	3.40797700
H	-3.52527400	6.43326800	4.08887000	H	5.89085100	-0.18624000	3.02235400
H	-2.43927600	5.03047300	4.14312600	H	6.92068800	-1.06552200	4.16130700
C	-4.72735500	5.84805800	1.79449300	H	6.54095600	-1.77456600	2.58058500
H	-5.33211600	5.21688300	1.13775100	C	4.35479800	-1.08037700	5.22120500
H	-5.40685600	6.38733000	2.46722400	H	3.92639100	-0.12173100	4.91010900
H	-4.21626800	6.59812700	1.16816300	H	3.56714900	-1.64408100	5.72806400
C	6.79928600	0.20504000	-1.37030800	H	5.15415500	-0.88267800	5.94454400
H	7.43844300	0.71384900	-2.09395700	C	1.99834300	-5.00085400	1.18177200
C	6.50125800	-1.19184900	-1.94952200	H	2.73558200	-5.69366600	1.59342800
H	5.92251900	-1.80849000	-1.25170600	C	0.65429200	-5.31989800	1.86021900
H	5.93682700	-1.11954300	-2.88623200	H	-0.13587400	-4.66296200	1.48113600
H	7.43777200	-1.72194400	-2.15564400	H	0.36320700	-6.35843700	1.66295500



H	0.71658700	-5.17826000	2.94351600
C	1.89934200	-5.25080200	-0.32750400
H	1.10120000	-4.66022600	-0.78682000
H	2.84122900	-5.01530500	-0.83721600
H	1.66710600	-6.30504200	-0.51696000
C	-4.64195400	2.55610200	3.79097500
H	-4.39653500	3.39299300	4.45497200
C	-4.59354100	1.25611000	4.61111300
H	-5.02546900	0.41466800	4.05481000
H	-3.57282000	0.97890300	4.88894000
H	-5.18526100	1.37270100	5.52540200
C	-6.08030900	2.78372700	3.28039900
H	-6.36608500	1.99228700	2.57629100
H	-6.79035200	2.76374800	4.11545500
H	-6.17746500	3.74589400	2.77414500
C	-2.03514800	5.10561900	0.15708500
H	-2.28662000	5.95574200	0.79405300
C	-0.51791900	5.18714300	-0.09924100
H	-0.17519500	4.41127200	-0.79423800
H	-0.26287900	6.15646000	-0.54239700
H	0.04752200	5.06753800	0.82939000
C	-2.82291600	5.25116800	-1.16055800
H	-2.61911600	4.41174700	-1.83415300
H	-3.90185800	5.27291500	-0.97845300
H	-2.54484100	6.17703800	-1.67785900
Rh	0.09880000	0.11792900	-1.31611200
C	-0.17598800	-3.01013100	-5.03414600
C	0.23947100	-1.83819600	-4.42346000
C	1.19118100	-1.86652000	-3.38047400
C	1.72591200	-3.10953100	-2.99023400
C	1.31235000	-4.29455700	-3.58984000
C	0.35306000	-4.22501100	-4.59427200
H	-0.91455200	-3.00881600	-5.82769600
H	-0.19019200	-0.89707800	-4.74271100
H	2.47058200	-3.14011700	-2.20138700
H	1.70139400	-5.25822300	-3.28211500
F	-0.09409900	-5.36099500	-5.14905300
C	1.69411200	-0.66595000	-2.72260700
H	2.58683100	-0.82090300	-2.12179800
C	1.41080700	0.66912900	-3.10586400
H	2.19503200	1.39928000	-2.93240400
H	0.79108000	0.86508800	-3.97242600
C	-1.45028800	1.79807500	-4.13014200
C	-1.61789400	1.47826000	-5.48509800
C	-1.25185900	2.39102100	-6.47960200
C	-0.71135000	3.63067200	-6.13460900
C	-0.54675900	3.95786100	-4.78566200
C	-0.91632200	3.05100700	-3.79188900
H	-2.04062700	0.51645300	-5.76314200
H	-1.38745000	2.12747900	-7.52514800
H	-0.42484100	4.33741200	-6.90792900
H	-0.13285500	4.92227400	-4.50371200
H	-0.78725100	3.31576800	-2.74785500
Se	-2.00705100	0.50005700	-2.76762900
H	0.55723600	1.46613500	-2.01265400

Cartesian coordinates

ATOM	X	Y	Z
C	-0.26313300	-1.63447300	3.77216500
C	-0.50261000	-0.77609900	2.67484900
C	-1.17188500	-1.30147300	1.54779400
C	-1.62156800	-2.63074400	1.55478500
C	-1.41564500	-3.43797000	2.66950400
C	-0.72804400	-2.95193500	3.77572600
C	-0.09025100	0.65396900	2.84236800
C	0.94215700	1.26944400	2.10499500
C	-0.71873100	1.39907400	3.87059500
C	1.35033800	2.57704200	2.41194400
C	-0.33022500	2.71378000	4.14402900
C	0.71554100	3.28640500	3.42507700
P	-1.55660500	-0.23317300	0.08858500
P	1.66535600	0.38136900	0.66173000
C	-2.48949800	1.13536500	0.87508300
C	-2.26291100	2.47314600	0.56398900
C	-3.44628700	0.81364900	1.84837300
C	-2.96722300	3.50114400	1.20265800
C	-4.20225700	1.80305900	2.47600300
C	-3.95827000	3.16356800	2.14959800
C	-2.73776800	-1.21683900	-0.89489300
C	-4.11288500	-1.02758900	-0.78005300
C	-2.24847300	-2.27742600	-1.67151500
C	-5.01984100	-1.89871300	-1.39693700
C	-3.12193700	-3.18005200	-2.28257100
C	-4.52243400	-2.97747300	-2.15687400
C	2.24068500	-1.21530500	1.35470500
C	1.99369700	-2.45604700	0.75424300
C	3.00107100	-1.15553500	2.52646200
C	2.47103600	-3.63838800	1.33817600
C	3.52017500	-2.30733400	3.12168600
C	3.21542900	-3.56013700	2.54395900
C	3.20998500	1.23378800	0.16049300
C	4.39853100	0.51686000	0.01706200
C	3.16841000	2.56254600	-0.29203100
C	5.54185100	1.09431400	-0.55454100
C	4.28779700	3.18052300	-0.84695300
C	5.48440800	2.43069300	-1.00252000
H	-2.15411100	-3.03318400	0.70317300
H	-1.78239200	-4.45955900	2.66900000
H	2.17589500	3.03542400	1.88534100
H	1.03786900	4.29667900	3.65959900
H	-1.52774800	2.72815800	-0.18719200
H	-3.59644400	-0.22449900	2.11695900
H	-4.49664300	-0.20468200	-0.19025400
H	-1.17608300	-2.40683200	-1.77227500
H	1.39623900	-2.50203400	-0.15180600
H	3.19648300	-0.19042400	2.98439700
H	4.44586000	-0.51301700	0.34989100
H	2.23368900	3.11082200	-0.24843200
N	6.58584600	3.09659500	-1.62968600
C	7.61177200	3.62205400	-0.74037600
H	7.13792100	4.12738900	0.10742600
H	8.29576000	2.85296600	-0.33867400
H	8.21661100	4.35930100	-1.28167400
C	7.06570400	2.59402600	-2.90889800
H	6.21855700	2.22936300	-3.49747100
H	7.53373300	3.41692300	-3.46386100

**19-R**

B3LYP-D3 SCF energy: -4539.861470 a.u.

B3LYP-D3 enthalpy: -4537.949071 a.u.

B3LYP-D3 free energy: -4538.200754 a.u.

M06 SCF energy in solution: -4538.833756 a.u.

H	7.80564000	1.77893600	-2.83787300	H	-6.31682100	-1.14598500	0.97011200
N	3.61553600	-4.79727200	3.14548800	H	-7.92282700	-1.72993800	0.50737000
N	-5.37348300	-3.92096500	-2.82157300	H	-6.57340200	-2.87236000	0.67300100
N	-4.75290400	4.14655200	2.83077300	C	-6.95539100	-0.27478500	-1.64333000
C	3.02927500	-5.13737500	4.43191000	H	-6.45804300	0.52957100	-1.08856100
H	3.06119500	-6.22609100	4.56551000	H	-6.72605100	-0.13856400	-2.70564300
H	3.52734400	-4.68036700	5.30477600	H	-8.03594100	-0.15368700	-1.50646400
H	1.97974800	-4.82554300	4.43966000	H	-0.55629300	-3.59160500	4.63369800
C	4.98925100	-5.22587300	2.93335800	H	-0.82332300	3.28654900	4.91945700
H	5.25822500	-5.07633900	1.88237100	O	-1.69666300	0.75560600	4.56376300
H	5.73374200	-4.69429000	3.55248100	O	0.43489700	-1.09953400	4.81149500
H	5.07294100	-6.29652500	3.15593900	C	-2.24255500	1.38488800	5.71657200
C	-6.18797300	-3.43887800	-3.92899000	H	-2.82414500	2.27450900	5.44781000
H	-6.41109700	-4.27703400	-4.60145200	H	-2.90921200	0.65054900	6.16972500
H	-7.15008600	-2.98720100	-3.63173400	H	-1.45717300	1.65806500	6.43225000
H	-5.62612300	-2.68974100	-4.49395600	C	0.15872400	-1.58969700	6.11933900
C	-6.00012700	-4.93141500	-1.98250200	H	0.56870200	-2.59442200	6.27901900
H	-6.86372000	-4.56487300	-1.39899600	H	0.64984300	-0.89906300	6.80677100
H	-6.34953600	-5.75794800	-2.61312500	H	-0.92154800	-1.60113000	6.30787200
H	-5.26243100	-5.33071800	-1.27861000	C	4.40355100	-2.15370600	4.35715100
C	-4.10499600	4.85474600	3.92278000	H	4.79047800	-3.13730200	4.62710300
H	-3.38891000	5.63233500	3.59997200	C	5.62578900	-1.26307200	4.06344500
H	-4.86806000	5.33957400	4.54366800	H	5.33220100	-0.24172800	3.79517800
H	-3.56070800	4.14158300	4.55026700	H	6.27076300	-1.20212100	4.94730200
C	-5.66814600	4.95646300	2.03525600	H	6.21888000	-1.66802500	3.23715700
H	-6.08124300	4.34897500	1.22536600	C	3.60796100	-1.62663500	5.56420000
H	-6.49920400	5.28797600	2.67092000	H	3.12976300	-0.66668900	5.34257200
H	-5.21404700	5.85517200	1.58546600	H	2.81932600	-2.33099900	5.84279700
C	6.78764000	0.22646200	-0.69562500	H	4.26862500	-1.49296600	6.42846000
H	7.61980400	0.86550000	-0.99478000	C	2.16907700	-5.00652600	0.73121000
C	6.58358700	-0.83153200	-1.79849700	H	2.89745600	-5.70153800	1.15451300
H	5.75981600	-1.50849300	-1.53860700	C	0.77657100	-5.50284200	1.15849600
H	6.34433400	-0.36473900	-2.75998300	H	-0.00592700	-4.85287200	0.75292000
H	7.48786200	-1.43700200	-1.92769000	H	0.60349200	-6.52069700	0.78965400
C	7.18855800	-0.43983800	0.63316500	H	0.67663500	-5.50865800	2.24843000
H	8.14062100	-0.96948000	0.51636200	C	2.29972100	-5.05153100	-0.79545500
H	7.30326200	0.30053900	1.43207800	H	1.52484300	-4.45999000	-1.29166200
H	6.44273700	-1.17263900	0.96022800	H	3.27909700	-4.68542000	-1.12519600
C	4.20106300	4.61246100	-1.36110600	H	2.18982900	-6.08308100	-1.14894100
H	5.19411000	5.05730500	-1.24876500	C	-5.28806200	1.41970100	3.47884100
C	3.87266300	4.60620500	-2.86787400	H	-5.22836200	2.13291700	4.30925200
H	2.90070300	4.13658900	-3.05437100	C	-5.13001500	-0.00008700	4.04949400
H	3.82746200	5.62970700	-3.25814000	H	-5.38189600	-0.76385800	3.30315700
H	4.63642800	4.06234900	-3.43088000	H	-4.11037000	-0.19751700	4.39302200
C	3.20110000	5.48430200	-0.58504300	H	-5.81647000	-0.13847900	4.89174100
H	2.16331200	5.17010500	-0.74753600	C	-6.69016300	1.56809300	2.85237700
H	3.39578400	5.45986200	0.49346300	H	-6.79153600	0.91687800	1.97603400
H	3.27730100	6.52452900	-0.91974500	H	-7.46308000	1.28129300	3.57504700
C	-2.58737200	-4.37215300	-3.06998400	H	-6.88159300	2.59622000	2.54092300
H	-3.26644400	-5.20999500	-2.88017900	C	-2.64332700	4.93994500	0.81077100
C	-1.17795800	-4.80175500	-2.63572300	H	-3.20298400	5.61015900	1.46392500
H	-0.42181600	-4.05455700	-2.89487900	C	-1.15478600	5.27495800	1.01991900
H	-1.12315000	-4.97861000	-1.55481800	H	-0.49987900	4.64661500	0.40649100
H	-0.89752000	-5.73032900	-3.14461800	H	-0.96074400	6.31949300	0.75064000
C	-2.63500700	-4.08600500	-4.58381200	H	-0.86269600	5.12443800	2.06353900
H	-2.15754700	-4.89609600	-5.14794700	C	-3.08952800	5.22492900	-0.63686800
H	-3.66658000	-3.98821000	-4.92913400	H	-2.56265700	4.58568100	-1.35293600
H	-2.10579000	-3.15686800	-4.81179600	H	-4.16329800	5.04626700	-0.75801200
C	-6.50665400	-1.66322300	-1.15166200	H	-2.88372300	6.26798100	-0.90395500
H	-7.07414500	-2.40627700	-1.71210300	Rh	0.21029300	0.58057600	-1.17259700
C	-6.84865000	-1.86607100	0.33772200	C	0.34456700	-2.36084100	-5.30935300

C	0.45369000	-1.38784100	-4.32586200	C	4.75616700	-0.56645700	2.71817000
C	1.37074800	-1.53371200	-3.26428000	C	2.81373700	-1.50810700	3.88353800
C	2.15004100	-2.70575900	-3.21387600	C	4.16254700	-1.06845700	3.89922800
C	2.03606000	-3.70059300	-4.18125500	C	-2.19068000	-1.57957400	-0.36220500
C	1.12936500	-3.51078400	-5.21761100	C	-2.04568200	-2.10625900	0.92527000
H	-0.34874400	-2.25784300	-6.13648600	C	-2.97397600	-2.25798900	-1.29985800
H	-0.18409800	-0.51116900	-4.36125000	C	-2.64747400	-3.31403600	1.28274900
H	2.88039700	-2.82038800	-2.42034600	C	-3.65869300	-3.42975900	-0.95508400
H	2.63156400	-4.60605300	-4.14349700	C	-3.46044200	-3.98010000	0.33173600
F	0.99163900	-4.46488700	-6.15137300	C	-2.75040100	1.23171700	-1.00289900
C	1.69253500	-0.46401600	-2.30631400	C	-4.09065700	0.86002500	-1.13647400
H	2.48397400	-0.78771800	-1.63307500	C	-2.43084600	2.59312400	-0.95161000
C	1.92900000	0.93543700	-2.83714900	C	-5.11079800	1.81770200	-1.19858600
H	2.98446500	1.20916300	-2.73906000	C	-3.41350400	3.57883200	-1.05724900
H	1.56422500	1.07674900	-3.85422900	C	-4.77058000	3.18967500	-1.18231200
C	-0.74408100	2.95143900	-3.52648200	H	1.89667100	-3.43221600	1.15097600
C	-0.75545100	3.18032100	-4.91028000	H	1.14674000	-5.64374300	0.36354600
C	-0.22442900	4.36037100	-5.43483000	H	-1.51946300	1.59482000	-3.22626000
C	0.32164000	5.32835400	-4.58834400	H	-0.37440500	1.44817700	-5.40619800
C	0.33744100	5.10558600	-3.21062100	H	1.88208100	1.78843300	-1.45637800
C	-0.18611500	3.92337400	-2.68230700	H	3.73686300	-2.05550200	-1.42649000
H	-1.18421800	2.43697700	-5.57632300	H	4.45745900	-0.13812000	0.63512500
H	-0.23968200	4.52304000	-6.50918700	H	1.03889900	-1.71483500	2.68983500
H	0.72822200	6.24812600	-4.99846800	H	-1.43851700	-1.56284900	1.63995400
H	0.75501900	5.85290700	-2.54212500	H	-3.06295000	-1.86650000	-2.30920400
H	-0.17076700	3.76339600	-1.60919700	H	-4.35901800	-0.18936700	-1.14797900
Se	-1.57405900	1.31732900	-2.82846100	H	-1.39643300	2.88781700	-0.80097800
H	1.43504200	1.75900500	-2.24295500	N	-5.74661800	4.23294600	-1.26851300

## 20-ts-R

B3LYP-D3 SCF energy: -4539.841822 a.u.

B3LYP-D3 enthalpy: -4537.930944 a.u.

B3LYP-D3 free energy: -4538.180692 a.u.

M06 SCF energy in solution: -4538.808597 a.u.

Imaginary frequency: -35.57 cm<sup>-1</sup>

## Cartesian coordinates

ATOM	X	Y	Z		X	Y	Z
C	-0.00392900	-3.74851900	-2.20755700	N	-4.05206000	-5.21733300	0.74423800
C	0.42181000	-2.47122000	-1.78519700	N	4.86223400	-1.14084600	5.14674900
C	1.09585600	-2.36495600	-0.55085900	N	5.34404600	0.97645800	-4.45535600
C	1.35732300	-3.50924200	0.21504300	C	-3.71552700	-6.43048900	0.01782800
C	0.94052900	-4.76044200	-0.23324700	H	-3.79278000	-7.29027600	0.69648800
C	0.25328500	-4.88606700	-1.43680700	H	-4.35661800	-6.64069700	-0.85552900
C	0.19942800	-1.32317700	-2.72215200	H	-2.68016500	-6.36527200	-0.33050100
C	-0.65547200	-0.23222400	-2.45721300	C	-5.40887500	-5.15189800	1.26271600
C	0.86886300	-1.36585600	-3.96968300	H	-5.50759500	-4.28278700	1.92129600
C	-0.85430500	0.76332000	-3.42678900	H	-6.18498300	-5.07334200	0.47948200
C	0.66910300	-0.36693100	-4.92702700	H	-5.61896900	-6.05273900	1.85253600
C	-0.20442500	0.68342800	-4.65352600	C	5.11492400	0.11352100	5.83790900
P	1.61875500	-0.70077200	0.03283600	H	5.33142200	-0.09426300	6.89273300
P	-1.39486300	0.01237800	-0.78238700	H	5.95679400	0.70322600	5.43344700
C	2.74825500	-0.15480000	-1.30069000	H	4.21575900	0.73724400	5.79552000
C	2.66328600	1.13357000	-1.82414400	C	5.88475900	-2.16790600	5.27826800
C	3.69059000	-1.04746300	-1.82214000	H	6.84722300	-1.92587800	4.79371700
C	3.50883800	1.56237800	-2.85564300	H	6.08282200	-2.34305000	6.34261500
C	4.54451100	-0.66857600	-2.85764000	H	5.51525900	-3.10264500	4.84496400
C	4.45758100	0.65125400	-3.37471700	C	4.76824000	0.94629900	-5.78971300
C	2.66975800	-0.94482000	1.51203300	H	4.14039500	1.82253600	-6.03460800
C	3.99928600	-0.51985900	1.54083000	H	5.57410900	0.89471500	-6.53185200
C	2.08450500	-1.42054300	2.69434300	H	4.14776100	0.05112200	-5.90017300
				C	6.36887800	1.98926200	-4.25057100
				H	6.72927300	1.94023600	-3.21919600

H	7.21742100	1.78198700	-4.91539600	H	-3.21860500	-3.99099000	-3.65354400
H	6.03858700	3.02326600	-4.44763300	H	-3.18476900	-5.51227700	-2.75518100
C	-6.55517400	1.33061900	-1.25425500	H	-4.53905200	-5.16681400	-3.84886600
H	-7.21138600	2.19342100	-1.13045500	C	-2.39697900	-3.93855900	2.65270200
C	-6.87496500	0.36462100	-0.09663600	H	-3.32470200	-4.42591700	2.96829500
H	-6.29775300	-0.56490700	-0.16843600	C	-1.31969700	-5.03610000	2.54862000
H	-6.65076300	0.82594700	0.87155800	H	-0.36353800	-4.60129100	2.23853200
H	-7.93707900	0.09499100	-0.11112100	H	-1.17547000	-5.52472600	3.51954800
C	-6.87437500	0.69228600	-2.61887800	H	-1.59878500	-5.79924000	1.81725100
H	-7.92005200	0.36597400	-2.65878800	C	-2.00986100	-2.92089500	3.73170600
H	-6.70589600	1.40130900	-3.43642300	H	-1.03508100	-2.46628400	3.52732700
H	-6.24206000	-0.18376200	-2.79841100	H	-2.74084800	-2.11554600	3.81440500
C	-3.00324100	5.04215500	-0.97770100	H	-1.93186000	-3.41771300	4.70505000
H	-3.89183300	5.63568700	-1.20861900	C	5.57150500	-1.65461000	-3.40406900
C	-2.55283300	5.39101600	0.45442900	H	5.65132000	-1.47469200	-4.48132900
H	-1.71773500	4.75817300	0.77381600	C	5.18502600	-3.12739000	-3.18814200
H	-2.23292300	6.43774500	0.51355100	H	5.29472900	-3.42568000	-2.13825600
H	-3.36677200	5.23985800	1.17180100	H	4.14904100	-3.32402300	-3.48093800
C	-1.91680100	5.39281300	-2.01027700	H	5.84517900	-3.77479600	-3.77537100
H	-1.00794500	4.79858600	-1.86314400	C	6.95957200	-1.37796400	-2.79196800
H	-2.27082700	5.21307200	-3.03160300	H	6.93189600	-1.51224900	-1.70324600
H	-1.63662300	6.44933900	-1.92491300	H	7.70484300	-2.07182300	-3.19802100
C	2.13090700	-2.04323300	5.13486600	H	7.29219600	-0.35887300	-3.00445600
H	2.88207100	-2.03626700	5.92872000	C	3.40576500	3.00260900	-3.35150300
C	1.66350700	-3.49716600	4.93625600	H	3.91238100	3.06538300	-4.31652400
H	0.91032100	-3.58148400	4.14596700	C	1.95634600	3.46417700	-3.58634800
H	2.50509800	-4.14621200	4.66838000	H	1.37485400	3.50567700	-2.65774100
H	1.21705700	-3.88397000	5.85944800	H	1.95014300	4.47028500	-4.02099400
C	0.97099900	-1.12793700	5.57596700	H	1.43171200	2.78839800	-4.26650900
H	0.48491700	-1.53273000	6.47099400	C	4.13301900	3.96097300	-2.38533800
H	1.33515200	-0.12241500	5.81699500	H	3.65560100	3.96230600	-1.39956300
H	0.20430500	-1.02670000	4.79971600	H	5.17899300	3.67310500	-2.24435000
C	6.18901000	-0.04679600	2.66307900	H	4.11092800	4.98726700	-2.77051900
H	6.64990500	-0.19359200	3.64044000	Rh	0.06100900	0.78837700	0.74446200
C	7.03687800	-0.82554200	1.63921400	Se	-1.08453000	2.04184300	2.57499000
H	6.66235200	-0.68921000	0.61777700	C	-2.49167200	0.91386500	3.32954100
H	8.07533500	-0.47643500	1.66050300	C	-3.52773600	0.42703100	2.51958000
H	7.03184900	-1.89885800	1.85817200	C	-2.54431000	0.71629500	4.71801700
C	6.21275900	1.46593300	2.36877000	C	-4.61484300	-0.23005500	3.09726500
H	5.77634100	1.68805900	1.38746000	H	-3.50035600	0.58199500	1.44882500
H	5.64612800	2.02361200	3.12352700	C	-3.62975600	0.05007100	5.28802900
H	7.24189200	1.84245800	2.37012400	H	-1.74627200	1.09507900	5.35011900
H	-0.07704300	-5.86155100	-1.77518100	C	-4.67137100	-0.41788100	4.48084600
H	1.18212400	-0.40256500	-5.88016600	H	-5.41395700	-0.59865500	2.46021800
O	1.70168400	-2.42632500	-4.16264300	H	-3.66463800	-0.09919100	6.36365000
O	-0.67463000	-3.79544900	-3.39263900	H	-5.51859100	-0.92975000	4.92838600
C	2.26487100	-2.62498000	-5.45209600	C	0.56890800	6.03506400	2.18184000
H	2.97774700	-1.83053900	-5.70539500	C	0.92328300	4.78424200	2.66470800
H	2.79750100	-3.57558500	-5.40196300	C	1.39892400	3.77074900	1.78817400
H	1.48738500	-2.68110200	-6.22446000	C	1.48288300	4.07713100	0.40189700
C	-0.54483300	-4.97295200	-4.18319600	C	1.14409700	5.32428000	-0.08714900
H	-1.12347900	-5.80921900	-3.77450900	C	0.67582100	6.28363800	0.81387900
H	-0.94552000	-4.71815000	-5.16612100	H	0.18838400	6.81269900	2.83456300
H	0.50875100	-5.26333600	-4.27428300	H	0.82115200	4.57571200	3.72285100
C	-4.60838200	-4.05515400	-1.97273500	H	1.84064900	3.31275200	-0.27424900
H	-5.18672400	-4.82858700	-1.46417800	H	1.21908500	5.56787800	-1.14031400
C	-5.62278400	-3.02908200	-2.51027100	F	0.29037900	7.47486600	0.34043700
H	-5.13363100	-2.25168200	-3.10810900	C	1.76412000	2.46556500	2.23215100
H	-6.35830900	-3.52293000	-3.15528600	H	2.18633500	1.81467100	1.46466300
H	-6.16218800	-2.53768700	-1.69308700	C	2.15864300	2.11221700	3.63001400
C	-3.84271600	-4.72124600	-3.12894300	H	1.57520900	2.63409600	4.39054000

H	3.21961100	2.37860400	3.76686500
H	2.07474100	1.03834900	3.79306500

## 21

B3LYP-D3 SCF energy: -4539.857869 a.u.

B3LYP-D3 enthalpy: -4537.948211 a.u.

B3LYP-D3 free energy: -4538.199113 a.u.

M06 SCF energy in solution: -4538.825417 a.u.

### Cartesian coordinates

ATOM	X	Y	Z
C	0.32186200	-2.60813000	3.14820300
C	-0.24897000	-1.56224800	2.38679300
C	-1.00849000	-1.89240600	1.24841600
C	-1.24292800	-3.23911500	0.92250200
C	-0.71970900	-4.24916600	1.72145700
C	0.07708900	-3.94538300	2.82271100
C	-0.07225200	-0.16917500	2.89874200
C	0.75500900	0.79325500	2.29150100
C	-0.73206000	0.16119500	4.10707300
C	0.92442500	2.05042100	2.89404500
C	-0.58740900	1.42829500	4.67817900
C	0.25275900	2.35874300	4.07217800
P	-1.69798200	-0.57444000	0.15952600
P	1.53842900	0.41717900	0.65745900
C	-2.75534800	0.40888600	1.26354200
C	-2.78226100	1.79865500	1.22487200
C	-3.55930500	-0.27248300	2.18772200
C	-3.56158900	2.53472900	2.12547400
C	-4.39349200	0.41980300	3.06358600
C	-4.38057200	1.84039600	3.04350900
C	-2.78886400	-1.46112000	-1.00814200
C	-4.17622400	-1.40783600	-0.90287900
C	-2.20835600	-2.14484200	-2.08789200
C	-5.00071900	-2.01988500	-1.85530000
C	-2.99579100	-2.73012500	-3.07870000
C	-4.40847000	-2.65054300	-2.97051200
C	2.49014100	-1.12404200	0.91281700
C	2.21119800	-2.24922400	0.12816000
C	3.51076200	-1.19316100	1.86309800
C	2.95124700	-3.42876100	0.24616800
C	4.34091500	-2.31796900	1.94970300
C	4.06609700	-3.43775400	1.12917700
C	2.73949700	1.78541800	0.38992200
C	4.11527600	1.59120200	0.26009800
C	2.21869600	3.06787400	0.14518100
C	4.96709100	2.62890600	-0.15489600
C	3.03093200	4.12905500	-0.25091900
C	4.41819200	3.89669600	-0.44212400
H	-1.84728500	-3.49921300	0.06346300
H	-0.92453200	-5.28731900	1.47800800
H	1.58690400	2.78652400	2.46008100
H	0.38928200	3.33474700	4.52925800
H	-2.17316300	2.31866200	0.49736100
H	-3.52324000	-1.35447200	2.22074200
H	-4.63306900	-0.87199400	-0.07951900
H	-1.12582000	-2.18805000	-2.17720700
H	1.38910700	-2.19769900	-0.57462200
H	3.69617400	-0.34171800	2.51105000
H	4.54020600	0.61540200	0.46137100
H	1.14859800	3.22669600	0.21769900

N	5.19282400	4.99252800	-0.94311700
C	6.02954300	5.71289400	0.00408400
H	5.49816000	5.82085400	0.95485900
H	7.00030200	5.22696400	0.20637600
H	6.23577000	6.71747400	-0.38590000
C	5.73434400	4.88973900	-2.29027100
H	5.04246700	4.32517100	-2.92172900
H	5.83990200	5.89619300	-2.71533100
H	6.72277600	4.40095800	-2.35044500
N	4.90206000	-4.59654700	1.11010300
N	-5.17206800	-3.21091000	-4.04441400
N	-5.20982200	2.50475200	4.00622400
C	5.11038100	-5.37293000	2.32110100
H	5.27191200	-6.42532100	2.05103100
H	5.96960500	-5.05852300	2.93638900
H	4.21158400	-5.32150400	2.94281300
C	6.02296100	-4.55897300	0.18346000
H	5.69792300	-4.16491300	-0.78464800
H	6.86921400	-3.94276300	0.54007000
H	6.39510300	-5.57770700	0.02156800
C	-5.96373500	-2.30024800	-4.85962100
H	-6.11727100	-2.74805400	-5.84956100
H	-6.95755900	-2.05584500	-4.44694900
H	-5.41415800	-1.36368000	-4.99173500
C	-5.75193900	-4.52578800	-3.81805000
H	-6.65134400	-4.52111100	-3.17633200
H	-6.03156500	-4.96808800	-4.78187600
H	-5.00693000	-5.17714500	-3.34906900
C	-4.53978200	2.96286500	5.21237800
H	-3.93798800	3.87979400	5.07370800
H	-5.28663200	3.16575000	5.98942500
H	-3.87036400	2.17809400	5.58044400
C	-6.28758700	3.36479300	3.53619400
H	-6.70142100	2.95625700	2.61019900
H	-7.08744900	3.37991100	4.28783000
H	-5.99271800	4.40982500	3.34443300
C	6.46542800	2.35838700	-0.23953400
H	6.92893500	3.17496800	-0.79388700
C	6.79545500	1.05887800	-0.99700800
H	6.45085300	0.17053100	-0.45435500
H	6.33349500	1.04799600	-1.99075400
H	7.87899600	0.96037300	-1.12357200
C	7.08743700	2.35619900	1.17076700
H	8.16812200	2.18134100	1.11529300
H	6.92112800	3.31232300	1.67737400
H	6.64781600	1.56959300	1.79016400
C	2.42772500	5.49789800	-0.54490600
H	3.18320300	6.24346300	-0.27781300
C	2.14679500	5.65008300	-2.05328700
H	1.40875400	4.91410300	-2.38794700
H	1.73842100	6.64431600	-2.26824400
H	3.05881300	5.52390700	-2.64142800
C	1.15426100	5.79165600	0.26375400
H	0.30820300	5.18586800	-0.07914000
H	1.29547000	5.60602200	1.33482300
H	0.86754900	6.84113200	0.13575300
C	-2.34297400	-3.34994400	-4.30709300
H	-3.06701600	-4.04207100	-4.74447400
C	-1.05665700	-4.12795700	-3.99402300
H	-0.24037700	-3.46573300	-3.68550000
H	-1.20883900	-4.86194200	-3.19508000

H	-0.71660800	-4.66317000	-4.88788900	H	-2.04506000	5.67695900	2.10321800
C	-2.07148100	-2.24664700	-5.35015600	H	-1.48964100	4.19594600	2.91713400
H	-1.60590500	-2.66839300	-6.24919100	C	-4.27346600	4.58317800	0.83438900
H	-2.99980600	-1.74866200	-5.64673600	H	-3.84174100	4.20325500	-0.09827700
H	-1.40564900	-1.47874800	-4.93569800	H	-5.32234800	4.27142300	0.86351900
C	-6.50858200	-1.95155700	-1.63984700	H	-4.24323000	5.67844600	0.79940700
H	-6.99705200	-2.52344100	-2.42992300	Rh	-0.09060600	0.51008000	-1.10617500
C	-6.90986300	-2.60275100	-0.30210400	C	4.35550300	-1.58994700	-2.47333300
H	-6.48220300	-2.06480000	0.55229200	C	3.49360000	-0.50384400	-2.50507600
H	-7.99957500	-2.59474200	-0.18654000	C	2.33558900	-0.51528100	-3.30926700
H	-6.56721900	-3.64217100	-0.24887800	C	2.09435100	-1.64127900	-4.12032900
C	-7.02082800	-0.50141200	-1.72917200	C	2.96280600	-2.73108300	-4.11544300
H	-6.58718100	0.12239200	-0.93858200	C	4.06715700	-2.69470300	-3.27055200
H	-6.75955100	-0.04825800	-2.69122300	H	5.23006700	-1.60102900	-1.83257900
H	-8.11093300	-0.47280800	-1.61905200	H	3.71286600	0.35360500	-1.88157400
H	0.49651400	-4.74772400	3.41687100	H	1.21331700	-1.66486300	-4.75613100
H	-1.10904500	1.68870900	5.59078300	H	2.77886300	-3.61138600	-4.72121700
O	-1.49158700	-0.82423700	4.65667400	F	4.87158100	-3.77398100	-3.19435500
O	1.09969100	-2.21568800	4.18965500	C	1.39017400	0.60526000	-3.34472200
C	-2.00733900	-0.63006500	5.96805600	H	0.53338600	0.47332600	-4.00235300
H	-2.78468900	0.14412600	5.98091400	C	1.50893200	1.79194300	-2.68687600
H	-2.45092600	-1.58290300	6.25893900	H	2.39012700	2.03937400	-2.11196100
H	-1.21053700	-0.36627700	6.67446900	H	0.81321500	2.59755500	-2.88390700
C	1.60000200	-3.20865300	5.07500500	C	-1.59989900	2.99090700	-3.16476200
H	2.26741500	-3.90784700	4.55604200	C	-1.30410000	3.33882500	-4.49038600
H	2.16909800	-2.67048300	5.83383900	C	-1.06947800	4.67326400	-4.83542500
H	0.78312400	-3.76579900	5.55143200	C	-1.12532600	5.67373500	-3.86349900
C	5.53063700	-2.27702000	2.90531300	C	-1.41618600	5.33282900	-2.53974200
H	6.19324400	-3.10636200	2.65478100	C	-1.64991500	4.00208300	-2.19306900
C	6.36468400	-0.99488800	2.74772200	H	-1.26231600	2.56608100	-5.25267200
H	5.80969900	-0.10470900	3.06363200	H	-0.84281800	4.92844500	-5.86716500
H	7.26756900	-1.05155100	3.36580500	H	-0.94268600	6.70974400	-4.13375700
H	6.67532800	-0.85121300	1.70751600	H	-1.46034700	6.10246400	-1.77385300
C	5.07586600	-2.45063600	4.36632300	H	-1.88236700	3.74733100	-1.16554300
H	4.36106900	-1.66642900	4.64373400	Se	-2.03119200	1.13079200	-2.71240000
H	4.58865600	-3.41852600	4.51784700	H	-0.50658600	1.80534500	-0.43875200
H	5.93045000	-2.39028100	5.04982800				
C	2.59044900	-4.67152300	-0.57648200				
H	3.46971900	-4.92679200	-1.18227100	<b>22-ts-S</b>			
C	2.26332100	-5.89331300	0.30979000	B3LYP-D3 SCF energy: -4539.837648 a.u.			
H	1.43206100	-5.66246400	0.98194300	B3LYP-D3 enthalpy: -4537.929507 a.u.			
H	1.96321000	-6.73838300	-0.32062100	B3LYP-D3 free energy: -4538.178897 a.u.			
H	3.11887500	-6.20387000	0.90605700	M06 SCF energy in solution: -4538.806800 a.u.			
C	1.41300300	-4.45000100	-1.53624400	Imaginary frequency: -869.71 cm <sup>-1</sup>			
H	0.48038800	-4.27954500	-0.98697000				
H	1.57257200	-3.60481900	-2.20613800	Cartesian coordinates			
H	1.27085000	-5.33896200	-2.15959100	ATOM X Y Z			
C	-5.32577300	-0.34149400	4.00274900	C 0.23586000 -2.64266500 3.09370200			
H	-5.29353300	0.16087600	4.97642000	C -0.27359000 -1.57104100 2.32531300			
C	-4.93486500	-1.81459200	4.20587400	C -1.08732000 -1.86592400 1.21543600			
H	-5.13926500	-2.41078700	3.30769500	C -1.42998500 -3.19534800 0.92235500			
H	-3.87486200	-1.93287900	4.44772000	C -0.96169900 -4.22806700 1.72736800			
H	-5.52849500	-2.24627500	5.01872800	C -0.11610900 -3.96373700 2.80219400			
C	-6.78115900	-0.26318500	3.49598100	C -0.00607400 -0.18455700 2.82183000			
H	-6.86583800	-0.72028900	2.50236600	C 0.84977300 0.74420600 2.19710900			
H	-7.45098900	-0.80534900	4.17352400	C -0.62552900 0.17706200 4.04428900			
H	-7.12708000	0.76995200	3.43028600	C 1.08887400 1.98892300 2.80383000			
C	-3.49779000	4.05757800	2.05863500	C -0.40870700 1.43221900 4.61798300			
H	-3.97495800	4.45925000	2.95414500	C 0.46240800 2.32327500 3.99860400			
C	-2.04997000	4.58197500	2.06024600	P -1.70048600 -0.51658200 0.12063400			
H	-1.50612500	4.29044000	1.15529600	P 1.60085200 0.35724300 0.54447500			
				C -2.66244200 0.54042100 1.24853200			

C	-2.57812200	1.92797500	1.19503200	H	-6.44159900	-4.94765700	-4.36540100
C	-3.49756300	-0.06784200	2.19424200	H	-5.37198800	-5.07522800	-2.95714900
C	-3.29361500	2.73042600	2.09315700	C	-4.23666200	3.26903800	5.17338600
C	-4.27658000	0.69514800	3.06163700	H	-3.56388100	4.13310100	5.02083200
C	-4.16042600	2.11016000	3.02055500	H	-4.96538700	3.54311600	5.94584000
C	-2.88749100	-1.33950900	-1.00387200	H	-3.63170000	2.43941400	5.55298000
C	-4.26035900	-1.33959200	-0.76359200	C	-5.95377800	3.77392000	3.49215000
C	-2.39873500	-1.95922300	-2.16050800	H	-6.39360700	3.38497300	2.56972600
C	-5.15611400	-1.94773100	-1.64994900	H	-6.75181900	3.85432500	4.24167900
C	-3.26063300	-2.56187800	-3.07886200	H	-5.58612900	4.79349200	3.28850600
C	-4.65511200	-2.55714100	-2.82230900	C	6.70214600	1.92771100	-0.21612300
C	2.41772100	-1.26518800	0.77593700	H	7.23180900	2.71548800	-0.75307600
C	2.04354100	-2.36415400	-0.00744100	C	6.94704900	0.61924300	-0.98947500
C	3.42423700	-1.42112000	1.73066000	H	6.53010000	-0.24913000	-0.46608000
C	2.68270400	-3.60209300	0.11362700	H	6.50166600	0.65943800	-1.99022900
C	4.16127000	-2.60843100	1.81490800	H	8.02218800	0.44296600	-1.10226600
C	3.79982100	-3.69869400	0.98949100	C	7.30349500	1.85925900	1.20157000
C	2.92731200	1.62800900	0.33378200	H	8.36900900	1.60592700	1.15667800
C	4.28772400	1.33178500	0.22414800	H	7.20142200	2.81756600	1.72070300
C	2.52155600	2.95601300	0.11910600	H	6.79870000	1.09856100	1.80320800
C	5.22744900	2.30981900	-0.14604500	C	2.92394800	5.37436700	-0.50915700
C	3.42055900	3.95978000	-0.23625000	H	3.75497600	6.05122700	-0.29053100
C	4.78772500	3.62444900	-0.41038300	C	2.57969200	5.53840300	-2.00326300
H	-2.07387300	-3.42156000	0.08161400	H	1.75866900	4.87129800	-2.28910400
H	-1.24806300	-5.25270900	1.50981200	H	2.25732400	6.56459100	-2.21432900
H	1.77736000	2.69575500	2.36343600	H	3.44400700	5.31838400	-2.63588700
H	0.65824800	3.28859700	4.45669400	C	1.72618800	5.78137600	0.36406900
H	-1.93443800	2.38646700	0.45471100	H	0.81322100	5.24316900	0.08503200
H	-3.53357200	-1.14899200	2.24806100	H	1.91506300	5.59712800	1.42783300
H	-4.65203800	-0.84340100	0.11562900	H	1.51904000	6.84947600	0.23608700
H	-1.33120100	-1.94296800	-2.36667600	C	-2.69299700	-3.13952300	-4.36763100
H	1.23026600	-2.24119500	-0.71122600	H	-3.50513500	-3.68696800	-4.85281000
H	3.67121500	-0.59227700	2.38694400	C	-1.53026300	-4.11431400	-4.12120700
H	4.63042800	0.31938500	0.40000400	H	-0.65540700	-3.60825400	-3.69860400
H	1.46829300	3.20612500	0.19355900	H	-1.81572200	-4.91297400	-3.42766400
N	5.65329500	4.66655300	-0.87595600	H	-1.21819700	-4.57780800	-5.06439000
C	6.55397000	5.28144000	0.08724200	C	-2.26397400	-1.99726800	-5.30990600
H	6.04206600	5.39190300	1.04823800	H	-1.86170000	-2.39740800	-6.24835000
H	7.48660500	4.71568600	0.25761800	H	-3.10859300	-1.34284800	-5.54995100
H	6.83292300	6.28203500	-0.26615600	H	-1.49548900	-1.36886800	-4.84116800
C	6.17458100	4.56367700	-2.23082800	C	-6.63967500	-1.90404500	-1.29805900
H	5.42240200	4.10621900	-2.87991800	H	-7.20066200	-2.39088400	-2.09655900
H	6.38814200	5.56980800	-2.61358900	C	-6.92264900	-2.68457400	0.00030100
H	7.10295600	3.97199700	-2.32025500	H	-6.40669500	-2.23380600	0.85704400
N	4.55328100	-4.91305200	0.95503000	H	-7.99607700	-2.68483300	0.22127200
N	-5.50282600	-3.16846000	-3.80257900	H	-6.58939500	-3.72514900	-0.08173700
N	-4.93994800	2.84563400	3.97377300	C	-7.15390300	-0.45508200	-1.19750000
C	4.70574100	-5.72072000	2.15371000	H	-6.66993000	0.08824400	-0.37723700
H	4.80180500	-6.77680100	1.86691400	H	-6.96137000	0.09775300	-2.12322200
H	5.58049200	-5.47197900	2.77712600	H	-8.23367000	-0.44755300	-1.00971900
H	3.80894000	-5.62276500	2.77243300	H	0.25720300	-4.78305300	3.40416900
C	5.67771800	-4.93402500	0.03257200	H	-0.89816000	1.71287700	5.54217700
H	5.38702800	-4.48439700	-0.92204200	O	-1.42327500	-0.76964000	4.60885200
H	6.56777000	-4.39592100	0.40905100	O	1.06180600	-2.29241900	4.11510100
H	5.97154000	-5.97295600	-0.16037600	C	-1.91286400	-0.54519400	5.92511900
C	-6.30515800	-2.27807700	-4.62873700	H	-2.64820900	0.26921500	5.94493800
H	-6.61037000	-2.80962500	-5.53844000	H	-2.40248200	-1.47284600	6.22377100
H	-7.21922500	-1.89663000	-4.14050400	H	-1.09542400	-0.32257200	6.62227400
H	-5.69858400	-1.41695400	-4.92580500	C	1.39140900	-3.27745500	5.08513300
C	-6.11537600	-4.43993000	-3.44948300	H	1.99105300	-4.08702900	4.65123900
H	-6.99095500	-4.36100200	-2.78100800	H	1.98589700	-2.76351000	5.84158400

H	0.48782600	-3.69743900	5.54532700
C	5.33935300	-2.67101700	2.78334400
H	5.94436200	-3.54053900	2.52363600
C	6.26576100	-1.44983000	2.66635000
H	5.77162300	-0.52837600	2.99346200
H	7.15192000	-1.58465600	3.29640500
H	6.60343100	-1.30778400	1.63444100
C	4.84998900	-2.84145300	4.23356300
H	4.18503900	-2.01619100	4.51499300
H	4.29482600	-3.77613200	4.35598200
H	5.69506400	-2.85424700	4.93140300
C	2.21469200	-4.81709200	-0.70000400
H	3.05300400	-5.11812000	-1.34353100
C	1.85030800	-6.02780300	0.18823300
H	1.08949800	-5.74429600	0.92085400
H	1.43739600	-6.83078400	-0.43331800
H	2.71517300	-6.42158200	0.71674900
C	1.00902500	-4.52364500	-1.60463500
H	0.11662600	-4.29831400	-1.01158200
H	1.18477200	-3.68797200	-2.28051200
H	0.78545600	-5.40161900	-2.21977000
C	-5.27041800	0.01619500	4.00029800
H	-5.22132200	0.53294300	4.96552600
C	-4.98437200	-1.47636400	4.23421700
H	-5.21931600	-2.07405700	3.34435300
H	-3.93767600	-1.66330100	4.48992800
H	-5.61466900	-1.85163900	5.04747400
C	-6.70778100	0.18262800	3.46333000
H	-6.80367000	-0.28558400	2.47548000
H	-7.42618500	-0.30048000	4.13592100
H	-6.98133100	1.23558000	3.37272900
C	-3.12361700	4.24408000	2.00562100
H	-3.58690900	4.69275500	2.88584400
C	-1.64407600	4.66882500	2.02990800
H	-1.09161000	4.28802600	1.16442900
H	-1.56362700	5.76175200	2.01552000
H	-1.14078900	4.29354500	2.92569700
C	-3.84343300	4.79977000	0.76061300
H	-3.42962400	4.37336400	-0.15943600
H	-4.91200800	4.56276800	0.78343700
H	-3.73615300	5.88950400	0.70622900
Rh	-0.02691300	0.64868000	-1.21997900
C	4.21050300	-1.60769300	-2.54432300
C	3.33531800	-0.53312900	-2.51430500
C	2.10117800	-0.58004500	-3.19690700
C	1.80665100	-1.72079200	-3.97318200
C	2.68647000	-2.79679600	-4.03081200
C	3.86053800	-2.73363100	-3.28634400
H	5.14492400	-1.59386900	-1.99529800
H	3.60675900	0.34306900	-1.94066000
H	0.87254400	-1.76607100	-4.52585000
H	2.46319300	-3.68789300	-4.60669400
F	4.67988400	-3.80097400	-3.26840600
C	1.14187200	0.51743600	-3.18528200
H	0.32643500	0.41342100	-3.89620900
C	1.33694600	1.80792800	-2.63968300
H	2.29197400	2.06908600	-2.19938700
H	0.81304600	2.62723400	-3.12331100
C	-1.59988800	3.22311100	-3.07987500
C	-1.59299600	3.61439600	-4.42644900
C	-1.30042200	4.93569800	-4.77647100

C	-1.00870800	5.88042500	-3.79010600
C	-1.01399000	5.49699000	-2.44660700
C	-1.30711200	4.17905800	-2.09408800
H	-1.81710700	2.88515400	-5.19967600
H	-1.29774000	5.22437000	-5.82413300
H	-0.78117900	6.90617300	-4.06526500
H	-0.79049400	6.22249100	-1.66923200
H	-1.31121800	3.89084800	-1.04935700
Se	-2.07502300	1.37986800	-2.60590400
H	0.41466200	2.15085900	-1.30297900

### 23-S

B3LYP-D3 SCF energy: -4539.862316 a.u.

B3LYP-D3 enthalpy: -4537.949860 a.u.

B3LYP-D3 free energy: -4538.199155 a.u.

M06 SCF energy in solution: -4538.830812 a.u.

### Cartesian coordinates

ATOM	X	Y	Z
C	0.20803300	-2.69832500	2.98640400
C	-0.26303700	-1.60331700	2.22512000
C	-1.02593400	-1.87052300	1.07027800
C	-1.37588700	-3.18853700	0.74011800
C	-0.96289800	-4.24128200	1.54925200
C	-0.15629500	-4.00792200	2.66001100
C	-0.00252000	-0.23287700	2.76950000
C	0.85762500	0.71337400	2.17831700
C	-0.63240600	0.09929900	3.99443000
C	1.08150500	1.95148400	2.80248900
C	-0.42393200	1.34438600	4.59445900
C	0.44291600	2.25685600	3.99885500
P	-1.63780000	-0.50181700	0.00155600
P	1.60258900	0.35471500	0.52510700
C	-2.64680600	0.46059900	1.18872100
C	-2.63830200	1.85162700	1.23894800
C	-3.45529500	-0.25237900	2.08521600
C	-3.40981000	2.55024900	2.17715700
C	-4.28622300	0.40471000	2.99024800
C	-4.25753300	1.82317600	3.04146100
C	-2.79464700	-1.28383900	-1.17716500
C	-4.16897000	-1.30516300	-0.93831200
C	-2.29689500	-1.85834500	-2.35233900
C	-5.05782000	-1.89576100	-1.84146000
C	-3.15296500	-2.46379200	-3.27641500
C	-4.54672400	-2.49158700	-3.01643500
C	2.41516100	-1.27568800	0.73245400
C	2.05218900	-2.38412700	-0.04523900
C	3.41792100	-1.41858100	1.69338400
C	2.70916200	-3.61282100	0.08323400
C	4.17137300	-2.59466200	1.78436800
C	3.83210900	-3.68830800	0.95540300
C	2.92638000	1.62366900	0.30064200
C	4.29477700	1.34323400	0.23310100
C	2.50690300	2.93898500	0.04803000
C	5.22991900	2.32710400	-0.12549200
C	3.40549800	3.95245900	-0.28644100
C	4.78156800	3.63707600	-0.40684600
H	-1.98334800	-3.39019100	-0.13336900
H	-1.25482000	-5.25753700	1.30232400
H	1.76494700	2.67069900	2.37140700
H	0.62429200	3.21505300	4.47713100



H	-2.02368600	2.40494300	0.54102700	H	0.87945200	5.23098800	0.30011200
H	-3.43553100	-1.33473000	2.06773900	H	2.14244900	5.72954200	1.43970200
H	-4.56696300	-0.83814800	-0.04690300	H	1.54452200	6.86029600	0.21100600
H	-1.23006400	-1.82294300	-2.55428700	C	-2.57659300	-3.04522700	-4.55922600
H	1.23703800	-2.27552300	-0.74820900	H	-3.40461700	-3.53035400	-5.08233700
H	3.64927800	-0.58689800	2.35172600	C	-1.50413100	-4.11180100	-4.27878100
H	4.64359500	0.33596800	0.42480600	H	-0.64138400	-3.69750200	-3.74669700
H	1.44881000	3.17962700	0.09963900	H	-1.90694000	-4.92446000	-3.66400700
N	5.65280500	4.68805800	-0.83919100	H	-1.14040400	-4.54478500	-5.21798600
C	6.58092700	5.25879600	0.12484000	C	-2.03787300	-1.92308500	-5.46709000
H	6.10292100	5.30555900	1.10797300	H	-1.63533900	-2.33670500	-6.39912300
H	7.52838000	4.70229700	0.22910600	H	-2.82761800	-1.20817700	-5.72191100
H	6.83154900	6.28301500	-0.17931000	H	-1.23966100	-1.35503800	-4.97347000
C	6.13480000	4.63722600	-2.21098500	C	-6.54385600	-1.86391300	-1.49934300
H	5.34230800	4.26317300	-2.86543000	H	-7.10383400	-2.24119600	-2.35619900
H	6.39826300	5.64999000	-2.54078300	C	-6.84569400	-2.78590500	-0.30170600
H	7.02414700	3.99771200	-2.35667600	H	-6.31024100	-2.45075400	0.59525500
N	4.61541300	-4.88322400	0.90755900	H	-7.91744300	-2.78367700	-0.07254900
N	-5.38319700	-3.12372900	-3.99176900	H	-6.54111800	-3.81801400	-0.50678100
N	-5.11146800	2.45103800	4.00832600	C	-7.04266600	-0.43073300	-1.23226600
C	4.80637100	-5.69638900	2.09686200	H	-6.58643900	-0.00073800	-0.33285800
H	4.91614600	-6.74865900	1.80070000	H	-6.81252500	0.23171300	-2.07352500
H	5.68913300	-5.43632800	2.70415000	H	-8.12813200	-0.43264500	-1.08155500
H	3.92123200	-5.61957700	2.73489300	H	0.18029100	-4.84322600	3.26148700
C	5.73002500	-4.86603900	-0.02750600	H	-0.92174100	1.60270900	5.52080200
H	5.41893300	-4.41746100	-0.97635300	O	-1.43215600	-0.86037000	4.53207000
H	6.60773900	-4.30542600	0.34504500	O	1.01086600	-2.38093700	4.03499100
H	6.05111800	-5.89491700	-0.23056100	C	-1.93561400	-0.66798100	5.84792600
C	-6.10910600	-2.24456400	-4.89650000	H	-2.67146200	0.14493100	5.87908200
H	-6.42906700	-2.81607200	-5.77621500	H	-2.42831600	-1.60241600	6.11875600
H	-7.00650500	-1.77715100	-4.45327200	H	-1.12588600	-0.46151700	6.55876900
H	-5.44510600	-1.44278300	-5.23464700	C	1.34780600	-3.40132400	4.96511500
C	-6.06523200	-4.35106600	-3.61093200	H	1.95022100	-4.18952900	4.49674000
H	-6.99968100	-4.20568300	-3.04187700	H	1.94179700	-2.91375300	5.73901400
H	-6.31498700	-4.91704200	-4.51707100	H	0.44819200	-3.84369700	5.41194300
H	-5.39215100	-4.96525400	-3.00463800	C	5.33762700	-2.64176300	2.76765700
C	-4.47573400	2.87870400	5.24354700	H	5.96347900	-3.49648200	2.50881300
H	-3.87520500	3.80194700	5.14813900	C	6.24226400	-1.40253300	2.67674500
H	-5.24425500	3.05620000	6.00555700	H	5.72595800	-0.49253200	3.00185000
H	-3.81333100	2.08661700	5.60823700	H	7.11965300	-1.52596800	3.32124000
C	-6.17933200	3.32130500	3.53283200	H	6.59534900	-1.24693000	1.65217700
H	-6.56667300	2.93694900	2.58526200	C	4.82894100	-2.83557700	4.20860800
H	-6.99885000	3.31564500	4.26307100	H	4.14558300	-2.02437400	4.48733300
H	-5.88169500	4.37144900	3.37569000	H	4.28748100	-3.78048600	4.31344000
C	6.70945300	1.96079400	-0.18037000	H	5.66300700	-2.84091700	4.91967300
H	7.23239600	2.75235400	-0.71910500	C	2.26057800	-4.84889300	-0.71185300
C	6.97424400	0.65430000	-0.95013300	H	3.10304400	-5.14235200	-1.35345700
H	6.55362600	-0.21762900	-0.43611800	C	1.92776900	-6.05468900	0.19636300
H	6.54523900	0.69526600	-1.95789400	H	1.16573400	-5.77782900	0.93034700
H	8.05221400	0.48510700	-1.04604300	H	1.52723600	-6.87426500	-0.41147900
C	7.30338100	1.90267500	1.24071700	H	2.80314100	-6.42475100	0.72421100
H	8.37203300	1.66183700	1.20283700	C	1.04393100	-4.60399900	-1.61610600
H	7.18721300	2.86031500	1.75782500	H	0.14574900	-4.40829000	-1.02375600
H	6.80403900	1.13721500	1.84071800	H	1.18799800	-3.76697100	-2.29528000
C	2.89182500	5.35409800	-0.58287100	H	0.85293000	-5.49389100	-2.22553400
H	3.74629200	6.02934700	-0.48627500	C	-5.23871400	-0.39441800	3.87554800
C	2.40128300	5.43680900	-2.04216800	H	-5.23308400	0.07068800	4.86790700
H	1.56449300	4.75234900	-2.21668700	C	-4.84695900	-1.87340200	4.03144800
H	2.04934800	6.44695800	-2.27828300	H	-5.03433600	-2.43769500	3.10905500
H	3.20518700	5.18531700	-2.74142800	H	-3.79041100	-1.99806200	4.28554800
C	1.80245100	5.81252500	0.40111800	H	-5.45296900	-2.33613900	4.81768900

C	-6.68056300	-0.30002700	3.33394800	C	0.78357500	1.48298200	1.65273900
H	-6.73702000	-0.71467500	2.31973300	C	-0.64339600	1.65131200	3.60914300
H	-7.36646800	-0.87207000	3.96968000	C	1.16510700	2.82156300	1.83719000
H	-7.02878400	0.73407600	3.30224400	C	-0.25484700	2.98089600	3.78826100
C	-3.32389900	4.07340300	2.19410300	C	0.66001700	3.55225000	2.90758700
H	-3.86380700	4.43684700	3.06955200	P	-1.66937300	-0.24281800	-0.05753400
C	-1.87536600	4.57407500	2.34482400	P	1.46907600	0.52767300	0.22589300
H	-1.23818600	4.26591700	1.50898500	C	-2.55388300	1.21430700	0.62713900
H	-1.85697000	5.66905100	2.38766700	C	-2.24743300	2.51850100	0.23446600
H	-1.41967500	4.18237400	3.25911400	C	-3.47547400	1.00677300	1.66066200
C	-4.00500100	4.67125200	0.94704600	C	-2.82958200	3.62614100	0.87217200
H	-3.52279400	4.33081200	0.02514800	C	-4.08426800	2.07538600	2.31527800
H	-5.05873200	4.37760200	0.89745800	C	-3.74996700	3.39755300	1.92434500
H	-3.95598400	5.76620800	0.96860400	C	-2.95649300	-1.33362800	-0.79675000
Rh	-0.08566100	0.83838600	-1.08295100	C	-4.31371900	-1.01808100	-0.76883400
C	4.25098100	-1.52451200	-2.57067000	C	-2.55874300	-2.55699400	-1.35888300
C	3.27744100	-0.54410400	-2.44772400	C	-5.28169800	-1.89370500	-1.27848500
C	1.99812800	-0.70124800	-3.02123800	C	-3.49513300	-3.48293300	-1.83058100
C	1.76656800	-1.84926900	-3.80518800	C	-4.87404500	-3.14281600	-1.79750400
C	2.74259700	-2.82960800	-3.96402000	C	2.21490400	-0.93970000	1.02440000
C	3.95764200	-2.66830500	-3.30805500	C	1.87273200	-2.21738200	0.56920500
H	5.22051500	-1.42395500	-2.09687600	C	3.10011100	-0.81171200	2.09524400
H	3.51008000	0.34355000	-1.87558900	C	2.40308600	-3.36971200	1.15073400
H	0.80755700	-1.97649700	-4.29675900	C	3.73027900	-1.93432300	2.64551000
H	2.56278300	-3.72308700	-4.55159600	C	3.37042800	-3.21997000	2.18046800
F	4.87723900	-3.64988300	-3.37770500	C	2.80115000	1.63465700	-0.39813100
C	0.93813200	0.30743000	-2.90760400	C	4.14171700	1.53681100	-0.03202200
H	0.09658300	0.09342000	-3.56143200	C	2.42707100	2.61151400	-1.33001700
C	1.29531700	1.77209400	-2.85566500	C	5.12148000	2.34984600	-0.62434400
H	2.36703500	1.96265800	-2.79185900	C	3.36536700	3.44773100	-1.93118300
H	0.83233700	2.31737900	-3.68366200	C	4.73508200	3.29467100	-1.59784000
C	-1.59536000	3.54841300	-2.72578300	H	-2.30278300	-2.97695200	0.92225900
C	-1.61514600	4.06236700	-4.03144900	H	-1.72086600	-4.23699400	2.92814800
C	-1.35641300	5.41533600	-4.26130700	H	1.86254200	3.29093900	1.15554300
C	-1.07834700	6.27354200	-3.19435400	H	0.97368800	4.58189600	3.05466300
C	-1.04603200	5.76593700	-1.89485000	H	-1.49984900	2.66705200	-0.53594100
C	-1.29255900	4.41122900	-1.66262900	H	-3.68516900	-0.00663400	1.98122300
H	-1.84526800	3.40479200	-4.86490700	H	-4.63411900	-0.07401100	-0.34431200
H	-1.37833600	5.79987800	-5.27749700	H	-1.50315500	-2.81662500	-1.36766700
H	-0.88857600	7.32758900	-3.37511300	H	1.16902000	-2.29154900	-0.25023500
H	-0.82562100	6.42111500	-1.05714100	H	3.31566200	0.17139000	2.50214000
H	-1.26658100	4.02932800	-0.64872000	H	4.45080300	0.80128700	0.70080000
Se	-2.10288600	1.67820700	-2.42636300	H	1.38230600	2.68724900	-1.61298100
H	0.87728500	2.33019300	-1.96444300	N	5.67023300	4.12375300	-2.30038500

#### 24-ts-S

B3LYP-D3 SCF energy: -4539.834164 a.u.

B3LYP-D3 enthalpy: -4537.922311 a.u.

B3LYP-D3 free energy: -4538.169374 a.u.

M06 SCF energy in solution: -4538.800694 a.u.

Imaginary frequency: -62.74 cm<sup>-1</sup>

#### Cartesian coordinates

ATOM	X	Y	Z				
C	-0.09434800	-1.35032800	3.63796400	N	-5.80177500	-4.11915500	-2.28473800
C	-0.47654400	-0.57325500	2.51790700	N	-4.34114200	4.45464300	2.69390100
C	-1.23857000	-1.17947500	1.49844600	C	3.81392300	-4.73343500	4.10938100
C	-1.67652200	-2.50416500	1.66405800	H	3.83521200	-5.82432300	4.23704300
C	-1.34697500	-3.22461000	2.80675800	H	4.59199100	-4.31182200	4.76798200
C	-0.53505400	-2.66611300	3.78824400	H	2.84171500	-4.37257200	4.45887300
C	-0.10879500	0.87402200	2.55327900	C	5.22060900	-4.82687400	2.09600800
				H	5.16841400	-4.68255300	1.01350300

H	6.09930000	-4.26980800	2.47194600	O	0.70957900	-0.73061300	4.54598000
H	5.39079200	-5.89258900	2.29413000	C	-1.85765800	1.61023100	5.67543500
C	-6.37715000	-3.87649300	-3.59817800	H	-2.46563700	2.51454600	5.55170300
H	-6.80315800	-4.81042000	-3.98380800	H	-2.44485900	0.86408100	6.21305600
H	-7.17514800	-3.11220600	-3.61436300	H	-0.95366000	1.85170800	6.24860600
H	-5.58855600	-3.55531600	-4.28692700	C	0.74441800	-1.24501900	5.87075600
C	-6.66920300	-4.77848800	-1.31937000	H	1.25293700	-2.21542000	5.92079000
H	-7.57625700	-4.21045900	-1.04939600	H	1.31321700	-0.52169700	6.45707300
H	-6.99208900	-5.74420500	-1.72755800	H	-0.26930400	-1.34306500	6.27944500
H	-6.10721100	-4.97178200	-0.40075400	C	4.79478600	-1.71631400	3.71758800
C	-3.52914100	5.00420700	3.76504600	H	5.32726100	-2.65717600	3.86500900
H	-2.76308800	5.72732800	3.42900500	C	5.84936900	-0.68350900	3.28283500
H	-4.17616500	5.51551000	4.48878300	H	5.42245400	0.32148100	3.19706000
H	-3.01133500	4.19176800	4.28213100	H	6.65805800	-0.63154300	4.02045100
C	-5.25048500	5.40056700	2.06866600	H	6.28805200	-0.94833700	2.31493000
H	-5.81522200	4.89893200	1.27819500	C	4.15978200	-1.31264400	5.06067200
H	-5.96757000	5.75817100	2.81970600	H	3.54998500	-0.40916300	4.94609100
H	-4.76030200	6.28625100	1.63105900	H	3.51037300	-2.10678700	5.44036200
C	6.57048200	2.17242100	-0.18347400	H	4.93203600	-1.11526800	5.81321900
H	7.19836200	2.81666700	-0.79925400	C	1.96652400	-4.75809000	0.67168100
C	7.06151700	0.72824300	-0.39780200	H	2.87602800	-5.30174100	0.38588900
H	6.51368300	0.01864100	0.23226900	C	1.26307200	-5.57123200	1.77837100
H	6.93343400	0.41626600	-1.43996500	H	0.35369000	-5.05756200	2.10208800
H	8.12352600	0.64475200	-0.14101900	H	0.97683300	-6.55678200	1.39203700
C	6.75906800	2.62218900	1.27752700	H	1.90653700	-5.72054300	2.64388200
H	7.80709700	2.51654700	1.58055100	C	1.03944900	-4.71738800	-0.55272700
H	6.46905500	3.67077200	1.40641500	H	0.08539900	-4.24047400	-0.29718800
H	6.15096900	2.01995600	1.96061200	H	1.48116700	-4.17934100	-1.39397000
C	2.92824500	4.44083000	-2.99959200	H	0.81632400	-5.73747500	-0.88362000
H	3.70167000	5.21155600	-3.05804300	C	-5.09256000	1.82105500	3.43211200
C	2.87600000	3.74151200	-4.37265600	H	-4.90848600	2.56731400	4.21260100
H	2.16490800	2.90514100	-4.35646500	C	-4.97269100	0.42685200	4.06899800
H	2.56670100	4.44243400	-5.15697500	H	-5.32523700	-0.36031300	3.39053700
H	3.85351900	3.33233300	-4.64436100	H	-3.93957300	0.19384900	4.34423800
C	1.58963600	5.12634700	-2.68519800	H	-5.59642700	0.37616300	4.96814400
H	0.74775100	4.42470500	-2.73543400	C	-6.53001800	2.04444600	2.92023400
H	1.58751400	5.57210800	-1.68474300	H	-6.76297600	1.34250600	2.10999000
H	1.39172200	5.91929500	-3.41487600	H	-7.25500300	1.88003800	3.72594700
C	-3.05563300	-4.88754600	-2.23088600	H	-6.66494000	3.06057000	2.54260100
H	-3.89679800	-5.33974400	-2.76208800	C	-2.46227100	5.04866900	0.44779100
C	-2.81633800	-5.72012300	-0.95303400	H	-2.65491500	5.69929800	1.30428500
H	-1.99059400	-5.30667700	-0.36200600	C	-0.97914100	5.22160200	0.08389300
H	-3.71038100	-5.73678300	-0.32009000	H	-0.70986800	4.65225900	-0.81193100
H	-2.56183700	-6.75512600	-1.20880200	H	-0.76829900	6.27564900	-0.12982600
C	-1.82710200	-4.93726600	-3.15123300	H	-0.32624100	4.89208600	0.89366800
H	-1.59280400	-5.97866900	-3.39838200	C	-3.33633600	5.55175600	-0.71938200
H	-2.01152300	-4.40740300	-4.09193700	H	-3.07179400	5.04489900	-1.64837300
H	-0.93316700	-4.50988100	-2.68250200	H	-4.40132100	5.37783000	-0.54965900
C	-6.74665700	-1.47790700	-1.18273900	H	-3.18407300	6.62713000	-0.86834200
H	-7.35435800	-2.23620900	-1.67749500	Rh	0.08597600	0.04094600	-1.53545100
C	-7.19538000	-1.41317900	0.29050300	Se	2.15638500	-0.45305400	-3.10115700
H	-6.62652600	-0.65636000	0.84337500	C	3.29115200	-1.91446700	-2.44242200
H	-8.25737800	-1.15189700	0.35962200	C	4.32022900	-1.65275500	-1.53117900
H	-7.04574900	-2.37552300	0.79167400	C	3.16396300	-3.19392500	-2.99579700
C	-7.02262500	-0.14544800	-1.90291000	C	5.20142100	-2.66883400	-1.16162700
H	-6.47718300	0.68689900	-1.44241900	H	4.43817600	-0.65895300	-1.12128200
H	-6.73810600	-0.20277700	-2.96037400	C	4.04668600	-4.20933100	-2.61984900
H	-8.08980500	0.09800600	-1.85675800	H	2.38191400	-3.39807800	-3.72176700
H	-0.25829700	-3.24848900	4.65865200	C	5.06585900	-3.95065300	-1.70077800
H	-0.65071200	3.56755200	4.60798300	H	5.99568100	-2.45405300	-0.45167700
O	-1.53159600	1.01823400	4.42504200	H	3.93903500	-5.20089100	-3.05108400

H	5.75878300	-4.73901500	-1.42028000	C	2.66602000	2.29193800	-1.34706500
C	-3.65309300	1.18793600	-3.19575800	C	5.26270800	1.26683900	-1.09878500
C	-2.71098900	0.20865600	-3.42878400	C	3.70751000	2.92205000	-2.02689900
C	-1.33575700	0.54868900	-3.60419000	C	5.01851500	2.38284100	-1.93272600
C	-0.95167400	1.91590700	-3.42763800	H	-2.37957400	-2.90139900	1.05667600
C	-1.90287400	2.90104700	-3.18815200	H	-1.79388800	-4.00280600	3.17301500
C	-3.23790200	2.51954400	-3.09351700	H	2.07462700	3.16046900	0.89469900
H	-4.70472500	0.95297200	-3.09312700	H	1.04131000	4.77987900	2.43326100
H	-3.02778900	-0.82198400	-3.52367500	H	-1.41250300	2.41031300	-1.11669400
H	0.08190300	2.19837700	-3.59943200	H	-3.82691100	0.44644400	1.81159700
H	-1.62678600	3.94485700	-3.09929000	H	-4.66847600	-0.01016100	-0.60536400
F	-4.17639300	3.45324500	-2.90354100	H	-1.56664500	-2.88164700	-1.29861100
C	-0.39523100	-0.37758900	-4.15768400	H	1.22851000	-2.48171600	-0.26599600
H	0.38007100	0.07740000	-4.76033400	H	3.07898300	0.03543100	2.66279600
C	-0.74204100	-1.79020000	-4.49927800	H	4.37601400	-0.19525900	0.19992900
H	0.15380600	-2.35397900	-4.76338100	H	1.65657300	2.68306300	-1.44350600
H	-1.42448200	-1.80010000	-5.36400500	N	6.04182000	3.00549500	-2.71209200
H	-1.24608400	-2.29736800	-3.67730700	C	6.82998400	4.04177200	-2.06406000

## 25

B3LYP-D3 SCF energy: -4298.369141 a.u.

B3LYP-D3 enthalpy: -4296.568849 a.u.

B3LYP-D3 free energy: -4296.804949 a.u.

M06 SCF energy in solution: -4297.379621 a.u.

### Cartesian coordinates

ATOM	X	Y	Z				
C	-0.31738200	-0.99618100	3.71618000	N	-5.73635100	-3.91464900	-2.87913300
C	-0.64338900	-0.33778900	2.50979800	N	-4.35858400	4.97575200	1.40849500
C	-1.38242200	-1.04222900	1.53550400	C	3.08656300	-4.83890500	4.40031700
C	-1.79404600	-2.36006100	1.78833800	H	3.11404100	-5.92157800	4.57825200
C	-1.46890200	-2.98293000	2.99016100	H	3.64990000	-4.35438000	5.21662700
C	-0.72687600	-2.31059300	3.95610700	H	2.04432600	-4.51056600	4.46656000
C	-0.20430900	1.08827200	2.38467600	C	4.94949300	-4.99374300	2.79034700
C	0.81718200	1.51011400	1.51085100	H	5.15287200	-4.89930300	1.71854800
C	-0.78087800	2.03751600	3.26073000	H	5.72427300	-4.42375700	3.33409600
C	1.26910600	2.83830900	1.54168700	H	5.05732800	-6.05007700	3.06514600
C	-0.34859100	3.36733900	3.26042000	C	-6.31243500	-3.44989800	-4.13308100
C	0.68686900	3.75313100	2.41287800	H	-6.57079900	-4.31880100	-4.75132000
P	-1.74453800	-0.27174300	-0.10549400	H	-7.22321700	-2.83637600	-4.02551000
P	1.45159700	0.34408500	0.23058800	H	-5.57003400	-2.85721600	-4.67597500
C	-2.56671800	1.30298100	0.30009500	C	-6.60280500	-4.75607500	-2.06605200
C	-2.18778000	2.46938600	-0.35909100	H	-7.47549200	-4.22889300	-1.64085300
C	-3.55186500	1.35729900	1.29296800	H	-6.97794400	-5.58586200	-2.67706300
C	-2.74672900	3.70771400	-0.02373200	H	-6.02742500	-5.17833400	-1.23566600
C	-4.16363500	2.56402900	1.63115100	C	-3.58785600	5.76694600	2.35417800
C	-3.74486600	3.75361700	0.97544500	H	-2.75128300	6.32739500	1.89774200
C	-3.01082400	-1.34760200	-0.87731000	H	-4.24797500	6.49096400	2.84703000
C	-4.34391000	-0.96490100	-1.00305400	H	-3.16673700	5.10970300	3.12243300
C	-2.60721600	-2.58782800	-1.39662100	C	-5.14743300	5.74702700	0.45807000
C	-5.28620300	-1.79627700	-1.62788800	H	-5.66230800	5.06564600	-0.22494800
C	-3.50919800	-3.43896800	-2.03267900	H	-5.90887500	6.31887800	1.00414900
C	-4.86200800	-3.02699100	-2.17141500	H	-4.56821100	6.46267400	-0.14924800
C	2.10189400	-1.10381700	1.12383600	C	6.66798800	0.75645600	-0.79479000
C	1.85045300	-2.38152900	0.61835600	H	7.36812500	1.23553100	-1.47947200
C	2.88938400	-0.95868000	2.26837400	C	6.81019500	-0.76538800	-0.97835900
C	2.35481700	-3.51987900	1.24988700	H	6.20758900	-1.31854500	-0.24758200
C	3.44347900	-2.07219700	2.90880900	H	6.49560500	-1.07441300	-1.97839200
C	3.14197400	-3.36474000	2.41664800	H	7.85381800	-1.06581000	-0.83304100
C	2.88895300	1.16037000	-0.55033600	C	7.07292400	1.17721000	0.63323800
C	4.18703500	0.66191500	-0.43581900	H	8.09782100	0.85537000	0.85173400
				H	7.02157800	2.26468800	0.75601400

H	6.41024200	0.72317300	1.37879000	H	3.17206900	-4.68200700	-1.13262700
C	3.41573600	4.18938600	-2.82093300	H	2.02487300	-6.03757600	-1.14526100
H	4.33098300	4.44293100	-3.36276300	C	-5.28358900	2.59694000	2.66801800
C	2.29243400	4.00689400	-3.85783100	H	-5.12218200	3.47978000	3.29725600
H	1.34110000	3.72936900	-3.38678400	C	-5.32382700	1.35706000	3.57625800
H	2.12549900	4.94241800	-4.40319400	H	-5.67968400	0.47288400	3.03264500
H	2.54602900	3.23593500	-4.59345100	H	-4.34083400	1.11737000	3.99112200
C	3.08053000	5.35050100	-1.86281800	H	-6.02092000	1.52638000	4.40391900
H	2.15930400	5.14653600	-1.30321200	C	-6.65261700	2.77224000	1.97840600
H	3.88391700	5.51152800	-1.13540500	H	-6.85173300	1.93054400	1.30340600
H	2.93507700	6.28281200	-2.42062200	H	-7.45546200	2.80173600	2.72426400
C	-3.03917600	-4.76666500	-2.61668300	H	-6.69341000	3.69606500	1.39827800
H	-3.88972900	-5.45339200	-2.58114500	C	-2.26442800	4.94492000	-0.77541600
C	-1.87878100	-5.40564300	-1.83801600	H	-2.61501900	5.83038000	-0.24241400
H	-0.94392700	-4.84193100	-1.94899000	C	-0.72916100	5.04405000	-0.83574500
H	-2.09778600	-5.47765100	-0.76693300	H	-0.29307900	4.24236700	-1.44366200
H	-1.68724800	-6.41611100	-2.21489900	H	-0.43048000	5.99470000	-1.29161600
C	-2.66455500	-4.59375600	-4.10185400	H	-0.28668400	4.97946700	0.16217100
H	-2.37816600	-5.55521000	-4.54353300	C	-2.86296500	4.97711800	-2.19562200
H	-3.50388900	-4.19069800	-4.67550600	H	-2.52777600	4.10601500	-2.77282100
H	-1.81390200	-3.90814500	-4.21207600	H	-3.95719800	4.95938400	-2.17048000
C	-6.73471100	-1.32097100	-1.67299100	H	-2.54642700	5.87971600	-2.73104100
H	-7.34528300	-2.11332100	-2.10765500	Rh	-0.00616000	-0.09825900	-1.50679700
C	-7.28398500	-1.06087600	-0.25661100	C	3.01565300	0.32456500	-4.10894300
H	-6.75152100	-0.24145000	0.24035300	C	1.62582800	0.33242000	-4.05792300
H	-8.34336700	-0.78503600	-0.30536700	C	0.90795100	-0.82468000	-3.67528700
H	-7.19060800	-1.95214400	0.37364800	C	1.64517100	-1.98590100	-3.32559400
C	-6.88554800	-0.07398300	-2.56470900	C	3.03401100	-1.99609400	-3.35900100
H	-6.30851800	0.76929800	-2.16628500	C	3.69327300	-0.83605600	-3.75830500
H	-6.53400800	-0.27087300	-3.58346300	H	3.57770400	1.20241200	-4.40053100
H	-7.93543800	0.23544500	-2.61902200	H	1.09394600	1.23339200	-4.34191700
H	-0.46948900	-2.80326600	4.88676200	H	1.10770600	-2.88226900	-3.03259100
H	-0.79800800	4.09671200	3.92276500	H	3.60460900	-2.87637000	-3.08512600
O	-1.75473700	1.56993100	4.08977300	F	5.04003300	-0.83896400	-3.81932400
O	0.42001600	-0.27845400	4.60999900	C	-0.55234300	-0.83865900	-3.50041300
C	-2.23865900	2.42741800	5.11646300	H	-1.03304400	-1.81228300	-3.45598100
H	-2.80490300	3.27081700	4.70115800	C	-1.32863500	0.29739800	-3.34442900
H	-2.90733600	1.81705800	5.72469100	H	-0.98198300	1.29185100	-3.61158200
H	-1.41892200	2.80494600	5.74052500	H	-2.40028600	0.19042400	-3.20917800
C	0.23225300	-0.54978300	5.99546300				
H	0.68996000	-1.49930100	6.29596600	<b>26</b>			
H	0.73067600	0.26187400	6.52853200	B3LYP-D3 SCF energy: -4539.860002 a.u.			
H	-0.83536600	-0.56065100	6.24631900	B3LYP-D3 enthalpy: -4537.950348 a.u.			
C	4.36245900	-1.84211600	4.10423100	B3LYP-D3 free energy: -4538.202402 a.u.			
H	4.80294100	-2.79941100	4.38757000	M06 SCF energy in solution: -4538.832033 a.u.			
C	5.53165500	-0.90623300	3.74273700				
H	5.18406600	0.10563900	3.50467800	Cartesian coordinates			
H	6.22851700	-0.82517600	4.58455800	ATOM	X	Y	Z
H	6.08587800	-1.28414400	2.87630500	C	-0.31365800	1.20111900	3.99798700
C	3.58008800	-1.31176300	5.31860000	C	0.08356500	0.50889800	2.83385900
H	3.06608400	-0.37490600	5.07925900	C	0.89325600	1.17910600	1.89688600
H	2.82058300	-2.03473200	5.63339100	C	1.31537700	2.49361700	2.14264900
H	4.25344600	-1.13282300	6.16474300	C	0.93804100	3.14286300	3.31502200
C	2.00540400	-4.89998200	0.70864100	C	0.11768400	2.50770600	4.24181400
H	2.68895800	-5.61291300	1.17617500	C	-0.29353600	-0.93419800	2.72502100
C	0.57509700	-5.28739100	1.12908100	C	-1.16987100	-1.46004900	1.75174400
H	-0.15542400	-4.57807800	0.72332600	C	0.23675000	-1.80836700	3.70767100
H	0.32022100	-6.28954500	0.76449800	C	-1.53816700	-2.81462600	1.81482100
H	0.47326200	-5.27929500	2.21942100	C	-0.10480200	-3.16218300	3.72912700
C	2.17262000	-5.00299300	-0.81656800	C	-1.01028200	-3.64999900	2.79200000
H	1.43616400	-4.38741800	-1.34685600	P	1.42727500	0.30660200	0.36097300

P	-1.75517400	-0.40776400	0.32894100	C	6.03251900	5.21004500	-1.06072200
C	2.34864200	-1.12941400	1.02386000	H	6.83978000	4.84370900	-0.40134100
C	2.22152600	-2.39102600	0.44749900	H	6.43592300	6.03942000	-1.65408600
C	3.17845800	-0.96530500	2.14058200	H	5.23213800	5.60482200	-0.42634800
C	2.88575700	-3.50384900	0.98317700	C	3.71327200	-5.23148100	3.62745500
C	3.89808800	-2.03338300	2.67261100	H	3.03963900	-5.95619100	3.13433300
C	3.74058100	-3.32016500	2.09251000	H	4.40979500	-5.79697000	4.25844400
C	2.70854700	1.42781500	-0.33443700	H	3.10124700	-4.59903900	4.27881600
C	4.07141200	1.25238100	-0.10019700	C	5.47454100	-5.09825100	1.92499400
C	2.28659100	2.52232700	-1.10402300	H	5.96220800	-4.39482400	1.24432400
C	5.02239000	2.15401900	-0.59817500	H	6.23884000	-5.49965000	2.60320700
C	3.20215000	3.44747200	-1.61202700	H	5.08966200	-5.93962800	1.32451800
C	4.58754900	3.24851900	-1.37477200	C	-6.86710400	-0.68829300	-1.21722200
C	-2.47844400	1.06607000	1.14888400	H	-7.52066300	-1.27310000	-1.86532900
C	-2.18152100	2.36718500	0.72529500	C	-6.73123200	0.70574700	-1.85948300
C	-3.35107400	0.87539300	2.22497600	H	-6.13561100	1.38344800	-1.23647900
C	-2.71348600	3.47799300	1.39387600	H	-6.25205300	0.64261100	-2.84299600
C	-3.92904100	1.95668000	2.89608400	H	-7.71949400	1.16106800	-1.98924000
C	-3.56867700	3.26596000	2.50474800	C	-7.54204500	-0.60035200	0.16336000
C	-3.19727300	-1.31210600	-0.37544300	H	-8.52461400	-0.12137900	0.08258900
C	-4.47228700	-0.74991000	-0.45442800	H	-7.68111100	-1.59464600	0.60155800
C	-2.98099400	-2.55725700	-0.98545300	H	-6.93617600	-0.01065000	0.85830300
C	-5.52049600	-1.39849600	-1.12663900	C	-3.71172300	-4.61336200	-2.24964000
C	-4.00661700	-3.26042600	-1.61534800	H	-4.67714200	-5.10270400	-2.40512100
C	-5.29356900	-2.66937800	-1.69816600	C	-3.05736200	-4.42843300	-3.63313300
H	1.95124000	3.00706000	1.43269800	H	-2.09372300	-3.91194900	-3.54964500
H	1.27767000	4.15687600	3.50224500	H	-2.87617800	-5.39915200	-4.10970600
H	-2.25552700	-3.22488100	1.12000500	H	-3.69468200	-3.83892900	-4.30003700
H	-1.30813500	-4.69419500	2.82474600	C	-2.84866500	-5.51924300	-1.35411100
H	1.56620400	-2.51805500	-0.40768900	H	-1.83167400	-5.12807800	-1.22075900
H	3.24846000	0.01238100	2.60117500	H	-3.29209600	-5.63692100	-0.35888500
H	4.41180100	0.41101500	0.49087700	H	-2.75660800	-6.51456700	-1.80336900
H	1.22558700	2.64915600	-1.29761000	C	2.72126200	4.62873800	-2.44537900
H	-1.49840200	2.50632300	-0.10816600	H	3.42959700	5.44736200	-2.28721900
H	-3.58507100	-0.13516500	2.54767100	C	1.32207800	5.12139700	-2.04650800
H	-4.66033900	0.21648000	-0.00010400	H	0.54580200	4.38907900	-2.28797200
H	-1.98145700	-2.98071800	-0.97872900	H	1.25953300	5.34035700	-0.97404700
N	-6.30954100	-3.41307400	-2.38207800	H	1.07700300	6.03582700	-2.59771600
C	-7.40969700	-3.93712100	-1.58587900	C	2.77048500	4.26280500	-3.94233400
H	-7.02112400	-4.31725800	-0.63611600	H	2.34172500	5.06499900	-4.55452000
H	-8.20467300	-3.20495600	-1.36145100	H	3.80029000	4.09027600	-4.26799200
H	-7.87275900	-4.77456200	-2.12244200	H	2.19231400	3.35202000	-4.12948700
C	-6.65957600	-2.98331200	-3.72802700	C	6.48417800	1.91429400	-0.23514000
H	-5.75322700	-2.69050500	-4.26592000	H	7.08807600	2.70311500	-0.68448800
H	-7.12028200	-3.82028300	-4.26727100	C	6.69287600	2.00175900	1.28965900
H	-7.36379300	-2.13303900	-3.76544500	H	6.13175400	1.22158100	1.81730400
N	-4.01944900	4.42817200	3.21178900	H	7.75271900	1.87570000	1.53844400
N	5.48704000	4.20104800	-1.95661600	H	6.36251700	2.97154600	1.67790200
N	4.46561300	-4.39616400	2.70583600	C	6.99360400	0.57077500	-0.78985700
C	-3.56043400	4.59894900	4.58055000	H	6.45325600	-0.27535800	-0.34838500
H	-3.59793300	5.66398000	4.84288900	H	6.86944300	0.51971400	-1.87737700
H	-4.14529700	4.04911800	5.33890100	H	8.05733600	0.44081900	-0.56083000
H	-2.51930600	4.26797300	4.65125400	H	-0.18044800	3.02228900	5.14816700
C	-5.36067800	4.90839500	2.92018400	H	0.31220800	-3.82982900	4.47263400
H	-5.52670700	4.88750000	1.83795600	O	1.08423800	-1.24577300	4.61462400
H	-6.16827700	4.32507000	3.39775200	O	-1.12304600	0.52056200	4.85731800
H	-5.45514500	5.94766500	3.25811500	C	1.51170000	-2.02895600	5.72108200
C	6.38954100	3.73233700	-2.99826500	H	2.17033800	-2.84627400	5.40231900
H	6.68654100	4.58308000	-3.62435600	H	2.07404400	-1.35290900	6.36628000
H	7.31325900	3.25269600	-2.63017800	H	0.65810500	-2.43794400	6.27609900
H	5.86657900	3.01113700	-3.63329900	C	-0.98579500	0.79244000	6.24780000

H	-1.41457700	1.76352800	6.52443200	C	2.70523400	-2.86273300	-4.45984700
H	-1.54151200	0.00671800	6.76264000	C	2.64506100	-4.20065700	-4.85759100
H	0.06926800	0.76094400	6.54510000	C	1.65198000	-5.04141900	-4.35014000
C	-4.94466400	1.67849400	4.00130300	C	0.72095500	-4.54742000	-3.43575800
H	-5.33834300	2.63325900	4.35232800	C	0.78110600	-3.21431500	-3.02223000
C	-6.14418000	0.88015700	3.45857500	H	3.46927100	-2.20760000	-4.86753700
H	-5.84359500	-0.11046800	3.09874000	H	3.37165500	-4.58059300	-5.56980800
H	-6.89397100	0.73473900	4.24461200	H	1.60570800	-6.07936200	-4.66620300
H	-6.62232300	1.41054800	2.62793000	H	-0.04684300	-5.19859700	-3.03005400
C	-4.30878800	0.97444800	5.21167900	H	0.07103600	-2.82502200	-2.29996000
H	-3.82625900	0.03439700	4.92494800	Se	1.87216600	-0.47313500	-3.00425700
H	-3.54486700	1.60985600	5.66721400	H	3.02729800	-0.63617600	-2.07355200
H	-5.07051000	0.75618100	5.96913200				
C	-2.35047100	4.90237500	0.98219900				
H	-3.11656900	5.55632500	1.40465400	<b>27-ts</b>			
C	-1.00719300	5.32656800	1.60196000	B3LYP-D3 SCF energy: -4539.830098 a.u.			
H	-0.19033900	4.70638400	1.21701800	B3LYP-D3 enthalpy: -4537.923370 a.u.			
H	-0.78789700	6.37377700	1.36158200	B3LYP-D3 free energy: -4538.172868 a.u.			
H	-1.02482600	5.21818800	2.69071300	M06 SCF energy in solution: -4538.805603 a.u.			
C	-2.32273800	5.11771700	-0.53522400	Imaginary frequency: -930.49 cm <sup>-1</sup>			
H	-1.50262300	4.57068500	-1.00851600				
H	-3.26289300	4.80361900	-1.00382300	Cartesian coordinates			
H	-2.17176400	6.18007600	-0.75913400	ATOM X Y Z			
C	4.85967800	-1.81018200	3.83710400	C 0.06288700 -1.18487400 3.96311900			
H	4.73707600	-2.65001400	4.53076200	C -0.27788000 -0.50010900 2.77761500			
C	4.60534300	-0.50482800	4.60947000	C -0.98802700 -1.19500600 1.77865600			
H	4.90826700	0.37292400	4.02473600	C -1.37313900 -2.52687500 1.98736500			
H	3.55144600	-0.37781500	4.87290300	C -1.05854700 -3.16869800 3.18263200			
H	5.19958500	-0.49720800	5.52951900	C -0.33377000 -2.50907900 4.16974100			
C	6.32117200	-1.83638600	3.34254400	C 0.04909100 0.95711200 2.70226000			
H	6.49211000	-1.03915400	2.60857600	C 0.96314700 1.52124900 1.78779300			
H	7.01100200	-1.67574000	4.17932300	C -0.57600100 1.80944800 3.64711000			
H	6.56831900	-2.79212900	2.87681700	C 1.26319700 2.89227400 1.85329300			
C	2.66605600	-4.86597700	0.33278600	C -0.29405200 3.17742900 3.67910500			
H	3.08999000	-5.62948100	0.98676100	C 0.63897900 3.70524100 2.79156900			
C	1.17117700	-5.20527600	0.18322700	P -1.47536200 -0.33000500 0.22022300			
H	0.65926400	-4.51439800	-0.49350300	P 1.69161700 0.49209200 0.43023900			
H	1.05334500	-6.21522000	-0.22644300	C -2.50818800 1.03785400 0.86083100			
H	0.66099100	-5.15867800	1.14991600	C -2.43982700 2.32965400 0.34428500			
C	3.40465700	-4.94634300	-1.01767500	C -3.38007300 0.76708200 1.92467900			
H	3.03890400	-4.18476900	-1.71262800	C -3.21981600 3.36436400 0.88261500			
H	4.48101800	-4.79382300	-0.88544800	C -4.20985100 1.75396500 2.45219700			
H	3.25278100	-5.92559800	-1.48579400	C -4.12654500 3.06872800 1.92504000			
Rh	-0.15375500	-0.15770400	-1.29312300	C -2.60193800 -1.52520700 -0.58809600			
C	-0.17864200	2.94782000	-5.28018500	C -3.97892900 -1.49433900 -0.38328800			
C	-0.49886300	1.76602700	-4.62346600	C -2.04565800 -2.56154300 -1.35120200			
C	-1.40955500	1.75599000	-3.54886500	C -4.81589900 -2.49085200 -0.90152900			
C	-2.01101300	2.97047900	-3.17794700	C -2.84806500 -3.56698900 -1.89474200			
C	-1.70054800	4.16421900	-3.82407900	C -4.25059000 -3.52241200 -1.68013400			
C	-0.77157600	4.13523300	-4.85711400	C 2.38558800 -0.97655900 1.27239000			
H	0.52653400	2.96910200	-6.10356000	C 2.16430200 -2.27408400 0.79766700			
H	-0.04202900	0.84380900	-4.96397800	C 3.17156500 -0.78371300 2.41374200			
H	-2.73095700	2.97420000	-2.36621100	C 2.68481700 -3.38362600 1.47721600			
H	-2.14735000	5.10642200	-3.52732300	C 3.74135300 -1.86243500 3.09501000			
F	-0.41878400	5.28652100	-5.45701500	C 3.45479300 -3.17315200 2.64856200			
C	-1.82178500	0.53061400	-2.85024400	C 3.15144900 1.42574700 -0.18998500			
H	-2.69160900	0.64920100	-2.20869900	C 4.44398900 0.89737400 -0.14535400			
C	-1.42319800	-0.75409300	-3.15449800	C 2.95237100 2.64132900 -0.86133800			
H	-2.01998300	-1.59176300	-2.82436200	C 5.52491400 1.55005000 -0.75581200			
H	-0.76685500	-0.95883600	-3.99416300	C 4.01024100 3.35526000 -1.42475100			
C	1.77454500	-2.37964000	-3.53686500	C 5.31689200 2.80407300 -1.37320300			

H	-1.37422900	-4.19528100	3.34107100	H	2.90970600	5.42840400	-3.99061500
H	1.99925200	3.33018000	1.19500300	H	3.65201500	3.82540200	-4.12489800
H	0.88099700	4.76318000	2.83242300	C	2.90162700	5.63460500	-1.22497400
H	-1.76334400	2.54184400	-0.47532200	H	1.89273600	5.24645700	-1.03472700
H	-3.40185400	-0.22994600	2.34635800	H	3.38433300	5.79793200	-0.25492200
H	-4.41879000	-0.69477700	0.19968200	H	2.78941200	6.60798500	-1.71577300
H	-0.97238100	-2.57823600	-1.51443000	C	-2.23504700	-4.67185300	-2.74701800
H	1.54778000	-2.41753400	-0.08563500	H	-2.83165100	-5.57531700	-2.58808800
H	3.34535700	0.22512300	2.77707600	C	-0.77998900	-4.99502600	-2.37576900
H	4.61789400	-0.05064200	0.35018700	H	-0.10326300	-4.16233800	-2.59097000
H	1.94709400	3.04275900	-0.94488500	H	-0.68210500	-5.24371600	-1.31301800
N	6.37194600	3.56185700	-1.97026600	H	-0.42547900	-5.85128500	-2.96020800
C	7.45659400	4.03509900	-1.12300900	C	-2.36276100	-4.30242000	-4.23850400
H	7.06038400	4.29434600	-0.13698900	H	-1.86800200	-5.05108200	-4.86898000
H	8.28042600	3.31482400	-0.98376500	H	-3.41333000	-4.24452200	-4.53473600
H	7.88477300	4.94354000	-1.56540400	H	-1.89937600	-3.32935300	-4.43169500
C	6.74831100	3.21466500	-3.33221700	C	-6.29883800	-2.42340500	-0.55125600
H	5.85006900	3.00830800	-3.92141300	H	-6.80344000	-3.27510500	-1.00825900
H	7.27022600	4.06189400	-3.79339200	C	-6.50737700	-2.54494200	0.97137700
H	7.41019100	2.33245800	-3.40212000	H	-6.04551100	-1.70799400	1.50793200
N	3.89753900	-4.33565000	3.35779100	H	-7.57653200	-2.54495400	1.21228400
N	-5.03089500	-4.56132300	-2.28631400	H	-6.06902700	-3.47217500	1.35717500
N	-4.99381800	4.05299500	2.50857700	C	-6.95630700	-1.14468200	-1.10262000
C	3.36404200	-4.55300000	4.69271300	H	-6.51874200	-0.24458400	-0.65452500
H	3.40888300	-5.62394400	4.92815300	H	-6.83104000	-1.07248600	-2.18846000
H	3.89257900	-4.01339600	5.49797100	H	-8.02932900	-1.13980200	-0.87966500
H	2.31376400	-4.24471400	4.71106900	H	-0.08330000	-3.01743900	5.09391300
C	5.26433100	-4.77663100	3.13070700	H	-0.78382200	3.82856900	4.39218800
H	5.48779400	-4.73099100	2.05958600	O	-1.44958800	1.21332800	4.50377200
H	6.02900000	-4.18207200	3.66215300	O	0.78599100	-0.48098700	4.87881200
H	5.36761500	-5.81941100	3.45460600	C	-2.00236700	1.98685900	5.56090300
C	-5.98761800	-4.18246500	-3.31685800	H	-2.66840900	2.76807700	5.17615800
H	-6.16212300	-5.04168600	-3.97696900	H	-2.58448000	1.29146000	6.16647200
H	-6.96964900	-3.85118600	-2.93755200	H	-1.21686800	2.44074600	6.17804600
H	-5.56952100	-3.37077700	-3.91917000	C	0.55224500	-0.75547700	6.25640100
C	-5.45224200	-5.64639400	-1.41296200	H	0.98536600	-1.71409300	6.56697500
H	-6.29654800	-5.39011600	-0.74777800	H	1.04622600	0.04556000	6.80916300
H	-5.75636800	-6.50519900	-2.02359400	H	-0.52256400	-0.75189700	6.47301700
H	-4.61084800	-5.95739600	-0.78491900	C	4.67376000	-1.58042200	4.27001000
C	-4.40044000	4.93867300	3.49591600	H	5.08384000	-2.53025700	4.61575500
H	-3.76428100	5.73513300	3.06823100	C	5.87090300	-0.71894100	3.82740300
H	-5.19646200	5.42156700	4.07578400	H	5.55350000	0.27297900	3.48568800
H	-3.78418600	4.35637600	4.18863100	H	6.56745900	-0.57530700	4.66113800
C	-6.01002000	4.66830400	1.66502600	H	6.41646900	-1.20036400	3.00841100
H	-6.37420100	3.93399600	0.94121900	C	3.93562500	-0.94052400	5.45771700
H	-6.85687000	4.97842200	2.29104800	H	3.43883100	-0.00870400	5.16884500
H	-5.66824800	5.55472400	1.10506100	H	3.16730400	-1.61672500	5.84217100
C	6.88542600	0.86092100	-0.74359400	H	4.63812600	-0.72182400	6.27017900
H	7.54651400	1.40401200	-1.42107500	C	2.39523000	-4.80261200	0.99763600
C	6.79924900	-0.58429900	-1.27246700	H	3.08967300	-5.46023400	1.52483800
H	6.21774000	-1.23023400	-0.60389900	C	0.97335500	-5.23703800	1.39314100
H	6.33381400	-0.61592700	-2.26427800	H	0.22239500	-4.59223400	0.92349300
H	7.80303700	-1.01609200	-1.35261300	H	0.78668200	-6.27025600	1.07700500
C	7.51445700	0.89645400	0.66126300	H	0.83270600	-5.17649200	2.47662600
H	8.50306000	0.42329500	0.65477000	C	2.61043800	-4.98350600	-0.50955500
H	7.62977100	1.92400100	1.02127100	H	1.87799400	-4.42210700	-1.09539000
H	6.88746000	0.35891600	1.37979600	H	3.61207100	-4.65742700	-0.81376900
C	3.73194800	4.68660900	-2.10898100	H	2.50030500	-6.03935100	-0.78250800
H	4.70469800	5.15285800	-2.28771700	C	-5.21064700	1.40915500	3.55190100
C	3.05151400	4.47148100	-3.47532600	H	-5.21263900	2.24043800	4.26611300
H	2.06341600	4.01090300	-3.36343500	C	-4.87036400	0.11800200	4.31578900



H	-5.05348200	-0.77295300	3.70207600	C	0.72456600	-4.82143100	-0.86233200
H	-3.82400300	0.08871500	4.63407500	C	0.15609300	-1.43562500	-2.45152900
H	-5.50889600	0.03233500	5.20165000	C	-0.94638400	-0.57644400	-2.25218900
C	-6.63621700	1.30394900	2.97121300	C	0.82980200	-1.39687300	-3.69500800
H	-6.68445400	0.51338000	2.21229400	C	-1.35375700	0.29447300	-3.27686100
H	-7.35445400	1.05561600	3.76147300	C	0.44464400	-0.49195100	-4.68959300
H	-6.94859400	2.24279400	2.51001500	C	-0.65206700	0.33892800	-4.47649000
C	-3.07097200	4.76900700	0.30632400	P	1.63643900	-0.38293900	0.17506000
H	-3.62298300	5.45945400	0.94554100	P	-1.71889900	-0.45508100	-0.57959000
C	-1.60692100	5.24566700	0.31955500	C	2.71705700	0.08000500	-1.22390900
H	-0.96737300	4.62066300	-0.31022600	C	2.68811200	1.33853200	-1.81358500
H	-1.54177700	6.27186500	-0.06024400	C	3.64212200	-0.87034000	-1.68296200
H	-1.19944400	5.22313500	1.33500900	C	3.56234500	1.67301300	-2.85663100
C	-3.68537700	4.85055700	-1.10421300	C	4.58168600	-0.55127300	-2.66227900
H	-3.18551900	4.16680400	-1.79468400	C	4.54730700	0.74098100	-3.24995900
H	-4.74901600	4.59008700	-1.08282900	C	2.73026200	-0.50961600	1.64945300
H	-3.58891800	5.86412700	-1.50938800	C	4.11918400	-0.55861200	1.51989100
Rh	0.20248900	0.25442700	-1.31695900	C	2.17883200	-0.57247600	2.93348700
C	0.79241300	-3.07912300	-5.07466500	C	4.95751400	-0.66689100	2.63538800
C	0.84201200	-1.90076900	-4.34256000	C	2.97796800	-0.67961100	4.07226300
C	1.80940000	-1.72151200	-3.32939700	C	4.38555500	-0.73556500	3.92611300
C	2.70101700	-2.77571100	-3.05671500	C	-2.12387900	-2.14439000	-0.02892300
C	2.65535800	-3.96439400	-3.77807300	C	-1.94287500	-2.49331100	1.30828500
C	1.69831100	-4.09668200	-4.77818000	C	-2.77639700	-3.03584100	-0.88787000
H	0.05854500	-3.23384600	-5.85664800	C	-2.39941200	-3.71403200	1.80996500
H	0.12062600	-1.11806000	-4.55548100	C	-3.26631300	-4.26002400	-0.42163500
H	3.44438300	-2.65356000	-2.27453400	C	-3.06006500	-4.60943500	0.93700100
H	3.33364400	-4.78445300	-3.57130500	C	-3.37302900	0.33481700	-0.74449700
F	1.62906100	-5.24511100	-5.46849800	C	-4.47945200	-0.29795000	-0.17002600
C	2.00333900	-0.44803400	-2.63906900	C	-3.54471500	1.63035600	-1.25872800
H	2.83721100	-0.41938400	-1.94590200	C	-5.73455500	0.31642700	-0.10979400
C	1.53007600	0.78657100	-3.14512700	C	-4.80977700	2.22234700	-1.33626600
H	2.01581800	1.69785200	-2.82127900	C	-5.92218300	1.55860100	-0.75366100
H	1.19716800	0.81844500	-4.18365600	H	2.05204700	-2.91554600	1.61253500
C	-1.66279200	2.66479600	-3.50054800	H	1.58878000	-5.27090400	1.05323900
C	-2.53915900	3.21218700	-4.44582200	H	-2.23065500	0.91472600	-3.15818500
C	-2.46911600	4.57129300	-4.75685800	H	-0.96671500	1.02178100	-5.26025700
C	-1.52269300	5.39246400	-4.13927300	H	1.97941600	2.07785000	-1.47384000
C	-0.64874300	4.84533800	-3.20027700	H	3.63681000	-1.86330000	-1.25202400
C	-0.71981800	3.48810500	-2.87509800	H	4.57076600	-0.49016100	0.53902000
H	-3.27432900	2.58323700	-4.93982800	H	1.10373700	-0.51485600	3.06137700
H	-3.15637000	4.98649600	-5.48876100	H	-1.42385100	-1.81059900	1.97171800
H	-1.47058900	6.44878800	-4.38546900	H	-2.91341700	-2.76708000	-1.93098200
H	0.08512600	5.47434400	-2.70508600	H	-4.36504900	-1.27325300	0.28427700
H	-0.05310900	3.07433300	-2.12455700	H	-2.68928200	2.19169200	-1.61576000
Se	-1.84383400	0.75016300	-3.07650100	N	-7.19763500	2.19257100	-0.85052200
H	0.00491800	0.80999500	-2.98024800	C	-8.28291800	1.48191100	-1.51065000

## 28

B3LYP-D3 SCF energy: -4539.851772 a.u.

B3LYP-D3 enthalpy: -4537.942739 a.u.

B3LYP-D3 free energy: -4538.197600 a.u.

M06 SCF energy in solution: -4538.817284 a.u.

### Cartesian coordinates

ATOM	X	Y	Z				
C	0.36446100	-3.80852200	-1.75521900	N	-3.49077400	-5.85724300	1.49007400
C	0.58945800	-2.45234200	-1.44370100	N	5.16602200	-0.84466600	5.12192100
C	1.21686800	-2.13569800	-0.22219800	N	5.55867400	1.03964200	-4.22399900
C	1.56756500	-3.15527100	0.67418300	C	-2.85080700	-7.07382500	1.01614400
C	1.31514500	-4.48734500	0.35300800	H	-2.92266400	-7.84485000	1.79375200
				H	-3.28131900	-7.49408400	0.09080100
				H	-1.78992100	-6.87346600	0.83547300

C	-4.89542900	-5.96750100	1.85024800	H	0.97788700	-0.44102700	-5.63037600
H	-5.21235600	-5.05220400	2.36111000	O	1.85018700	-2.28181300	-3.84572000
H	-5.57359900	-6.13003700	0.99312200	O	-0.24061100	-4.05909400	-2.95157100
H	-5.02691400	-6.80659800	2.54408300	C	2.55614000	-2.29415400	-5.08069500
C	5.81138500	0.37167700	5.59293700	H	3.06470500	-1.33839100	-5.24985400
H	6.08447800	0.25011500	6.64817500	H	3.30081300	-3.08499300	-4.99197000
H	6.72621200	0.64608000	5.03763000	H	1.88754800	-2.51482400	-5.92214200
H	5.10900900	1.20787700	5.51786700	C	0.17842600	-5.21929000	-3.66809200
C	5.89869900	-2.08167400	5.34457500	H	-0.22652600	-6.13981500	-3.23268300
H	6.86456700	-2.15056000	4.81471500	H	-0.21815100	-5.10503900	-4.67871100
H	6.10198500	-2.18897100	6.41738700	H	1.27273200	-5.27479100	-3.70241400
H	5.28038700	-2.92899900	5.03206900	C	-4.00314800	-5.17753400	-1.39343300
C	5.17297300	0.95378600	-5.62297500	H	-4.44778000	-5.99238300	-0.82015300
H	4.52349400	1.77836800	-5.96784100	C	-5.15867600	-4.45849000	-2.11336700
H	6.07524700	0.95503000	-6.24599100	H	-4.79959700	-3.64173700	-2.74963100
H	4.64557300	0.01135800	-5.80394500	H	-5.69768400	-5.16363400	-2.75605300
C	6.49715100	2.11034400	-3.90824500	H	-5.87215100	-4.03781100	-1.39780600
H	6.72234600	2.08953800	-2.83819500	C	-3.02796100	-5.79795900	-2.40977500
H	7.43208700	1.93919700	-4.45683200	H	-2.55337900	-5.01933600	-3.01423100
H	6.14447600	3.12450400	-4.15966400	H	-2.23418700	-6.35509800	-1.89984800
C	-6.82538000	-0.37554800	0.70129800	H	-3.55515300	-6.48745500	-3.07912000
H	-7.70064500	0.27546200	0.72580300	C	-2.14217900	-4.05400800	3.27108400
C	-6.37625500	-0.57271900	2.16400000	H	-2.72335900	-4.95134300	3.49802600
H	-5.52725400	-1.26348000	2.23655900	C	-0.65470600	-4.39289000	3.48591300
H	-6.07493100	0.37842800	2.61691900	H	-0.01428400	-3.54062600	3.22994000
H	-7.19614400	-0.99074700	2.75901600	H	-0.46481400	-4.65660400	4.53273100
C	-7.24651500	-1.71580400	0.07274000	H	-0.35149000	-5.23660200	2.85652400
H	-8.06365000	-2.16995000	0.64452400	C	-2.59613600	-2.93098500	4.22092300
H	-7.58228300	-1.58505800	-0.96150600	H	-1.99645400	-2.02014000	4.09656000
H	-6.40886900	-2.42290400	0.06791400	H	-3.64666800	-2.66624700	4.05327400
C	-4.98653800	3.54206900	-2.07866200	H	-2.48640200	-3.24877800	5.26367400
H	-6.06498600	3.70553500	-2.15294400	C	5.64721700	-1.56866900	-3.06414000
C	-4.37999500	4.73422600	-1.31806300	H	5.76353100	-1.50842700	-4.15244700
H	-3.29438200	4.63531000	-1.21320700	C	5.28624700	-3.01879600	-2.69843600
H	-4.57808500	5.66876800	-1.85607100	H	5.35491800	-3.18913200	-1.61659600
H	-4.81170200	4.82807600	-0.31522400	H	4.27163700	-3.28828600	-3.00898900
C	-4.42472000	3.46264100	-3.51036900	H	5.99113500	-3.70776500	-3.17586600
H	-3.33474900	3.33652600	-3.51518400	C	7.01116600	-1.20720900	-2.44039000
H	-4.86163700	2.62255200	-4.06125600	H	6.94792700	-1.21539200	-1.34582200
H	-4.64955500	4.38419900	-4.05908100	H	7.77300600	-1.93732900	-2.73796500
C	2.30760500	-0.68955000	5.43873400	H	7.34454000	-0.21814700	-2.75929100
H	3.09630600	-0.86441700	6.17542500	C	3.37010100	3.02309800	-3.53994700
C	1.26979300	-1.81847300	5.56764600	H	4.14328700	3.14167800	-4.29951500
H	0.42210300	-1.67328000	4.88652100	C	2.01451600	3.06129100	-4.27346400
H	1.71223000	-2.79532100	5.34303000	H	1.18077200	2.96645400	-3.57055300
H	0.86717900	-1.85234500	6.58645300	H	1.89695800	4.01092300	-4.80848300
C	1.66834200	0.68144200	5.73549600	H	1.93549300	2.24290000	-4.99776600
H	1.22216000	0.69169700	6.73668500	C	3.50395300	4.20027000	-2.55582700
H	2.41043900	1.48555500	5.68168900	H	2.71908100	4.18331000	-1.79245600
H	0.87728400	0.91370500	5.00987400	H	4.47231300	4.17769800	-2.04411500
C	6.46240400	-0.71638400	2.39088700	H	3.42175100	5.15265900	-3.09193100
H	6.97061200	-0.65600100	3.35445900	Rh	-0.24761400	0.85768900	0.71068000
C	6.85922800	-2.05526700	1.73844900	C	0.70982800	3.78649700	0.23205800
H	6.36793500	-2.17744100	0.76557000	C	0.83387400	5.17898900	0.34655200
H	7.94221000	-2.10176700	1.57642200	C	0.23065100	6.02146900	-0.58532700
H	6.56979200	-2.90452100	2.36694900	C	-0.52001700	5.49726300	-1.64396200
C	6.95281700	0.47780300	1.54994600	C	-0.65394100	4.11549600	-1.76839400
H	6.54621000	0.45678600	0.53224500	C	-0.03608800	3.26852600	-0.84401100
H	6.66083400	1.42924600	2.00737800	H	1.39185700	5.59998400	1.17633000
H	8.04539700	0.45619000	1.46765000	H	0.33709800	7.09748500	-0.47786600
H	0.53454900	-5.85934000	-1.11193800	H	-0.98411700	6.15889000	-2.36904400

H	-1.19930800	3.69034200	-2.60605400	C	-3.78492000	-3.55110000	2.32296000
H	-0.06703000	2.19076000	-1.05223000	C	-3.35067500	0.76358800	-0.86544200
Se	1.53897700	2.57567700	1.51036200	C	-4.65323900	0.45844300	-0.46219800
C	-2.43864700	5.78671600	1.51579900	C	-3.13579300	1.94871700	-1.58543200
C	-2.42465400	4.40486600	1.62970600	C	-5.73273100	1.30221000	-0.75562600
C	-1.60469200	3.76340500	2.57748300	C	-4.19249600	2.78603400	-1.94831600
C	-0.79040200	4.55311100	3.40942100	C	-5.50777100	2.46387400	-1.52729100
C	-0.79657900	5.94232000	3.31060600	H	1.50641500	-3.13072900	2.24686000
C	-1.61814200	6.53510200	2.35870600	H	0.47165000	-5.37716600	2.31901600
H	-3.05309400	6.29266400	0.78013100	H	-2.21130900	0.43996300	-3.22186600
H	-3.04836400	3.81700000	0.96708200	H	-1.05844800	-0.26617000	-5.27304500
H	-0.14221500	4.07027900	4.13405900	H	2.26563100	0.75091600	-2.02971200
H	-0.17446700	6.56470400	3.94450100	H	3.08113500	-3.19792500	-0.59724300
F	-1.61263400	7.87373200	2.23285000	H	4.32455000	-0.62372000	0.45898000
C	-1.58605100	2.31338900	2.73908900	H	0.95204400	-0.75618300	3.10351600
H	-0.92260700	1.94255400	3.51714400	H	-1.73374600	-0.83907100	2.43106500
C	-2.37411200	1.41327600	2.08466700	H	-3.67897800	-2.60949400	-0.95205900
H	-3.12943900	1.72840200	1.37652100	H	-4.83904900	-0.44189500	0.10955600
H	-2.45543600	0.39142700	2.43850800	H	-2.12784800	2.22601500	-1.87950300
H	-0.29284800	-0.19358100	1.80759700	N	-6.55221800	3.36743900	-1.89918300

### 29-ts-R

B3LYP-D3 SCF energy: -4539.839082 a.u.

B3LYP-D3 enthalpy: -4537.932147 a.u.

B3LYP-D3 free energy: -4538.184385 a.u.

M06 SCF energy in solution: -4538.805113 a.u.

Imaginary frequency: -121.95 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z				
C	-0.72544600	-4.33456500	-0.68412200	N	4.91939000	0.70125200	4.85770400
C	-0.18957900	-3.03348400	-0.72178800	N	5.59406600	-1.70796800	-4.12367900
C	0.62972900	-2.61084600	0.34276500	C	-3.87938900	-5.93328000	2.98639100
C	0.86449900	-3.45522600	1.43568500	H	-3.88040700	-6.47604200	3.94052800
C	0.29312800	-4.72645500	1.46797100	H	-4.53238900	-6.48677700	2.28983000
C	-0.49250200	-5.17531200	0.40858000	H	-2.86169300	-5.95335800	2.58441300
C	-0.45138400	-2.20460300	-1.94223200	C	-5.60213400	-4.35820600	3.77604500
C	-1.30387800	-1.07800100	-1.97019900	H	-5.73044300	-3.30882800	4.06069600
C	0.16930800	-2.61225500	-3.14828000	H	-6.42100000	-4.62409500	3.08333200
C	-1.52565800	-0.39565900	-3.18017100	H	-5.71468300	-4.97223100	4.67795500
C	-0.02800700	-1.90016600	-4.33581100	C	5.37588100	2.07918300	4.75860000
C	-0.88488600	-0.80300200	-4.34471300	H	5.55590800	2.47140200	5.76757500
P	1.42194200	-0.96132500	0.20914400	H	6.30324600	2.21944200	4.17661200
P	-1.92594000	-0.30534000	-0.40623800	H	4.59223400	2.68545100	4.29324100
C	2.57194700	-1.19886600	-1.19301600	C	5.81335800	-0.21811400	5.54447000
C	2.81748400	-0.17688000	-2.10295600	H	6.75591400	-0.42505400	5.00640500
C	3.28983400	-2.39775900	-1.29704000	H	6.07353100	0.19624200	6.52615400
C	3.76942900	-0.32095000	-3.12233700	H	5.30054700	-1.17207100	5.70403600
C	4.27773900	-2.56609300	-2.26593900	C	5.20684900	-2.08918700	-5.47197900
C	4.53245900	-1.50733600	-3.17879500	H	4.76829900	-1.26894700	-6.06879500
C	2.54192300	-0.75723400	1.64752500	H	6.08746700	-2.46035700	-6.00968500
C	3.89854300	-0.50326600	1.44724800	H	4.47496300	-2.90307500	-5.42836000
C	2.00919200	-0.57395900	2.93009600	C	6.75118500	-0.82691900	-4.03428200
C	4.72641400	-0.05401500	2.48388000	H	6.96043800	-0.61127100	-2.98248000
C	2.79334700	-0.10454000	3.98488500	H	7.62502500	-1.33865000	-4.45714400
C	4.16710800	0.17156400	3.75918200	H	6.64282000	0.13640500	-4.56122000
C	-2.63109300	-1.61748300	0.64625300	C	-7.11608300	0.91991500	-0.23884600
C	-2.38750900	-1.59925600	2.02176900	H	-7.76701200	1.79088800	-0.34027000
C	-3.48393000	-2.59184400	0.11645400	C	-7.10227800	0.54652700	1.25575900
C	-2.94046900	-2.55730800	2.87144200	H	-6.54923100	-0.38157700	1.44238800
C	-4.09768700	-3.54115200	0.94354000	H	-6.64508300	1.33846000	1.85915300
				H	-8.12704600	0.39279800	1.61189300

C	-7.71650300	-0.22299700	-1.08034900	H	-1.55260800	-4.50066400	4.22838300
H	-8.71906800	-0.48309000	-0.72142800	C	-2.33475800	-1.17566000	4.94009100
H	-7.79285000	0.05247700	-2.13676600	H	-1.43371100	-0.70269100	4.53264300
H	-7.09063500	-1.11869400	-1.01339300	H	-3.18190900	-0.50725000	4.74787900
C	-3.91815700	4.00614000	-2.81753100	H	-2.19304400	-1.24584000	6.02391400
H	-4.87258500	4.52376800	-2.94012300	C	5.09810300	-3.85182900	-2.31396000
C	-2.92243500	4.97872100	-2.16392500	H	5.28978400	-4.07778900	-3.36857200
H	-1.92485500	4.53345000	-2.07939900	C	4.38812400	-5.06187600	-1.68324200
H	-2.82137000	5.88702200	-2.76954100	H	4.34725700	-4.98236700	-0.59016800
H	-3.25500000	5.27380200	-1.16206900	H	3.35944800	-5.17380500	-2.04153200
C	-3.43555000	3.57829800	-4.21642400	H	4.93855900	-5.97914100	-1.91824200
H	-2.48534100	3.03242500	-4.16002500	C	6.46796100	-3.64409000	-1.63650400
H	-4.16820300	2.92561500	-4.70357100	H	6.33664900	-3.39936600	-0.57550900
H	-3.27957300	4.45439400	-4.85662600	H	7.07059500	-4.55779300	-1.69975400
C	2.13605600	0.17211300	5.32953500	H	7.02710400	-2.83452000	-2.11122100
H	2.92276500	0.53698200	5.99487000	C	3.90079400	0.80762300	-4.13938100
C	1.53270700	-1.10052500	5.94824700	H	4.69350900	0.55256000	-4.84335100
H	0.73584600	-1.51804600	5.32368000	C	2.60229600	0.94507300	-4.95883900
H	2.29656100	-1.87567400	6.07613800	H	1.75398600	1.20693000	-4.31841100
H	1.10144800	-0.88221600	6.93216500	H	2.70857700	1.73011500	-5.71668600
C	1.07981300	1.28798400	5.19648200	H	2.35696600	0.00547600	-5.46664000
H	0.63917200	1.52487400	6.17170700	C	4.28643900	2.14276600	-3.47412500
H	1.53023400	2.20292300	4.79205000	H	3.50811200	2.49453200	-2.78836200
H	0.26368800	0.99125500	4.52516400	H	5.21743500	2.04347800	-2.90476400
C	6.18766300	0.22673300	2.15052200	H	4.43145600	2.91910400	-4.23405400
H	6.71067100	0.48641400	3.07215800	Rh	-0.10039700	0.89876600	0.37032000
C	6.88989100	-1.01381700	1.56688000	C	1.49466200	3.40430800	-0.80527400
H	6.46029800	-1.30441700	0.60140700	C	1.93897900	4.70435700	-1.08033300
H	7.95395100	-0.80689500	1.40530000	C	1.63488000	5.30639500	-2.30376000
H	6.80706800	-1.87154300	2.24355600	C	0.87143800	4.62965800	-3.25818300
C	6.30557800	1.42893900	1.19214100	C	0.41501300	3.33718000	-2.98893300
H	5.81569900	1.21843400	0.23361600	C	0.72941700	2.72982200	-1.77316000
H	5.83328000	2.32135700	1.61664900	H	2.51534400	5.24474800	-0.33603900
H	7.35833900	1.65850700	0.99034200	H	1.99071200	6.31249600	-2.50662400
H	-0.92225100	-6.17067000	0.43001800	H	0.63526100	5.10301700	-4.20641200
H	0.46724600	-2.19878800	-5.25098400	H	-0.16768600	2.79205200	-3.72529000
O	0.95898200	-3.71552800	-3.06444900	H	0.41356600	1.68985200	-1.63421600
O	-1.48047200	-4.70382600	-1.75929200	Se	1.86185100	2.54918000	0.90383400
C	1.68697500	-4.11397200	-4.21997300	C	-0.40112500	6.95037400	0.63718900
H	2.37835200	-3.32455300	-4.53744700	C	-0.58158800	5.57156900	0.67998200
H	2.25866900	-4.99332100	-3.92369300	C	-0.14699000	4.81723300	1.78711500
H	1.01615200	-4.37916600	-5.04687000	C	0.49093600	5.49129500	2.85153800
C	-1.38009100	-6.05786100	-2.19616600	C	0.67624100	6.86578300	2.82347000
H	-1.92493700	-6.74415400	-1.53795500	C	0.22449400	7.57693800	1.71021200
H	-1.83595500	-6.08601800	-3.18772400	H	-0.73197000	7.54097600	-0.21008400
H	-0.32917100	-6.36271500	-2.26191900	H	-1.06116800	5.07852000	-0.15405600
C	-5.10162100	-4.51676900	0.33675900	H	0.84549900	4.92053100	3.70599900
H	-5.56535800	-5.07394500	1.15203900	H	1.15655000	7.39791000	3.63733100
C	-6.23733600	-3.77371400	-0.38947700	F	0.40240100	8.90655900	1.67546000
H	-5.86720600	-3.21584200	-1.25733600	C	-0.33719600	3.37345700	1.87230200
H	-6.98854600	-4.48509400	-0.75083600	H	-0.09780100	2.95096000	2.84709200
H	-6.73483700	-3.06521200	0.28174000	C	-1.26250900	2.59196400	1.07291000
C	-4.42119900	-5.53263800	-0.59541500	H	-1.72230600	3.11986200	0.24099100
H	-3.92882000	-5.02825700	-1.43178700	H	-2.02340100	2.10922600	1.69268200
H	-3.65762500	-6.10319300	-0.05587700	H	-0.34946100	0.33855500	1.75835200
H	-5.15662500	-6.23888800	-0.99762300				
C	-2.57386400	-2.57427500	4.35040100				
H	-3.40803900	-3.02864100	4.89184200				
C	-1.34573800	-3.48048700	4.56605700				
H	-0.48594400	-3.10751300	3.99765500				
H	-1.06927000	-3.51611500	5.62621700				

### 30-R

B3LYP-D3 SCF energy: -4539.841792 a.u.

B3LYP-D3 enthalpy: -4537.933929 a.u.

B3LYP-D3 free energy: -4538.188665 a.u.

M06 SCF energy in solution: -4538.817631 a.u.

Cartesian coordinates							
ATOM	X	Y	Z				
C	-1.14174600	-4.40611900	-0.08767400	H	-6.84271500	4.76538400	-1.00676200
C	-0.45746400	-3.19867800	-0.32259000	N	-4.82872400	-3.80693400	3.53289700
C	0.44255500	-2.73083600	0.65419200	N	4.88918900	0.95367800	4.70126900
C	0.62577600	-3.44355400	1.84670000	N	5.24813000	-2.53767300	-4.13201400
C	-0.08552400	-4.62145800	2.07028700	C	-4.62853700	-5.24376300	3.42991900
C	-0.96654700	-5.10930800	1.10794500	H	-4.71883000	-5.69164300	4.42795700
C	-0.63937200	-2.54087900	-1.65666700	H	-5.34137400	-5.76436300	2.76743000
C	-1.35935000	-1.34471400	-1.87172800	H	-3.61712000	-5.43887900	3.05983900
C	-0.07426700	-3.20008100	-2.77487500	C	-6.12386700	-3.38307500	4.04193300
C	-1.51065200	-0.84242200	-3.17674400	H	-6.10892000	-2.30406500	4.22670600
C	-0.20166700	-2.67131100	-4.06327600	H	-6.96793400	-3.59888700	3.36228300
C	-0.93095800	-1.50108300	-4.25511700	H	-6.32372200	-3.88921600	4.99428600
P	1.34951300	-1.17616500	0.30070200	C	5.26851300	2.33774500	4.46282600
P	-1.91367600	-0.29537400	-0.45020500	H	5.48531600	2.82273100	5.42287600
C	2.44399600	-1.62252900	-1.08941200	H	6.15333000	2.46899300	3.81524600
C	2.64915700	-0.71473500	-2.12319800	H	4.43019700	2.86565700	3.99663700
C	3.13747700	-2.83893300	-1.09358000	C	5.84969700	0.14473100	5.43560800
C	3.53082400	-0.99330100	-3.17601000	H	6.79282100	-0.05218100	4.89517700
C	4.06227000	-3.13593200	-2.09428400	H	6.10415200	0.65130500	6.37467500
C	4.26692800	-2.19765100	-3.14269900	H	5.39596700	-0.82015100	5.68323300
C	2.49189700	-0.86264200	1.69653400	C	4.74867800	-3.11135700	-5.37055400
C	3.84496700	-0.62936800	1.45497600	H	4.26515700	-2.38128200	-6.04529000
C	1.96787900	-0.53589500	2.95408800	H	5.57914000	-3.57366200	-5.91743000
C	4.67736900	-0.05447600	2.42438900	H	4.01808100	-3.89586400	-5.14492900
C	2.76205200	0.04047900	3.94677200	C	6.41363700	-1.67557900	-4.27217700
C	4.13066700	0.29950700	3.67641800	H	6.70008600	-1.29202500	-3.28871600
C	-2.79671300	-1.37311100	0.72412400	H	7.25177800	-2.26631300	-4.66356900
C	-2.55585600	-1.26088200	2.09566200	H	6.27342000	-0.81242800	-4.94460100
C	-3.77032700	-2.27049200	0.27262700	C	-6.88087300	1.65983600	-0.73907200
C	-3.23706300	-2.05126900	3.02098600	H	-7.38725600	2.59255000	-0.99573300
C	-4.51044700	-3.04637500	1.17308500	C	-6.98096300	1.50749900	0.79074500
C	-4.20657400	-2.96971600	2.55251000	H	-6.58027000	0.54679700	1.13490400
C	-3.16455200	0.87023300	-1.11567100	H	-6.43416500	2.30476700	1.30608200
C	-4.51298500	0.81073700	-0.75836900	H	-8.03020300	1.55422200	1.10310400
C	-2.74195200	1.90805800	-1.95806900	C	-7.61602000	0.50795000	-1.45127800
C	-5.43607400	1.76038100	-1.21803500	H	-8.66102400	0.45487700	-1.12467300
C	-3.63611200	2.84121800	-2.48059200	H	-7.60395800	0.63508900	-2.53839100
C	-5.00252200	2.77018900	-2.10733500	H	-7.14152800	-0.45186100	-1.22120500
H	1.33037300	-3.09030900	2.59096300	C	-3.12261600	3.90703800	-3.43919900
H	0.05328100	-5.16791500	2.99848000	H	-3.99377100	4.48211800	-3.76340700
H	-2.09503400	0.04955600	-3.35848200	C	-2.14044000	4.86785000	-2.74494500
H	-1.05021700	-1.10167900	-5.25816400	H	-1.21975800	4.34898500	-2.45387400
H	2.10965000	0.22631200	-2.11937300	H	-1.85568100	5.68274800	-3.42083800
H	2.96060300	-3.54654200	-0.29175600	H	-2.58047700	5.30931700	-1.84378800
H	4.26081700	-0.86201300	0.48151100	C	-2.47955400	3.27566700	-4.68804500
H	0.91043700	-0.69164700	3.15023600	H	-1.59293600	2.68137900	-4.42958600
H	-1.80579700	-0.56190600	2.44401300	H	-3.18437200	2.61553000	-5.20547100
H	-3.96191700	-2.36198500	-0.79258200	H	-2.16233800	4.05396000	-5.39175900
H	-4.85601800	0.02862800	-0.09201800	C	2.11765400	0.45147800	5.26300600
H	-1.69201300	1.99090700	-2.22333200	H	2.92018200	0.82432300	5.90462900
N	-5.87869600	3.76101500	-2.65020700	C	1.43973200	-0.73310900	5.97300700
C	-6.98332100	3.34515800	-3.49989400	H	0.61127700	-1.14387100	5.38503700
H	-6.67907600	2.47595600	-4.09021100	H	2.15399200	-1.54371300	6.15525300
H	-7.91003500	3.08617400	-2.96077600	H	1.03087700	-0.41618700	6.93937900
H	-7.22432900	4.15880700	-4.19616700	C	1.12439200	1.60896500	5.03431900
C	-6.12094500	4.93500500	-1.82615900	H	0.68893600	1.94317000	5.98302300
H	-5.17894500	5.27107400	-1.38078300	H	1.62468500	2.46544700	4.56581600
H	-6.50960800	5.74640100	-2.45342000	H	0.29956400	1.30096800	4.37868700
				C	6.12733700	0.21729300	2.03891400
				H	6.64919500	0.62018700	2.90794000
				C	6.86040300	-1.07347300	1.62716800

H	6.42262400	-1.51662800	0.72491700
H	7.91412600	-0.86111500	1.41340600
H	6.81756200	-1.82370600	2.42437100
C	6.20295900	1.27865800	0.92246500
H	5.72232900	0.92292800	0.00299100
H	5.70039300	2.20444600	1.22412200
H	7.24697200	1.51471500	0.68609900
H	-1.50944100	-6.03180200	1.28180300
H	0.24991400	-3.16640600	-4.91380300
O	0.59049800	-4.35526000	-2.50425100
O	-1.97308100	-4.82935500	-1.08394200
C	1.24268800	-5.02781600	-3.57408300
H	2.02859700	-4.39933400	-4.01057100
H	1.69574100	-5.91666500	-3.13459400
H	0.53206500	-5.33181200	-4.35308800
C	-2.04184600	-6.23300700	-1.32580700
H	-2.62133000	-6.75711500	-0.55723200
H	-2.55045900	-6.34627200	-2.28505400
H	-1.03454600	-6.66134200	-1.38587600
C	-5.63991700	-3.92192400	0.63857300
H	-6.18405600	-4.32961900	1.49194100
C	-6.65205100	-3.09369400	-0.17442500
H	-6.20306900	-2.68949600	-1.08899400
H	-7.50229000	-3.71721900	-0.47309700
H	-7.03620700	-2.25306900	0.41398000
C	-5.10819000	-5.10675100	-0.18479500
H	-4.52778800	-4.75946600	-1.04488900
H	-4.45261300	-5.73811000	0.42356300
H	-5.93694000	-5.72447200	-0.54951300
C	-2.88838500	-1.96880100	4.50242900
H	-3.77566200	-2.26949000	5.06598200
C	-1.77579600	-2.98278500	4.83230800
H	-0.86851800	-2.76051900	4.25890200
H	-1.52634900	-2.95252500	5.89942200
H	-2.08964100	-4.00031900	4.57918700
C	-2.49308700	-0.55630700	4.96122200
H	-1.53599000	-0.23553400	4.53351600
H	-3.25104300	0.18518600	4.68387300
H	-2.37627700	-0.53591600	6.05016400
C	4.89059900	-4.41522200	-2.02490400
H	5.02985500	-4.77553900	-3.04959600
C	4.23320700	-5.53776900	-1.20570200
H	4.24261400	-5.31531600	-0.13190500
H	3.19178700	-5.70730400	-1.49772100
H	4.78713700	-6.47220600	-1.34522200
C	6.29091900	-4.10657600	-1.45526600
H	6.21018000	-3.71571400	-0.43327000
H	6.90220600	-5.01603700	-1.42189200
H	6.81360700	-3.36734400	-2.06696100
C	3.65408900	0.03017600	-4.29954100
H	4.27547800	-0.39572600	-5.08882200
C	2.28444300	0.33728100	-4.93535600
H	1.59947300	0.80558500	-4.22038600
H	2.40456500	1.02399500	-5.78136900
H	1.80422700	-0.57829800	-5.29618700
C	4.34281200	1.31619500	-3.80166900
H	3.76212400	1.79367700	-3.00513500
H	5.34160200	1.09952800	-3.40753900
H	4.44701600	2.04066800	-4.61778400
Rh	-0.02522700	0.82180200	0.25961900
C	2.01822500	3.39180700	-0.75080500

C	2.79054700	4.55392400	-0.84404300
C	2.88034100	5.23330200	-2.06140200
C	2.19686900	4.76244300	-3.18418100
C	1.42425700	3.60227300	-3.09329300
C	1.33834800	2.91769400	-1.88034600
H	3.31011400	4.93289900	0.03040600
H	3.48034400	6.13617300	-2.12738700
H	2.26660800	5.29521300	-4.12784800
H	0.89197800	3.22771500	-3.96238600
H	0.73334700	2.01373500	-1.82707500
Se	1.86543500	2.47584300	0.97291400
C	0.05155400	7.02579000	0.42207200
C	-0.09980800	5.64111200	0.40554600
C	0.11557600	4.87566900	1.56370600
C	0.49997700	5.53852400	2.74321800
C	0.65548400	6.92079400	2.77723400
C	0.42711800	7.64497800	1.60944600
H	-0.11340300	7.62640400	-0.46595800
H	-0.38252400	5.15649500	-0.52016200
H	0.67811000	4.96046300	3.64705500
H	0.94276300	7.44366200	3.68313300
F	0.57531200	8.98137400	1.63148000
C	-0.01100100	3.39409400	1.57046500
H	-0.04198400	3.00747500	2.59154200
C	-0.98071800	2.66876000	0.67500800
H	-1.14593000	3.18583300	-0.27135200
H	-1.94777400	2.53192800	1.16932100
H	-0.43044900	0.50586800	1.68648300

### 31

B3LYP-D3 SCF energy: -4539.855762 a.u.

B3LYP-D3 enthalpy: -4537.946462 a.u.

B3LYP-D3 free energy: -4538.199028 a.u.

M06 SCF energy in solution: -4538.825775 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z	
C	-0.33174300	0.26276700	4.14176600	
C	0.06560600	-0.21255700	2.87322200	
C	0.94245100	0.57645500	2.10045200	
C	1.39725000	1.80734900	2.59981200	
C	0.99363400	2.25181000	3.85578000	
C	0.12969900	1.48598900	4.63190800	
C	-0.44672000	-1.55324800	2.45991100	
C	-1.36724600	-1.74033700	1.40821200	
C	-0.04466900	-2.67800200	3.22077200	
C	-1.87650700	-3.02397800	1.14655100	
C	-0.53223600	-3.95406800	2.92727100	
C	-1.45821400	-4.11362200	1.90080100	
P	1.52489400	0.00276900	0.44154800	
P	-1.84355400	-0.32673300	0.30575700	
C	2.16542600	-1.67375900	0.74585400	
C	1.87658300	-2.71816800	-0.12656300	
C	2.96149300	-1.91682700	1.87273100	
C	2.34324300	-4.01598100	0.11119400	
C	3.50096500	-3.17981900	2.11312300	
C	3.17606100	-4.24402400	1.22900000	
C	2.96054900	1.08356900	0.08918400	
C	4.26717300	0.66051900	0.32534800	
C	2.73853100	2.39271800	-0.36131900	
C	5.35650800	1.52177100	0.14173600	

C	3.79687800	3.28113600	-0.55333900	H	4.15398500	-6.75360400	-0.18764500
C	5.12277500	2.83490400	-0.31794000	C	-7.06263900	-0.15654400	-0.85277600
C	-2.41942700	1.01095900	1.40929200	H	-7.75805500	-0.45366000	-1.63847500
C	-2.04535200	2.33710800	1.17043000	C	-7.01875700	1.38264500	-0.84759100
C	-3.28181900	0.72513000	2.47306700	H	-6.40371900	1.77168000	-0.02747700
C	-2.48335500	3.37432900	1.99631800	H	-6.61212800	1.77109000	-1.78799200
C	-3.78183400	1.74266800	3.29415300	H	-8.02873800	1.78739800	-0.71904700
C	-3.34061700	3.06923200	3.08149600	C	-7.61519800	-0.70015000	0.47910900
C	-3.33543000	-0.92455900	-0.58251800	H	-8.60543100	-0.27831900	0.68648100
C	-4.59889300	-0.36860400	-0.38953700	H	-7.70620700	-1.79131000	0.45509000
C	-3.17995000	-1.92400900	-1.55604400	H	-6.95479800	-0.43732200	1.31148400
C	-5.70326800	-0.77878900	-1.15372400	C	-4.04099300	-3.43914600	-3.38937500
C	-4.25306500	-2.37079600	-2.32492000	H	-5.00982000	-3.91865300	-3.55419000
C	-5.52706900	-1.77205100	-2.13991100	C	-3.62474400	-2.78167800	-4.72026300
H	2.08238800	2.41339900	2.02189700	H	-2.67665600	-2.24215500	-4.61302200
H	1.35494400	3.20436700	4.23073800	H	-3.49064500	-3.53892300	-5.50182200
H	-2.61349700	-3.17937600	0.37171600	H	-4.38459500	-2.07313800	-5.06306500
H	-1.86118000	-5.10001800	1.69018200	C	-3.03419000	-4.52263300	-2.97024200
H	1.27749800	-2.52445500	-1.00746400	H	-2.01284300	-4.13349100	-2.88715900
H	3.15800500	-1.10615900	2.56352500	H	-3.29976100	-4.96770800	-2.00442700
H	4.45516700	-0.35288800	0.65648100	H	-3.01344700	-5.32326800	-3.71790800
H	1.72566200	2.71789300	-0.57032100	C	3.53074000	4.69129600	-1.06517200
H	-1.37557300	2.55726700	0.34712300	H	4.31877700	5.33704500	-0.66657200
H	-3.57483500	-0.30358400	2.66145000	C	2.17482700	5.25766300	-0.61527400
H	-4.73884500	0.39850400	0.36265100	H	1.33655000	4.73309900	-1.08544300
H	-2.19420500	-2.34637200	-1.73103500	H	2.04814600	5.19582100	0.47232300
N	-6.58215400	-2.22004000	-2.99981200	H	2.09465400	6.30990700	-0.90960100
C	-7.59981500	-3.08093600	-2.41542300	C	3.64933600	4.71134800	-2.60220700
H	-7.12387400	-3.80820400	-1.74999600	H	3.37124300	5.69348600	-3.00260500
H	-8.37317000	-2.54418600	-1.83863300	H	4.67231900	4.48548500	-2.91632300
H	-8.10623700	-3.63407300	-3.21602300	H	2.98272800	3.96356900	-3.04394200
C	-7.05790600	-1.29673300	-4.02012800	C	6.74607300	0.99086400	0.47866000
H	-6.21391800	-0.72784000	-4.42051100	H	7.47247200	1.78450300	0.30135800
H	-7.50492300	-1.86822300	-4.84323100	C	6.84636300	0.61720300	1.97048300
H	-7.81517100	-0.57459500	-3.66710200	H	6.15893000	-0.19739500	2.22645500
N	-3.70769100	4.15528600	3.93888700	H	7.86151300	0.28370000	2.21416600
N	6.17551300	3.77208900	-0.57750500	H	6.60374300	1.47329700	2.60993300
N	3.71737200	-5.53410000	1.54602000	C	7.13177400	-0.19858600	-0.42035200
C	-3.28983000	4.09872000	5.33067900	H	6.46026700	-1.05155300	-0.26544000
H	-3.19526800	5.12076200	5.71960200	H	7.08410300	0.07500300	-1.47984400
H	-3.97739500	3.55218000	5.99881600	H	8.15155300	-0.53200800	-0.19653800
H	-2.30723000	3.62019200	5.39073000	H	-0.18573000	1.83672300	5.60820500
C	-4.99084600	4.79405300	3.68956800	H	-0.20873700	-4.81657700	3.49619400
H	-5.13233300	4.92243600	2.61152800	O	0.82699100	-2.43378100	4.23741500
H	-5.85790600	4.23179600	4.08044600	O	-1.19526600	-0.52831300	4.84050300
H	-4.99916900	5.78723400	4.15492600	C	1.12535400	-3.49206400	5.14096600
C	7.09495600	3.47523100	-1.66702000	H	1.70900100	-4.28167200	4.65190100
H	7.52831200	4.41359000	-2.03576400	H	1.72643000	-3.04696300	5.93449100
H	7.93086400	2.80675500	-1.39735300	H	0.21100200	-3.91899200	5.57129800
H	6.54400000	3.00917500	-2.48891600	C	-1.02538200	-0.59498400	6.25414400
C	6.76559100	4.42381700	0.58166400	H	-1.37420600	0.31450500	6.75663600
H	7.46720300	3.78840400	1.15180700	H	-1.63712800	-1.43446800	6.58966800
H	7.31326100	5.31599600	0.25460800	H	0.02611000	-0.77507500	6.50616800
H	5.97107700	4.74456400	1.26355800	C	-4.80665600	1.38955900	4.36828400
C	2.81292200	-6.45307800	2.21756300	H	-5.18110900	2.32035900	4.79707600
H	2.05449400	-6.90690200	1.55339200	C	-6.02190300	0.66235800	3.76464800
H	3.39145400	-7.26668300	2.67152600	H	-5.74709000	-0.31922600	3.36199900
H	2.28208600	-5.92561200	3.01745800	H	-6.78824400	0.50052400	4.53100800
C	4.63810900	-6.15621500	0.60274100	H	-6.46927700	1.24817800	2.95417100
H	5.23891700	-5.38229200	0.11736600	C	-4.18461900	0.56806700	5.50981200
H	5.31785400	-6.82174100	1.15040400	H	-3.75368400	-0.36539000	5.13477700

H	-3.38276300	1.12954500	5.99895900
H	-4.94156700	0.32473700	6.26427200
C	-2.00147700	4.80372400	1.77253100
H	-2.77407900	5.47240400	2.16061800
C	-0.72083600	5.06884800	2.58734300
H	0.09496000	4.42579700	2.23847200
H	-0.40556900	6.11335500	2.48009000
H	-0.88364000	4.86490600	3.65002900
C	-1.77016800	5.14971600	0.29520500
H	-0.91009600	4.61346000	-0.11945700
H	-2.64867000	4.91589100	-0.31814500
H	-1.55777100	6.21981700	0.19245000
C	4.45741400	-3.39786300	3.28350100
H	4.18957100	-4.35090200	3.75454300
C	4.39431500	-2.29392600	4.35248700
H	4.84733800	-1.36163400	3.99307200
H	3.36905600	-2.06613300	4.65614500
H	4.95998800	-2.60370400	5.23768700
C	5.90925500	-3.53093100	2.77661400
H	6.21630800	-2.62002800	2.24844800
H	6.59503400	-3.67809100	3.61914800
H	6.02005000	-4.37708100	2.09670000
C	1.95120400	-5.11020900	-0.87742300
H	2.27441800	-6.07104800	-0.47486800
C	0.42590800	-5.20663100	-1.06386700
H	0.00659800	-4.28935300	-1.49150200
H	0.17927900	-6.02875100	-1.74528100
H	-0.07852500	-5.38141900	-0.10931100
C	2.66225700	-4.90168200	-2.22928800
H	2.36445400	-3.95395800	-2.69188400
H	3.75015200	-4.88574200	-2.10520100
H	2.40870400	-5.70937300	-2.92571700
Rh	-0.07522000	0.13028900	-1.23164700
C	-0.57054500	4.97462600	-3.00999400
C	-1.02422600	3.66644100	-2.89298200
C	-0.49978800	2.64601800	-3.70737200
C	0.48659300	2.97684200	-4.65437900
C	0.94526100	4.28318400	-4.78896600
C	0.41752900	5.25907300	-3.95105600
H	-0.95236400	5.77046700	-2.38097500
H	-1.78559000	3.43689800	-2.15496500
H	0.90282700	2.19375400	-5.28076300
H	1.71524500	4.55068100	-5.50385700
F	0.89510000	6.51334000	-4.02890300
C	-0.94181700	1.25759600	-3.62786200
H	-0.47579500	0.58831900	-4.34388400
C	-1.91862700	0.72514200	-2.83857200
H	-2.27253000	-0.27603400	-3.04696500
H	-2.55703100	1.33363300	-2.20565800
C	1.27146200	-1.11479100	-4.21678900
C	1.62534800	-0.81472000	-5.54261200
C	1.15397800	-1.59897200	-6.59681000
C	0.31921100	-2.69123200	-6.34660500
C	-0.03880400	-2.99624200	-5.03225900
C	0.43233900	-2.21462600	-3.97495700
H	2.27745400	0.03044900	-5.74535700
H	1.44041600	-1.35529700	-7.61634800
H	-0.04322500	-3.30274600	-7.16761500
H	-0.67660900	-3.85028100	-4.82588200
H	0.16079200	-2.47631200	-2.95599600
Se	1.99812300	-0.02521000	-2.76481000

H -0.17368800 1.59752100 -0.84892800

### 32-ts-S

B3LYP-D3 SCF energy: -4539.841232 a.u.

B3LYP-D3 enthalpy: -4537.934079 a.u.

B3LYP-D3 free energy: -4538.184888 a.u.

M06 SCF energy in solution: -4538.810831 a.u.

Imaginary frequency: -126.44 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z
C	0.66011600	-1.29014200	-3.99150500
C	0.11169100	-1.23804000	-2.69422600
C	-0.76548600	-0.18255600	-2.37215700
C	-1.06358500	0.79719800	-3.33056300
C	-0.49881200	0.73137300	-4.60244700
C	0.36221000	-0.30892000	-4.94032200
C	0.43954100	-2.36436500	-1.76504700
C	1.27619900	-2.24083400	-0.63464100
C	-0.07312700	-3.64364000	-2.09094100
C	1.58187500	-3.37500000	0.13809600
C	0.20671100	-4.75575800	-1.29192100
C	1.04422000	-4.61400600	-0.18913600
P	-1.48372100	-0.08038600	-0.67755300
P	1.86456200	-0.57900200	-0.06547500
C	-2.39418000	-1.64689500	-0.48196300
C	-2.33836700	-2.33336000	0.72801900
C	-3.14997900	-2.17016400	-1.53806100
C	-2.99521500	-3.55926700	0.89825600
C	-3.86246800	-3.36003300	-1.39476600
C	-3.77276100	-4.06779000	-0.16561500
C	-2.75232100	1.23568300	-0.77525800
C	-4.11497500	0.95270300	-0.82450600
C	-2.34034700	2.57611500	-0.74804500
C	-5.07460500	1.97491500	-0.85202400
C	-3.26175000	3.62191400	-0.76143500
C	-4.64790700	3.31737600	-0.79164800
C	2.61065900	0.25261500	-1.50642200
C	2.33639000	1.59734400	-1.76616400
C	3.51922400	-0.42872800	-2.32397700
C	2.92738900	2.26653400	-2.83894900
C	4.16265400	0.21706400	-3.38588300
C	3.83079800	1.56299900	-3.67039600
C	3.24154700	-0.90737300	1.10237100
C	4.56492800	-0.55347300	0.83647800
C	2.93693900	-1.46360800	2.35229500
C	5.57799100	-0.74019300	1.78865400
C	3.91746600	-1.70073300	3.31350100
C	5.25824700	-1.33230900	3.03162000
H	-1.74591400	1.60372000	-3.09123900
H	-0.73446800	1.49596100	-5.33664300
H	2.25347200	-3.30340600	0.98229500
H	1.28513800	-5.48234100	0.41723900
H	-1.76718900	-1.91956700	1.55401000
H	-3.17412800	-1.63414600	-2.47915700
H	-4.44966600	-0.07768900	-0.84134500
H	-1.28099500	2.80456200	-0.69057500
H	1.62530800	2.12348600	-1.14012600
H	3.73397800	-1.47512500	-2.12778600
H	4.81909700	-0.10949300	-0.11853700
H	1.90839400	-1.72454400	2.58468000



N	6.22906500	-1.57420800	4.05457600	H	-1.24036900	6.39580400	-1.40737700
C	7.29668900	-2.52802600	3.79554700	C	-2.66746100	5.46698300	0.82289000
H	6.90955500	-3.34903600	3.18493000	H	-2.31750100	6.50159500	0.91967900
H	8.17809000	-2.10582900	3.28377800	H	-3.63446700	5.38232200	1.32812700
H	7.63986300	-2.94853000	4.74948600	H	-1.95391200	4.81874200	1.34387100
C	6.58724900	-0.44503900	4.89914100	C	-6.54146900	1.57025200	-0.95437900
H	5.68711900	0.12227000	5.15457700	H	-7.14795800	2.47507800	-1.01044900
H	7.03238000	-0.81477700	5.83094400	C	-6.80849800	0.77192300	-2.24532400
H	7.30777000	0.25267300	4.43517700	H	-6.25274200	-0.17307200	-2.25631600
N	4.35841300	2.26951800	-4.79776400	H	-7.87426900	0.53156800	-2.33209700
N	-5.55522000	4.42564700	-0.74059200	H	-6.51284600	1.34395800	-3.13181100
N	-4.49148400	-5.30717600	-0.08134700	C	-6.99577300	0.78380600	0.28976500
C	4.01950600	1.78255000	-6.12542400	H	-6.44239700	-0.15765700	0.38945300
H	4.06499500	2.61685800	-6.83705800	H	-6.83488900	1.36497400	1.20433700
H	4.67801000	0.98374700	-6.50814800	H	-8.06202600	0.53936000	0.22115800
H	2.99377600	1.40059400	-6.11497100	H	0.79881800	-0.35890100	-5.93168200
C	5.67946800	2.86067600	-4.65281800	H	-0.20978900	-5.72720100	-1.52689500
H	5.75807800	3.34198900	-3.67246700	O	-0.83708000	-3.71027700	-3.21568900
H	6.51093600	2.13875900	-4.74387600	O	1.49755900	-2.33673100	-4.25133400
H	5.81928400	3.63010400	-5.42183600	C	-1.26689500	-4.98903400	-3.66674200
C	-6.40145100	4.55499300	0.43635900	H	-1.99195300	-5.43197700	-2.97299700
H	-6.69780600	5.60538600	0.55112200	H	-1.75294600	-4.81900900	-4.62789300
H	-7.32461300	3.95012000	0.41236700	H	-0.41874200	-5.67151600	-3.80317400
H	-5.83210200	4.26422700	1.32418500	C	1.42464400	-2.92393300	-5.54817000
C	-6.15986300	4.83140800	-2.00002400	H	1.89437300	-2.29636300	-6.31431400
H	-6.97692100	4.17224400	-2.34480600	H	1.97514300	-3.86438800	-5.48243800
H	-6.56876100	5.84377700	-1.89560000	H	0.38159800	-3.12102300	-5.82186000
H	-5.39315700	4.85392400	-2.78150000	C	5.22017500	-0.54412500	-4.17978900
C	-3.70703000	-6.51458300	-0.28029200	H	5.70007200	0.15739400	-4.86386500
H	-3.07820000	-6.79355200	0.58518700	C	6.32698100	-1.08874300	-3.25820600
H	-4.37949700	-7.35503100	-0.49079800	H	5.94275600	-1.85022100	-2.56983000
H	-3.04629600	-6.38495500	-1.14414500	H	7.12273900	-1.55301900	-3.85153000
C	-5.56606500	-5.42670300	0.89522800	H	6.77229000	-0.28582400	-2.66034200
H	-6.06876100	-4.46151700	1.00204300	C	4.60178400	-1.66931900	-5.02619600
H	-6.30236500	-6.15551200	0.53214200	H	4.07341100	-2.39201700	-4.39686100
H	-5.24327100	-5.75271200	1.89814200	H	3.87916000	-1.26314200	-5.74093400
C	6.99595500	-0.30373000	1.43419800	H	5.37952800	-2.19889000	-5.58838300
H	7.59096900	-0.30859200	2.34933900	C	2.55343400	3.71436100	-3.13104500
C	7.04666300	1.13215200	0.87873700	H	3.34005200	4.13097100	-3.76466600
H	6.55102100	1.21308600	-0.09581300	C	1.23975200	3.77094900	-3.93367200
H	6.56458200	1.83975500	1.56231400	H	0.41459500	3.33521100	-3.35865800
H	8.08814400	1.44383900	0.74189300	H	0.97935200	4.80764800	-4.17748400
C	7.64033800	-1.29598600	0.44683400	H	1.32954500	3.20752500	-4.86812200
H	8.66930600	-0.99781700	0.21481500	C	2.45082900	4.57578300	-1.86234400
H	7.66277800	-2.31089700	0.85659300	H	1.59526800	4.28217600	-1.24470300
H	7.07769000	-1.32624100	-0.49211200	H	3.35595600	4.50241700	-1.24839100
C	3.51923000	-2.31875100	4.64678500	H	2.30348600	5.62733300	-2.13350900
H	4.44921900	-2.57444300	5.16173800	C	-4.75133400	-3.86763300	-2.52777600
C	2.75980500	-1.30006100	5.51905600	H	-4.60798200	-4.95220500	-2.59811100
H	1.80948000	-1.00725400	5.05724200	C	-4.42657600	-3.24619800	-3.89650100
H	2.53047900	-1.72778200	6.50203800	H	-4.74507200	-2.19747500	-3.94566000
H	3.35003700	-0.39049800	5.67489400	H	-3.35731500	-3.27646700	-4.12454200
C	2.70011900	-3.61000400	4.46868000	H	-4.96607900	-3.78266200	-4.68436100
H	1.73331000	-3.42378400	3.98290100	C	-6.23929600	-3.62415500	-2.19919600
H	3.24135000	-4.34302700	3.86003100	H	-6.43354700	-2.55169300	-2.07507700
H	2.49340500	-4.06570200	5.44380300	H	-6.87495700	-3.98852800	-3.01469200
C	-2.78349500	5.06453100	-0.66081400	H	-6.53595200	-4.13633300	-1.28236300
H	-3.55511200	5.69492400	-1.11133000	C	-2.85445700	-4.27241100	2.23884400
C	-1.45946200	5.32223200	-1.39656200	H	-3.28419400	-5.27069100	2.14517400
H	-0.61588800	4.83144100	-0.89949200	C	-1.37942100	-4.46914000	2.63688900
H	-1.49375700	4.96931200	-2.43353500	H	-0.86833800	-3.51430900	2.79577100

H	-1.31405400	-5.03664200	3.57246500	C	-3.23684000	-2.28200100	-1.31794200
H	-0.83320200	-5.01323000	1.86027500	C	-3.13235100	-3.39661000	1.25780600
C	-3.64013900	-3.52259400	3.33260000	C	-3.98273800	-3.42926200	-1.04950500
H	-3.26509700	-2.50228600	3.46036300	C	-3.92033800	-3.99771700	0.25157600
H	-4.70376700	-3.46201000	3.07837700	C	-2.73899200	1.17751600	-0.90428200
H	-3.54686800	-4.03488500	4.29693800	C	-4.11163300	0.94010200	-0.89301900
Rh	0.09699200	0.45022400	1.04413300	C	-2.28276600	2.49776600	-1.03684200
C	1.02152800	5.59182700	1.39258400	C	-5.03721000	1.98731300	-1.01203500
C	1.06566100	4.23633500	1.70117900	C	-3.16879900	3.56837100	-1.14820900
C	0.47596700	3.74214300	2.88039400	C	-4.56456900	3.31221100	-1.11164900
C	-0.15893600	4.65518000	3.74587200	C	2.61343400	0.00011700	-1.52568800
C	-0.21021100	6.01195600	3.45268400	C	2.35701900	1.29949400	-1.96836000
C	0.37532700	6.45763900	2.27013000	C	3.51712200	-0.79748500	-2.23694300
H	1.46532900	5.98485300	0.48513200	C	2.96369900	1.80944400	-3.11745200
H	1.56399600	3.55865800	1.01754400	C	4.17375300	-0.31082500	-3.37256800
H	-0.63068900	4.28634900	4.65279600	C	3.86193000	0.98833000	-3.83939400
H	-0.70226700	6.72270000	4.10735400	C	3.21316000	-0.84454300	1.21243400
F	0.29902600	7.76123700	1.95735200	C	4.54352100	-0.54093800	0.92103700
C	0.50447100	2.31966300	3.23564600	C	2.88898800	-1.24368700	2.51628200
H	0.22263100	2.10887300	4.26441500	C	5.54441400	-0.62438100	1.90041100
C	1.35743400	1.34639300	2.58012000	C	3.85643900	-1.37739400	3.50981900
H	1.68149000	0.55159900	3.24809800	C	5.20452800	-1.06049400	3.20132500
H	2.20914400	1.76895100	2.04677100	H	-1.77350300	1.22414400	-3.27826300
C	-1.85306300	0.17063700	3.97361700	H	-0.76467700	0.83547800	-5.49520500
C	-2.86941900	0.27189600	4.93412200	H	2.17354500	-3.21980400	1.36576100
C	-2.94375900	-0.65278900	5.97723700	H	1.15231900	-5.42690200	1.06062900
C	-2.00176700	-1.67930800	6.08271900	H	-1.85296800	-1.73299100	1.73351900
C	-0.99099500	-1.78684000	5.12717800	H	-3.24291700	-1.85193200	-2.31232000
C	-0.92219900	-0.87323400	4.07310400	H	-4.48000900	-0.07446100	-0.79409400
H	-3.59988500	1.07320200	4.86809900	H	-1.21526100	2.69236500	-1.03334500
H	-3.73784300	-0.56489300	6.71343500	H	1.64795600	1.91442500	-1.42660200
H	-2.05981000	-2.39315300	6.89890100	H	3.71818200	-1.80966800	-1.89843900
H	-0.25864800	-2.58581400	5.19167600	H	4.81236600	-0.21588800	-0.07691500
H	-0.13044500	-0.97563100	3.33567500	H	1.85463800	-1.46146100	2.76613100
Se	-1.76817000	1.51583300	2.55209400	N	6.16170300	-1.18886900	4.25737000
H	0.36466600	1.70835800	0.24785500	C	7.22143800	-2.17698700	4.12552300

### 33-S

B3LYP-D3 SCF energy: -4539.842844 a.u.

B3LYP-D3 enthalpy: -4537.934740 a.u.

B3LYP-D3 free energy: -4538.188250 a.u.

M06 SCF energy in solution: -4538.815762 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z		X	Y	Z
C	0.62082200	-1.76863800	-3.81696400	N	4.40665300	1.52770300	-5.04797100
C	0.07317000	-1.55505600	-2.53635700	N	-5.43334900	4.45107400	-1.16699000
C	-0.79972400	-0.46426800	-2.34691300	N	-4.67778100	-5.19729800	0.46916900
C	-1.09513500	0.39095900	-3.41780100	C	4.06686100	0.87086800	-6.29993800
C	-0.53106500	0.16680200	-4.67207700	H	4.13530000	1.59915300	-7.11813400
C	0.32664300	-0.90979300	-4.87925800	H	4.71054200	0.01394400	-6.56382200
C	0.38193600	-2.56887400	-1.47838200	H	3.03290400	0.51514900	-6.24781200
C	1.22083600	-2.33279000	-0.36727700	C	5.73492300	2.11547500	-4.97360500
C	-0.16037300	-3.86568700	-1.65184600	H	5.81262900	2.72694300	-4.06859200
C	1.49946800	-3.37485900	0.53475900	H	6.55677000	1.37714400	-4.95575600
C	0.09202700	-4.88193800	-0.72585700	H	5.89168300	2.76918700	-5.84022200
C	0.93224300	-4.63083200	0.35516500	C	-6.24897300	4.73991700	0.00286400
P	-1.50627300	-0.15782500	-0.67228500	H	-6.51140100	5.80548300	0.00268000
P	1.84925900	-0.63006700	0.00431800	H	-7.19011100	4.16616600	0.06571100
C	-2.46985700	-1.66626300	-0.32168000	H	-5.66893400	4.53428500	0.90748900
C	-2.43829500	-2.21743900	0.95652200	C	-6.05183200	4.73689800	-2.45246100
				H	-6.89958800	4.07501000	-2.70578900
				H	-6.42179000	5.76944500	-2.45471900

H	-5.30293800	4.64284100	-3.24570400	C	5.22544800	-1.18688200	-4.04695700
C	-3.93285200	-6.44407600	0.41373900	H	5.71672400	-0.59289500	-4.81913800
H	-3.31831900	-6.64481500	1.31066500	C	6.32122800	-1.61010200	-3.05126900
H	-4.63168300	-7.28064000	0.29253700	H	5.92417300	-2.26342000	-2.26585700
H	-3.26379300	-6.43393800	-0.45327900	H	7.11420300	-2.16175400	-3.56868000
C	-5.76138900	-5.17167100	1.44233200	H	6.77325500	-0.73666000	-2.56832000
H	-6.23445200	-4.18581900	1.43323200	C	4.59781800	-2.41221600	-4.73235000
H	-6.51800200	-5.91452700	1.15802300	H	4.05127800	-3.03069400	-4.01354200
H	-5.45531600	-5.39060200	2.47917500	H	3.88948900	-2.10192700	-5.50668600
C	6.97099400	-0.24725600	1.51379000	H	5.37289500	-3.02756700	-5.20356400
H	7.55612100	-0.15056100	2.43018100	C	2.61407800	3.21208000	-3.59840100
C	7.04358400	1.11286300	0.79420000	H	3.38652200	3.51167600	-4.31062500
H	6.55944300	1.08329400	-0.18898400	C	1.27205300	3.19812300	-4.35401100
H	6.56172800	1.90051300	1.38388800	H	0.45823500	2.87136900	-3.69654700
H	8.08988100	1.39618600	0.63428200	H	1.02931500	4.19917900	-4.72946500
C	7.61482700	-1.35483800	0.65745600	H	1.30986700	2.50883300	-5.20380700
H	8.64956600	-1.09610200	0.40469700	C	2.58375300	4.24144600	-2.45717500
H	7.62135500	-2.31497000	1.18340600	H	1.75182100	4.05434000	-1.76973400
H	7.06234000	-1.48930300	-0.27834800	H	3.51346700	4.23001900	-1.87678500
C	3.43801800	-1.83006700	4.90215000	H	2.44383800	5.24976900	-2.86311700
H	4.36023500	-2.03736600	5.45176900	C	-4.87798900	-4.03711000	-2.12667500
C	2.68694100	-0.70761700	5.64464400	H	-4.76922600	-5.12635900	-2.06874200
H	1.74194900	-0.46115000	5.14599700	C	-4.52082200	-3.59027300	-3.55417500
H	2.44917000	-1.01459200	6.66989600	H	-4.80395600	-2.54502100	-3.72957900
H	3.28591700	0.20801700	5.69519900	H	-3.45102200	-3.68062800	-3.76324400
C	2.60000400	-3.12095700	4.86876800	H	-5.07018600	-4.19808900	-4.28105500
H	1.63663700	-2.97569100	4.36213700	C	-6.35999500	-3.71118000	-1.84675900
H	3.13027300	-3.92644900	4.34856900	H	-6.52099200	-2.62612400	-1.85212600
H	2.38474500	-3.45994800	5.88859400	H	-7.00038900	-4.14962800	-2.62103900
C	-2.64128700	4.99534100	-1.22959000	H	-6.68018600	-4.10224700	-0.87943700
H	-3.39963000	5.59269200	-1.74339600	C	-3.01793000	-3.96036000	2.67010600
C	-1.32272600	5.11641200	-2.00918000	H	-3.47356300	-4.95146100	2.68448400
H	-0.48643000	4.66143200	-1.46758200	C	-1.55101300	-4.14896000	3.10066100
H	-1.38702000	4.64211200	-2.99501000	H	-1.01628700	-3.19533800	3.15961300
H	-1.06938100	6.17264400	-2.15306000	H	-1.50545900	-4.61442800	4.09217000
C	-2.48573200	5.57382000	0.19094100	H	-1.01338900	-4.78605100	2.39180200
H	-2.11578700	6.60500600	0.15226200	C	-3.78944400	-3.07378400	3.66708500
H	-3.44274600	5.57173800	0.72175400	H	-3.38782800	-2.05548000	3.68206300
H	-1.77049300	4.98235300	0.77338200	H	-4.84980500	-3.01434000	3.39966900
C	-6.51918200	1.62778700	-1.03810900	H	-3.71474700	-3.47673100	4.68376700
H	-7.09521400	2.54170700	-1.18850700	Rh	0.11936500	0.55991100	0.97254100
C	-6.84513800	0.69431300	-2.22020000	C	1.22820200	5.65845000	0.68385500
H	-6.32513800	-0.26661300	-2.12989900	C	1.17188400	4.35261800	1.16925900
H	-7.92080400	0.48766200	-2.25799300	C	0.56355300	4.06525100	2.40183000
H	-6.54925300	1.14632900	-3.17336900	C	0.01384500	5.12933500	3.13927100
C	-6.97068700	1.00987500	0.29873900	C	0.05828400	6.43696400	2.66853900
H	-6.44580400	0.06796800	0.49837200	C	0.66095000	6.67894500	1.43715400
H	-6.77062100	1.68909500	1.13480000	H	1.69426200	5.89272600	-0.26626000
H	-8.04558400	0.79629300	0.28006600	H	1.61426100	3.55648000	0.58170600
H	0.76211400	-1.08273500	-5.85717100	H	-0.46635300	4.92387900	4.09289100
H	-0.34740300	-5.86424200	-0.84586700	H	-0.36739600	7.26256100	3.22830600
O	-0.92443500	-4.04719000	-2.76377400	F	0.68636400	7.93551700	0.95867700
O	1.44968800	-2.84598500	-3.94701800	C	0.46143600	2.67851100	2.94147400
C	-1.39029800	-5.35832500	-3.05782600	H	0.36621300	2.67903600	4.02950300
H	-2.12713100	-5.69291000	-2.31731500	C	1.33391000	1.58711100	2.38887200
H	-1.87183900	-5.29251200	-4.03389600	H	1.61327000	0.88153700	3.17195800
H	-0.56208400	-6.07620200	-3.10830400	H	2.25010400	1.96537300	1.92981400
C	1.37728000	-3.58061600	-5.16612300	C	-1.79394500	0.73754200	3.92536400
H	1.85202200	-3.04959600	-5.99938500	C	-2.83216100	1.00081200	4.82599000
H	1.92294300	-4.50943200	-4.98916400	C	-3.01656700	0.17275000	5.93604800
H	0.33396600	-3.80318500	-5.41872900	C	-2.16238400	-0.90915900	6.15932500

C	-1.13162600	-1.17657200	5.25694900
C	-0.95406000	-0.36319300	4.13644100
H	-3.49038400	1.84992500	4.66691500
H	-3.82475000	0.38183000	6.63096500
H	-2.30368200	-1.54502200	7.02810600
H	-0.46772900	-2.02078800	5.41589800
H	-0.14973800	-0.58435100	3.44172100
Se	-1.53969800	1.96399300	2.40828600
H	0.45452500	1.71942500	0.05844600

### 34

B3LYP-D3 SCF energy: -4539.851368 a.u.

B3LYP-D3 enthalpy: -4537.9420799 a.u.

B3LYP-D3 free energy: -4538.194248 a.u.

M06 SCF energy in solution: -4538.820827 a.u

#### Cartesian coordinates

ATOM	X	Y	Z
C	0.86367300	3.46917300	2.19333200
C	0.94595900	2.14423700	1.71568200
C	1.70819100	1.88874400	0.55939600
C	2.34578700	2.94830400	-0.10601300
C	2.23486000	4.25031900	0.37501200
C	1.49977300	4.51778400	1.52588200
C	0.25150000	1.09100900	2.51461800
C	-0.91004300	0.42065200	2.07534200
C	0.74266900	0.82787000	3.81587900
C	-1.56363100	-0.46894900	2.94432700
C	0.11047200	-0.09900200	4.64889500
C	-1.05125700	-0.72678500	4.21028900
P	1.88695900	0.16684400	-0.08496900
P	-1.49314900	0.59555400	0.31778900
C	2.49776700	-0.80197900	1.32364000
C	1.99694500	-2.07097100	1.58957100
C	3.50953100	-0.27082800	2.13449200
C	2.45753300	-2.81872400	2.68003900
C	4.05267000	-1.01443800	3.18077500
C	3.50870100	-2.29677800	3.46570500
C	3.26193800	0.29180800	-1.28904300
C	4.55138200	-0.13592000	-0.97344000
C	3.02455000	0.83887300	-2.55518800
C	5.60285900	-0.02275400	-1.89013500
C	4.04782800	0.98437700	-3.49170900
C	5.35695700	0.55827700	-3.15525200
C	-1.72890100	2.38252300	0.01246300
C	-1.32183200	2.92023800	-1.21217700
C	-2.32539000	3.22384200	0.95821100
C	-1.45308500	4.27799500	-1.49739600
C	-2.50926500	4.58886100	0.69688300
C	-2.02738000	5.12556700	-0.52080700
C	-3.16953900	-0.15999900	0.31179100
C	-4.32198200	0.61284200	0.14449900
C	-3.31701300	-1.52773300	0.59845300
C	-5.59938800	0.06234500	0.31490700
C	-4.56366000	-2.07690700	0.91712600
C	-5.72086600	-1.26488100	0.78938300
H	2.94434200	2.76208600	-0.98795000
H	2.72939100	5.06129600	-0.15084300
H	-2.48082200	-0.95418400	2.64802700
H	-1.56605600	-1.42430400	4.86486300
H	1.23296800	-2.48604300	0.94613700

H	3.87946200	0.72628500	1.93008200
H	4.74807200	-0.58719100	-0.00941700
H	2.02297100	1.15815800	-2.82505000
H	-0.86298800	2.27273200	-1.94686700
H	-2.64712900	2.81496400	1.91173900
H	-4.23200800	1.66143300	-0.11764900
H	-2.43369800	-2.15465000	0.67633600
N	-6.97020300	-1.81731400	1.20529100
C	-7.70608400	-1.14744200	2.26750100
H	-7.00130100	-0.67937500	2.96038900
H	-8.41252600	-0.37508400	1.92006900
H	-8.28525400	-1.89420700	2.82594000
C	-7.79963100	-2.49540500	0.22208000
H	-7.18922600	-3.11127500	-0.43849900
H	-8.50736800	-3.15517000	0.73831800
H	-8.38897500	-1.80348200	-0.40829300
N	-2.06788200	6.52347400	-0.82731100
N	6.37642000	0.73150900	-4.14460000
N	4.07545600	-3.00469000	4.57628800
C	-1.30482000	7.43026300	0.01595600
H	-1.03059600	8.31861200	-0.56741000
H	-1.83346700	7.77758900	0.92028400
H	-0.38239400	6.93378400	0.33308400
C	-3.31584700	7.05111900	-1.35694100
H	-3.72228700	6.35490000	-2.09769500
H	-4.09358500	7.22400800	-0.59134900
H	-3.12223600	8.00704400	-1.85857900
C	6.72704500	-0.44330200	-4.92844500
H	7.25097500	-0.12789700	-5.83884500
H	7.37523900	-1.16392400	-4.39801000
H	5.81356000	-0.96804500	-5.22586800
C	7.46332600	1.65497500	-3.85909700
H	8.28655900	1.23219100	-3.25776600
H	7.89300500	2.00500300	-4.80618200
H	7.06768000	2.52531300	-3.32654800
C	3.34236900	-2.91895700	5.82880300
H	2.43123500	-3.54408300	5.86146500
H	3.99372500	-3.23116100	6.65393300
H	3.04172800	-1.88112200	6.00860700
C	4.72435900	-4.28625800	4.32918700
H	5.20718500	-4.26552700	3.34832700
H	5.50124800	-4.44669900	5.08785100
H	4.04932600	-5.15759500	4.35589800
C	-6.81460600	0.92681700	-0.00674400
H	-7.70354700	0.29513700	0.05030700
C	-6.74843800	1.47497700	-1.44599400
H	-5.90621200	2.16411300	-1.57879800
H	-6.64036400	0.66795300	-2.17913400
H	-7.66538700	2.02572700	-1.68349900
C	-6.97903300	2.07799900	1.00128700
H	-7.87632500	2.66561200	0.77598800
H	-7.06284500	1.70632000	2.02729200
H	-6.11791300	2.75149100	0.95983500
C	-4.65686100	-3.48931900	1.48861000
H	-5.63310900	-3.54857600	1.97860600
C	-4.61487300	-4.57403700	0.39764100
H	-3.73698400	-4.45959500	-0.24413700
H	-4.57952800	-5.57058400	0.85428800
H	-5.49779500	-4.53745900	-0.24395500
C	-3.58201400	-3.75473500	2.55906300
H	-2.56964600	-3.77662200	2.13979600

H	-3.60121700	-2.99059200	3.34477500	H	6.73746100	-1.06392300	2.48238700
H	-3.75752800	-4.72715500	3.03238500	H	7.39579300	-0.82718000	4.11115500
C	3.71690500	1.58815400	-4.84888800	H	6.46387600	-2.28702100	3.73911200
H	4.65481900	1.64045400	-5.40807100	C	1.80086800	-4.16846100	2.95104000
C	3.16483400	3.01905000	-4.70980300	H	2.17386900	-4.54851400	3.90301100
H	2.20871600	3.03466300	-4.17180700	C	0.27314300	-4.03928500	3.09801100
H	3.86464300	3.66401000	-4.16616100	H	-0.19590400	-3.71410200	2.16353700
H	2.99224500	3.46086300	-5.69790000	H	-0.16522300	-5.00739800	3.36582200
C	2.73733300	0.69078000	-5.62900200	H	0.00767300	-3.31028400	3.86967600
H	2.54856500	1.10500100	-6.62611200	C	2.16603600	-5.19003300	1.85628600
H	3.13498100	-0.32299800	-5.74708200	H	1.79650700	-4.86774300	0.87631700
H	1.77252100	0.60552400	-5.11256200	H	3.25092400	-5.31918200	1.78172700
C	6.97577500	-0.53257400	-1.46387500	H	1.71917400	-6.16623100	2.07755600
H	7.63480900	-0.51319900	-2.33330300	Rh	-0.03194200	-0.56549300	-1.13140700
C	7.58817200	0.38816400	-0.39021700	C	0.40967200	-3.77083400	-2.05686100
H	6.96330500	0.40512800	0.51141100	C	0.39129400	-4.82682600	-2.98362300
H	8.58512000	0.03654800	-0.10085700	C	-0.34075200	-5.98665800	-2.72195400
H	7.67951800	1.41770700	-0.75274300	C	-1.07796200	-6.11087700	-1.53952600
C	6.92463400	-1.99230000	-0.97346400	C	-1.07645800	-5.06282400	-0.61850400
H	6.34787700	-2.09213600	-0.04641800	C	-0.33970400	-3.90532900	-0.87617000
H	6.46808600	-2.64632600	-1.72397100	H	0.95652900	-4.74037100	-3.90718500
H	7.93831600	-2.35568800	-0.77007200	H	-0.33432100	-6.79731900	-3.44575300
H	1.41890900	5.53153900	1.90231500	H	-1.63891300	-7.01796600	-1.33504600
H	0.50240700	-0.32090000	5.63350400	H	-1.62725000	-5.15237600	0.31240100
O	1.84759000	1.53062300	4.18967100	H	-0.32587300	-3.11436300	-0.12863400
O	0.12282400	3.65933000	3.32280800	Se	1.51831300	-2.19618100	-2.38680200
C	2.29936800	1.41281000	5.53357900	C	-5.52980200	-2.19759700	-2.56481600
H	2.69364200	0.40890700	5.73360500	C	-4.32756900	-1.51629200	-2.68692200
H	3.10490100	2.13939600	5.64346700	C	-3.13363200	-2.20683000	-2.97141400
H	1.49892000	1.64588800	6.24669300	C	-3.18255500	-3.60472200	-3.13441300
C	0.61687500	4.59651400	4.27741700	C	-4.38082300	-4.29999500	-3.01563200
H	0.46926600	5.63337000	3.95466500	C	-5.53363800	-3.58002000	-2.72877900
H	0.03822400	4.42891100	5.18781000	H	-6.45650400	-1.68333800	-2.34086800
H	1.68041000	4.41843700	4.47376200	H	-4.32164400	-0.44032800	-2.55758700
C	-3.23531000	5.45242900	1.72526200	H	-2.26884000	-4.14871800	-3.34913300
H	-3.38573900	6.44070500	1.28854900	H	-4.43047100	-5.37799200	-3.12108400
C	-4.63469500	4.89787500	2.04378600	F	-6.69397700	-4.24628900	-2.55218600
H	-4.58536800	3.90667300	2.50850300	C	-1.86728500	-1.52711300	-3.22069500
H	-5.15813200	5.56341800	2.73954900	H	-1.07451200	-2.15633800	-3.61463800
H	-5.23907300	4.81661700	1.13417100	C	-1.61131900	-0.19199000	-3.14251400
C	-2.40773600	5.63494100	3.00804900	H	-0.73624000	0.20680600	-3.64325500
H	-2.20256800	4.67292400	3.48694100	H	-2.36149700	0.52822900	-2.82986300
H	-1.44481200	6.10429300	2.78318200	H	0.25035400	0.74626700	-1.83544500
H	-2.94199700	6.27317200	3.72123100				
C	-0.91940000	4.83773900	-2.81134600				
H	-1.52467300	5.71248600	-3.06559400				
C	0.53120700	5.32461300	-2.62632800				
H	1.18294300	4.48992700	-2.34423200				
H	0.91460900	5.76025000	-3.55633200				
H	0.59144300	6.08251300	-1.83953500				
C	-1.00631000	3.84523400	-3.98252400				
H	-0.30489800	3.00883700	-3.86773700				
H	-2.01466500	3.42872600	-4.08861000				
H	-0.74577800	4.34989300	-4.91885200				
C	5.24670800	-0.47705700	3.96635800				
H	5.07312200	-0.69669300	5.02616700				
C	5.45992200	1.03818500	3.81365200				
H	5.83659500	1.29057500	2.81437300				
H	4.53973600	1.60751600	3.97222800				
H	6.20959400	1.38106100	4.53457100				
C	6.53728200	-1.21476700	3.55036200				

### 35-ts-R

B3LYP-D3 SCF energy: -4539.842756 a.u.

B3LYP-D3 enthalpy: -4537.935429 a.u.

B3LYP-D3 free energy: -4538.188528 a.u.

M06 SCF energy in solution: -4538.808461 a.u

Imaginary frequency: -743.30 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z
C	0.75161300	-4.27697600	-0.69477700
C	0.17612400	-3.09408100	-0.18197000
C	-0.82361400	-2.45034400	-0.94224000
C	-1.25311800	-2.99954100	-2.15886500
C	-0.68147400	-4.17741400	-2.63299600
C	0.32610100	-4.81372700	-1.91414100
C	0.59062200	-2.64911700	1.18614700
C	1.27320600	-1.44398300	1.45058700

C	0.28589100	-3.50216900	2.27398600	H	6.38157200	-3.88438600	-5.09586100
C	1.66796200	-1.11927700	2.75704400	C	-6.78615800	2.45089500	-3.18084700
C	0.68169300	-3.17115000	3.57395500	H	-7.17298700	2.92079200	-4.09461700
C	1.38292200	-1.99072600	3.80282500	H	-7.59456300	2.47084500	-2.43128300
P	-1.53340500	-0.87024400	-0.32172100	H	-5.96391500	3.06389800	-2.80378200
P	1.63640500	-0.26935400	0.07819300	C	-7.29997700	0.17573000	-3.96348700
C	-2.14364800	-1.30432700	1.33932900	H	-8.01862700	-0.12485200	-3.17970100
C	-1.89096900	-0.51278400	2.45416600	H	-7.86857700	0.62427500	-4.78700000
C	-2.92841900	-2.45677000	1.46948200	H	-6.81307800	-0.72917700	-4.34040400
C	-2.44040900	-0.82103900	3.70411900	C	-2.89020000	-3.02430000	6.01620500
C	-3.47106800	-2.81746500	2.70186100	H	-2.21824300	-2.31150200	6.52811800
C	-3.23268100	-1.98468000	3.82821600	H	-3.46315200	-3.55628300	6.78519900
C	-3.00796000	-0.44734300	-1.31280000	H	-2.26454300	-3.75575600	5.49279200
C	-4.20975900	-0.17542000	-0.65850600	C	-4.85177200	-1.58773700	5.67496400
C	-2.91355900	-0.19622800	-2.68863400	H	-5.46832300	-1.14659700	4.88695800
C	-5.31966700	0.32503500	-1.34292200	H	-5.49653000	-2.22374400	6.29504100
C	-4.00395600	0.29615100	-3.41165000	H	-4.47989600	-0.76793100	6.31178700
C	-5.21783100	0.57583100	-2.73160600	C	6.47017800	1.80393900	1.03469900
C	2.62570500	-1.30812100	-1.06501100	H	6.92362200	2.71715700	1.42496300
C	2.40311600	-1.32740100	-2.44119000	C	6.82562200	1.73336500	-0.46242300
C	3.63308700	-2.12708700	-0.53679300	H	6.47257200	0.80388700	-0.92437300
C	3.14527900	-2.14450300	-3.29555400	H	6.39051500	2.57113300	-1.01899900
C	4.42997100	-2.92811400	-1.36096400	H	7.91283400	1.77047700	-0.59227000
C	4.16092100	-2.96553900	-2.75071500	C	7.08186700	0.61001900	1.79253400
C	2.74612800	0.99171100	0.80504000	H	8.16808900	0.57612300	1.64989100
C	4.13234900	0.95514600	0.63492900	H	6.88023800	0.66937300	2.86632800
C	2.17879000	2.00437900	1.59528400	H	6.66462100	-0.33226100	1.42503100
C	4.96481400	1.88740300	1.26967900	C	2.34622200	3.97556100	3.17523500
C	2.97835700	2.93593800	2.25870300	H	3.02120200	4.83504900	3.20553800
C	4.38817600	2.85501400	2.12463600	C	0.97021800	4.46477200	2.69722100
H	-2.05277700	-2.53514400	-2.72067500	H	0.19780500	3.69290100	2.78111400
H	-1.02512000	-4.60382800	-3.57080900	H	0.64915400	5.31396900	3.31126100
H	2.20112400	-0.19885000	2.95801000	H	0.99892000	4.78616200	1.65102500
H	1.70534800	-1.74714200	4.81071400	C	2.26132500	3.41451700	4.60923300
H	-1.25063800	0.35329500	2.35880700	H	1.61456100	2.52866700	4.63968400
H	-3.10786700	-3.07715000	0.59894000	H	3.25160600	3.13107100	4.97969300
H	-4.27956900	-0.32656900	0.41098300	H	1.84142500	4.16257300	5.29165500
H	-1.97314600	-0.36475300	-3.20435800	C	-3.86353500	0.53097300	-4.90882000
H	1.60059800	-0.73876400	-2.86305700	H	-4.76780900	1.05789400	-5.22481300
H	3.80360000	-2.13880700	0.53520300	C	-3.79391600	-0.80780500	-5.66814700
H	4.57892200	0.19491900	0.00490600	H	-2.90355100	-1.37982400	-5.37482400
H	1.10075700	2.05920800	1.70052100	H	-4.67246900	-1.42927300	-5.46340500
N	5.16682500	3.77420700	2.89623300	H	-3.74176200	-0.63791100	-6.74972900
C	6.06656800	3.24401100	3.90870800	C	-2.65199700	1.41424100	-5.25621000
H	5.62909600	2.34379900	4.35039500	H	-2.67605200	1.69508900	-6.31492700
H	7.07580800	2.99103900	3.54182100	H	-2.63720400	2.33298400	-4.65843900
H	6.18407700	3.98876000	4.70643300	H	-1.70681300	0.88138300	-5.09005800
C	5.62209000	4.98793700	2.23606500	C	-6.57825200	0.61595800	-0.53411200
H	4.81783700	5.41616100	1.63561600	H	-7.39371600	0.82614700	-1.22827200
H	5.90664900	5.72553700	2.99610500	C	-7.01737100	-0.59261600	0.31470700
H	6.49477200	4.83704100	1.57420100	H	-6.28929300	-0.82897100	1.09900300
N	4.86786700	-3.81938400	-3.65264500	H	-7.97126500	-0.37692800	0.80876800
N	-6.29200500	1.11922400	-3.50385200	H	-7.14773500	-1.48723400	-0.30463300
N	-3.80936300	-2.40868600	5.07253100	C	-6.36401300	1.86259200	0.34867500
C	4.78768700	-5.25775700	-3.45944600	H	-5.55828600	1.69218400	1.07256200
H	4.91849500	-5.75814100	-4.42762500	H	-6.08417600	2.73397900	-0.25199300
H	5.53787000	-5.67635400	-2.76723400	H	-7.27774900	2.10351700	0.90409300
H	3.79363700	-5.51309100	-3.07859900	H	0.76977800	-5.72581100	-2.29588200
C	6.12070500	-3.31713600	-4.19430400	H	0.44992900	-3.82391100	4.40617500
H	6.00177500	-2.26639000	-4.47746600	O	-0.40355400	-4.63407100	1.96991700
H	6.97171200	-3.38638900	-3.49284900	O	1.72286400	-4.85069200	0.06601400

C	-0.65805800	-5.57526000	3.00597700
H	-1.32989800	-5.15778600	3.76643100
H	-1.14750900	-6.42248000	2.52437300
H	0.27314000	-5.91211300	3.47863200
C	1.89836600	-6.25986200	-0.03727800
H	2.39200200	-6.54358000	-0.97536500
H	2.54183400	-6.54327600	0.79662600
H	0.93507800	-6.77807400	0.04098900
C	5.57878400	-3.71126900	-0.73135400
H	6.19478300	-4.11392400	-1.53770900
C	6.49123500	-2.79918900	0.10809200
H	5.97859600	-2.43224000	1.00415600
H	7.37662900	-3.35142300	0.44215200
H	6.82821600	-1.93156700	-0.46989000
C	5.07019700	-4.89455500	0.11106400
H	4.37222500	-4.55451700	0.88407700
H	4.54552900	-5.62157800	-0.51399600
H	5.90710900	-5.40641200	0.59988900
C	2.84104400	-2.12032400	-4.78728300
H	3.48395300	-2.87175500	-5.25328200
C	1.38046400	-2.50430700	-5.08346500
H	0.67255000	-1.79070900	-4.64249000
H	1.20368800	-2.52330300	-6.16498000
H	1.14381900	-3.49151400	-4.67559100
C	3.18455200	-0.74820400	-5.39786700
H	2.54589800	0.04324400	-4.98411100
H	4.22650100	-0.47160600	-5.20157400
H	3.03382000	-0.76058700	-6.48324200
C	-4.33842400	-4.06688100	2.82192700
H	-4.11588200	-4.52130100	3.79364000
C	-4.06935200	-5.11050800	1.72461500
H	-4.47579900	-4.79205800	0.75670800
H	-2.99994100	-5.29681000	1.58777600
H	-4.55964100	-6.05558700	1.98188100
C	-5.83420800	-3.69123500	2.82502200
H	-6.10613100	-3.19558100	1.88502100
H	-6.45540400	-4.58897200	2.92578800
H	-6.07501000	-3.01793300	3.65065200
C	-2.23971900	0.17186200	4.84601900
H	-2.53018500	-0.31122000	5.78061800
C	-0.78090800	0.62872700	5.01717800
H	-0.41524900	1.17418700	4.13985500
H	-0.70149700	1.30503500	5.87557400
H	-0.11567900	-0.22208300	5.18485800
C	-3.16158500	1.39138300	4.63215900
H	-2.89464000	1.91834700	3.70861900
H	-4.21107900	1.08917100	4.55352800
H	-3.06960700	2.09457700	5.46819500
Rh	-0.17206900	0.90793100	-0.69532600
C	-2.45605800	3.80399800	-0.41257900
C	-3.07640100	3.51659300	-1.63916000
C	-3.56664900	4.55226900	-2.43812500
C	-3.47348500	5.88013600	-2.01097100
C	-2.88770900	6.16429500	-0.77511900
C	-2.37571400	5.13431100	0.02019000
H	-3.16894200	2.48641300	-1.96737800
H	-4.02406600	4.31831600	-3.39640700
H	-3.85908800	6.68363900	-2.63169400
H	-2.81912900	7.19246900	-0.42924000
H	-1.90388200	5.36420200	0.97106400
Se	-1.78873700	2.36064400	0.72226400

C	3.52720400	4.34314100	-1.00212500
C	2.60805600	3.42170000	-1.48592100
C	1.24873900	3.76389800	-1.63331900
C	0.83861600	5.06420400	-1.27701000
C	1.75057800	5.99831100	-0.79639200
C	3.08236500	5.62119300	-0.67218000
H	4.57186100	4.08836200	-0.87077400
H	2.95147600	2.42095000	-1.72540300
H	-0.20306000	5.34401900	-1.38615400
H	1.44931800	7.00457900	-0.52639200
F	3.97333200	6.51933300	-0.20433600
C	0.25201100	2.85819800	-2.20274400
H	-0.76082300	3.24401100	-2.25098900
C	0.53138100	1.70890600	-2.95335000
H	-0.22310000	1.38104500	-3.66292000
H	1.55796900	1.48398000	-3.23103700
H	0.34369300	0.38781000	-2.13120300

### 36-R

B3LYP-D3 SCF energy: -4539.874177 a.u.

B3LYP-D3 enthalpy: -4537.961271 a.u.

B3LYP-D3 free energy: -4538.214852 a.u.

M06 SCF energy in solution: -4538.839453 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z
C	-0.18579700	3.06595800	-2.55693000
C	-0.45320100	1.88157400	-1.83818700
C	-1.13642100	1.97898700	-0.60847700
C	-1.54215800	3.23275600	-0.12804700
C	-1.25628900	4.38775600	-0.85216300
C	-0.57505000	4.31350100	-2.06298900
C	-0.06089600	0.59536600	-2.50022000
C	1.01740900	-0.21147400	-2.07471200
C	-0.75877000	0.23269600	-3.67627200
C	1.40490900	-1.32674900	-2.83567900
C	-0.38373400	-0.89760400	-4.40959100
C	0.70615300	-1.65860600	-3.99229000
P	-1.66303300	0.40863200	0.20087100
P	1.73797700	0.10513800	-0.40075400
C	-2.89624600	-0.14452600	-1.05926000
C	-2.98785400	-1.42552600	-1.59091600
C	-3.83722100	0.81923300	-1.44755100
C	-4.03722900	-1.78879600	-2.44841400
C	-4.89410700	0.50111100	-2.29696600
C	-5.02202600	-0.82939800	-2.76927500
C	-2.71753900	0.80705100	1.64236200
C	-3.90068700	0.07800200	1.79994400
C	-2.37854400	1.75443900	2.61541700
C	-4.74957100	0.28048800	2.89155100
C	-3.21032200	2.00251300	3.71126700
C	-4.40475700	1.25260800	3.85824900
C	2.21737400	1.87102800	-0.43675300
C	1.95017900	2.71074900	0.64122400
C	2.97595700	2.35462600	-1.50928500
C	2.44852800	4.01630000	0.68763600
C	3.49481500	3.65240800	-1.50391400
C	3.22398500	4.49411700	-0.39496300
C	3.35807900	-0.75100000	-0.26769400
C	4.47106500	-0.02011400	0.15435500
C	3.49151800	-2.14078800	-0.43296800

C	5.71010500	-0.62818300	0.38457300	C	4.91071200	-4.24631800	-0.64136800
C	4.73587200	-2.76667300	-0.31085900	H	5.61823000	-4.66436500	0.08044000
C	5.86330400	-1.99733100	0.08621000	C	3.61882000	-5.06756600	-0.56422000
H	-2.11755200	3.31629500	0.78289400	H	2.92216500	-4.80393700	-1.36572300
H	-1.58041400	5.35282800	-0.47380200	H	3.84978200	-6.13228900	-0.67735400
H	2.25682200	-1.92358600	-2.54011000	H	3.09226300	-4.93557900	0.38480500
H	1.01214800	-2.51978400	-4.57960400	C	5.53676400	-4.39499300	-2.04410300
H	-2.26282900	-2.17470900	-1.31636100	H	4.86893500	-3.97586100	-2.80754100
H	-3.75893800	1.82943900	-1.06372500	H	6.49851100	-3.88102100	-2.10708100
H	-4.17379700	-0.66076900	1.05681500	H	5.69783800	-5.45334900	-2.28009800
H	-1.47287500	2.33995400	2.51242900	C	-2.83962200	3.10538800	4.69386000
H	1.33020600	2.35388400	1.45100600	H	-3.58280700	3.06702100	5.49431100
H	3.17432500	1.70489500	-2.35596400	C	-2.93546000	4.48793300	4.01950800
H	4.37785400	1.04258600	0.33905600	H	-2.20937300	4.58374700	3.20168500
H	2.61732800	-2.74317900	-0.65476600	H	-3.93500000	4.65864500	3.60409900
N	7.12165200	-2.67326400	0.17494600	H	-2.72688000	5.28459200	4.74288700
C	8.21963000	-2.19211000	-0.65166100	C	-1.45044600	2.89893400	5.32261700
H	7.82485800	-1.83531100	-1.60741000	H	-1.27893100	3.64149400	6.11007800
H	8.81568200	-1.37864200	-0.20436200	H	-1.35765800	1.90221200	5.76827600
H	8.90321300	-3.02581400	-0.85685200	H	-0.64618900	3.01734000	4.58696700
C	7.50629700	-3.18137700	1.48362000	C	-6.01624400	-0.56640800	2.96511400
H	6.65825000	-3.68774800	1.95187900	H	-6.59466500	-0.25188300	3.83458000
H	8.31259800	-3.91474100	1.36424000	C	-6.90851600	-0.35179000	1.72682900
H	7.86618000	-2.39859400	2.17711900	H	-6.40978400	-0.67557000	0.80569200
N	3.70621300	5.83942800	-0.30892600	H	-7.83591100	-0.92766600	1.82380200
N	-5.22167800	1.53481900	5.00028400	H	-7.17295600	0.70451600	1.60682700
N	-6.19095500	-1.13307900	-3.54348300	C	-5.67140300	-2.05661700	3.15295500
C	3.18296700	6.81746700	-1.24903900	H	-5.09462700	-2.44425800	2.30528900
H	3.26075400	7.81914300	-0.80731700	H	-5.07418500	-2.21166400	4.05822300
H	3.69807500	6.84439500	-2.22468200	H	-6.58742300	-2.65210200	3.24047100
H	2.12370400	6.60879000	-1.43016100	H	-0.35847500	5.21487900	-2.62494700
C	5.09150300	6.01855300	0.09568100	H	-0.92220600	-1.17962600	-5.30530100
H	5.31935300	5.34088100	0.92476400	O	-1.78784800	1.04687200	-4.02305800
H	5.82704600	5.83138100	-0.70750500	O	0.46396000	2.91190800	-3.74365000
H	5.23651500	7.04682400	0.44865000	C	-2.61984000	0.67007800	-5.11426900
C	-5.28384000	0.51846300	6.04087800	H	-3.06222300	-0.31774100	-4.94674900
H	-5.62601900	0.98283300	6.97374400	H	-3.41493200	1.41571600	-5.14909600
H	-5.95732200	-0.32795400	5.82122800	H	-2.06726900	0.67882700	-6.06255300
H	-4.28062800	0.11541800	6.21181500	C	0.12927100	3.80894400	-4.80102000
C	-6.44667400	2.28377100	4.76150600	H	0.56370300	4.80347500	-6.64966200
H	-7.27183300	1.68961700	4.33059400	H	0.55654900	3.37406300	-5.70625400
H	-6.79947400	2.70670600	5.70977600	H	-0.95903700	3.89026200	-4.90449500
H	-6.23682300	3.11342000	4.07863300	C	4.33108000	4.11611100	-2.69418600
C	-6.02105900	-1.25380300	-4.98176300	H	4.80469500	5.06257600	-2.42820200
H	-5.49828600	-2.17074600	-5.30898700	C	5.46599700	3.13435700	-3.03805300
H	-7.00643100	-1.24296100	-5.46214800	H	5.08286000	2.16084500	-3.36406500
H	-5.45818800	-0.39200200	-5.35659100	H	6.07450800	3.53758100	-3.85529700
C	-7.16828000	-2.02863800	-2.93913900	H	6.12098800	2.96611000	-2.17800700
H	-7.26679000	-1.78788300	-1.87611800	C	3.43842500	4.36882400	-3.92268100
H	-8.14351700	-1.86792000	-3.41497400	H	2.92307800	3.45100500	-4.22232300
H	-6.92736100	-3.10223600	-3.02185700	H	2.67496300	5.12218200	-3.70180300
C	6.82196700	0.22857100	0.98371200	H	4.03749600	4.72602800	-4.76821700
H	7.68353000	-0.41118900	1.17889600	C	2.18913100	4.86441400	1.92502100
C	6.39509600	0.82689400	2.33971500	H	2.56456300	5.86717600	1.70448900
H	5.54876600	1.51594300	2.23038300	C	0.69305300	4.97755600	2.26249800
H	6.10299700	0.04434000	3.04927700	H	0.25912200	4.00204000	2.51356200
H	7.22382400	1.38961200	2.78400900	H	0.54556500	5.63245200	3.12860000
C	7.26689700	1.34209700	0.01864400	H	0.12535400	5.38398200	1.42012100
H	8.10731200	1.90556500	0.43966700	C	2.97901700	4.31173500	3.12835400
H	7.57779400	0.93196000	-0.94800800	H	2.63002600	3.30805700	3.40310100
H	6.44828700	2.04818900	-0.16301000	H	4.04979500	4.24335900	2.90454500



H	2.85502800	4.95962100	4.00367500	C	0.67921800	-2.71756900	-1.13091500
C	-5.91987800	1.56835500	-2.65552800	C	1.31050400	-2.23101300	0.03081400
H	-6.40540100	1.24926300	-3.58224400	C	1.63344000	-3.11222700	1.07426600
C	-5.28962800	2.95224600	-2.89054200	C	1.34125000	-4.46893900	0.96244600
H	-4.92329500	3.40258800	-1.96015000	C	0.72894800	-4.97022800	-0.18256300
H	-4.44217300	2.89823500	-3.58372700	C	0.29114300	-1.87199200	-2.30174000
H	-6.03512200	3.63742800	-3.30878300	C	-0.81017200	-0.99035000	-2.27837100
C	-7.01036000	1.64235300	-1.56938300	C	0.98924200	-2.05798200	-3.51711200
H	-6.57255900	1.91902800	-0.60226100	C	-1.20482700	-0.33080100	-3.45391000
H	-7.76866400	2.39056300	-1.82838200	C	0.62496700	-1.34863800	-4.66622200
H	-7.51043700	0.67611300	-1.44810600	C	-0.48146000	-0.50438700	-4.62909700
C	-4.07934500	-3.22511100	-2.96142500	P	1.70288900	-0.43423000	0.20876600
H	-4.95207400	-3.33446300	-3.60656900	P	-1.60074200	-0.61478700	-0.65465700
C	-2.84422500	-3.55573400	-3.81993800	C	2.72023700	-0.05643000	-1.25043200
H	-1.91809400	-3.47770600	-3.24194200	C	2.56704400	1.13049800	-1.95726400
H	-2.91237900	-4.58023500	-4.20332300	C	3.70219300	-0.97639600	-1.64536400
H	-2.76479000	-2.87594300	-4.67603000	C	3.35666600	1.41105400	-3.08026800
C	-4.23391600	-4.22923700	-1.80245400	C	4.56626000	-0.69471000	-2.70201200
H	-3.36737300	-4.20714400	-1.13355600	C	4.38402200	0.51006900	-3.43409700
H	-5.12485400	-4.00553800	-1.20540100	C	2.81585400	-0.36378700	1.66612600
H	-4.32968900	-5.24900200	-2.19268000	C	4.20191000	-0.30662200	1.52237700
Rh	0.03671200	-1.01935800	0.80756300	C	2.27506500	-0.37399500	2.95636200
C	-0.92871900	-4.11975300	0.39278500	C	5.05156900	-0.26037200	2.63405800
C	-0.88746500	-5.42060900	0.91723200	C	3.08560800	-0.33280300	4.09042200
C	-0.29125000	-6.45532400	0.19344600	C	4.49296400	-0.28232900	3.93219000
C	0.27924900	-6.20917400	-1.05836200	C	-2.12408900	-2.20407900	0.06667400
C	0.25593800	-4.91457600	-1.57853900	C	-1.95792900	-2.44246200	1.43010400
C	-0.33920200	-3.87627800	-0.85998800	C	-2.85662600	-3.11226800	-0.70331500
H	-1.33222300	-5.62470400	1.88720000	C	-2.51807200	-3.56405200	2.04561200
H	-0.27661100	-7.45933600	0.60915400	C	-3.44644100	-4.23950300	-0.12440700
H	0.73897500	-7.01731400	-1.61936600	C	-3.26461000	-4.47507900	1.26173600
H	0.69259700	-4.70422200	-2.55146800	C	-3.19288900	0.26322600	-0.92492300
H	-0.35517800	-2.88282200	-1.29874900	C	-4.29362800	-0.13760100	-0.16218200
Se	-1.82748400	-2.69633300	1.39641100	C	-3.31982900	1.41328700	-1.72110700
C	3.98455100	-2.34063200	2.89198300	C	-5.49698900	0.57589700	-0.16331800
C	2.98299700	-1.38659700	2.85762300	C	-4.53677700	2.09320400	-1.82957500
C	1.61254400	-1.75422800	2.82287500	C	-5.62283700	1.70185000	-1.00396500
C	1.30800100	-3.13858200	2.82779500	H	2.12397400	-2.74743100	1.96757900
C	2.30695300	-4.10638100	2.82895700	H	1.59599500	-5.14199600	1.77545400
C	3.63067200	-3.68836800	2.84862700	H	-2.08819100	0.28974800	-3.47137400
H	5.02998700	-2.06205900	2.91419700	H	-0.78682100	0.01872300	-5.53055300
H	3.27083200	-0.34327000	2.86953300	H	1.82075100	1.84876300	-1.64867000
H	0.27098100	-3.44777900	2.83645900	H	3.79641500	-1.91102000	-1.10662400
H	2.07107000	-5.16434000	2.80656400	H	4.63981000	-0.27386900	0.53307000
F	4.60871100	-4.61255200	2.80285200	H	1.19864500	-0.39723300	3.08884100
C	0.53286500	-0.74104300	2.85575600	H	-1.37718600	-1.74850200	2.02690500
H	-0.37557500	-1.10854000	3.33237400	H	-2.98362700	-2.92797500	-1.76579100
C	0.89020300	0.63656600	3.35159800	H	-4.21786900	-1.01482800	0.46776800
H	1.08916200	0.59050300	4.43273200	H	-2.46577400	1.79228400	-2.26678300
H	1.77542400	1.05137300	2.86982600	N	-6.80874400	2.50312700	-1.07092300
H	0.06162300	1.32536400	3.20891400	C	-7.95594000	1.92492600	-1.75741300
				H	-7.62312500	1.45535900	-2.68867300
				H	-8.50606100	1.16733200	-1.17217000
				H	-8.66063500	2.72502800	-2.01344700
				C	-7.11853300	3.32002600	0.09509900
				H	-6.19483900	3.75351300	0.49126900
				H	-7.77770200	4.14274700	-0.20777900
				H	-7.61647600	2.77787900	0.91749400
				N	-3.81083600	-5.61630000	1.93127100
				N	5.28549900	-0.23995300	5.12419900
				N	5.28515700	0.74534600	-4.52548000

**37**  
B3LYP-D3 SCF energy: -4539.853959 a.u.  
B3LYP-D3 enthalpy: -4537.945371 a.u.  
B3LYP-D3 free energy: -4538.202518 a.u.  
M06 SCF energy in solution: -4538.822559 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.39894400	-4.09849700	-1.22320400

C	-3.28542500	-6.92646700	1.58198500	H	6.52625200	0.86260400	0.44955200
H	-3.44939700	-7.61491600	2.42049700	H	6.55739600	1.93183200	1.86059800
H	-3.73648300	-7.38318500	0.68392200	H	8.02246900	1.05492600	1.37037800
H	-2.20626600	-6.84716600	1.41593300	H	0.50333900	-6.02751700	-0.26158600
C	-5.22262100	-5.56082100	2.27727300	H	1.17820600	-1.46539000	-5.58965300
H	-5.45657300	-4.57345300	2.68908400	O	2.00449500	-2.96149500	-3.48609100
H	-5.90731200	-5.74598500	1.43011500	O	-0.22145900	-4.50772900	-2.36535000
H	-5.43604200	-6.30988100	3.04931900	C	2.67151100	-3.27032400	-4.70431600
C	5.82765500	1.05702300	5.50108200	H	3.23643800	-2.40669200	-5.07566600
H	6.11344500	1.03513200	6.55974100	H	3.36669200	-4.07637400	-4.46910700
H	6.71433100	1.36621500	4.91902700	H	1.96540300	-3.61027500	-5.47206100
H	5.05711300	1.82378500	5.37276700	C	0.04192000	-5.83075000	-2.82537200
C	6.12138200	-1.39188600	5.42573800	H	-0.46358500	-6.58695300	-2.21445900
H	7.08588200	-1.41861900	4.88952700	H	-0.35604900	-5.87782700	-3.84059100
H	6.34059300	-1.40301100	6.50071000	H	1.12068700	-6.02773300	-2.83850600
H	5.57440200	-2.30845700	5.18358900	C	-4.27600300	-5.16169500	-1.01224700
C	4.78193800	0.43597100	-5.85394000	H	-4.77439000	-5.89396700	-0.37543100
H	4.06101100	1.17521200	-6.24792900	C	-5.38380700	-4.39525900	-1.75963900
H	5.62229200	0.37918000	-6.55621600	H	-4.97116400	-3.67572400	-2.47584400
H	4.28665300	-0.54094200	-5.84142800	H	-6.01297300	-5.09494700	-2.32115000
C	6.15834000	1.91080700	-4.45535500	H	-6.02308800	-3.84379900	-1.06199000
H	6.45217700	2.08180200	-3.41604600	C	-3.37499600	-5.93379500	-1.99278700
H	7.06684700	1.71343900	-5.03878400	H	-2.80913400	-5.24576800	-2.62992200
H	5.71383800	2.84440200	-4.83879700	H	-2.65412100	-6.55401700	-1.44912400
C	-6.60218600	0.09333600	0.77037300	H	-3.97359100	-6.58962500	-2.63524500
H	-7.48764600	0.70889500	0.60866500	C	-2.30089300	-3.76889100	3.53826500
C	-6.18163300	0.26627500	2.24353100	H	-2.92875700	-4.61145700	3.83906300
H	-5.31572400	-0.36301400	2.48448200	C	-0.83615700	-4.14571100	3.82881200
H	-5.90983200	1.30525600	2.45991100	H	-0.15060200	-3.35267700	3.50738900
H	-7.00007700	-0.02123400	2.91310500	H	-0.68498700	-4.30963400	4.90197600
C	-7.00280900	-1.36552300	0.47777500	H	-0.55445800	-5.06080700	3.29681700
H	-7.84410100	-1.66198900	1.11424300	C	-2.72389800	-2.53392900	4.35541100
H	-7.30282200	-1.49205600	-0.56824900	H	-2.08239900	-1.66748800	4.14869400
H	-6.17699700	-2.05921500	0.67605300	H	-3.75829300	-2.24448700	4.13565700
C	-4.70793400	3.22896300	-2.83514300	H	-2.64945800	-2.74418800	5.42813000
H	-5.77315300	3.25606800	-3.08188300	C	5.71380000	-1.64672500	-3.03083600
C	-4.36224800	4.60068700	-2.22848800	H	5.77528500	-1.72566200	-4.12235100
H	-3.30758400	4.65171800	-1.93773600	C	5.53331600	-3.05995900	-2.45177300
H	-4.54834700	5.39894700	-2.95656800	H	5.67021800	-3.06716500	-1.36301000
H	-4.97821100	4.80264400	-1.34654700	H	4.54273900	-3.47404800	-2.66138400
C	-3.93228700	2.99406700	-4.14252400	H	6.28794000	-3.73224800	-2.87362900
H	-2.84636900	3.06111200	-4.00448800	C	7.05500100	-1.06347100	-2.53780600
H	-4.15610900	2.00951600	-4.56905000	H	7.03515800	-0.92254400	-1.45015300
H	-4.20731400	3.75475400	-4.88114800	H	7.87841800	-1.74805200	-2.77281500
C	2.42411700	-0.30357700	5.46073000	H	7.26874800	-0.10124200	-3.00606600
H	3.22719100	-0.36279400	6.20024500	C	3.02970000	2.66798200	-3.88002900
C	1.48314600	-1.50282500	5.67538200	H	3.72581300	2.73963800	-4.71606900
H	0.62302400	-1.47473100	4.99453500	C	1.61649200	2.56705800	-4.48768300
H	2.00462000	-2.45313600	5.51436200	H	0.85122800	2.50147900	-3.70788700
H	1.08911100	-1.49971600	6.69809000	H	1.39974300	3.45213000	-5.09719700
C	1.67509100	1.02771100	5.66902700	H	1.52277700	1.67726200	-5.11949300
H	1.23445400	1.07026400	6.67188800	C	3.18723800	3.94580200	-3.03368800
H	2.34835300	1.88406700	5.55289800	H	2.48896600	3.96367500	-2.19039800
H	0.86499000	1.14489700	4.93701200	H	4.20317500	4.02752500	-2.63203000
C	6.55357400	-0.19565300	2.37654700	H	2.98866500	4.83308600	-3.64558400
H	7.06011600	-0.03381400	3.32906700	Rh	-0.20666200	0.80246800	0.60055900
C	7.06335000	-1.53048600	1.79861700	C	0.64564100	3.82260600	0.15407500
H	6.58715300	-1.74730400	0.83441600	C	0.82656400	5.21035100	0.24935200
H	8.14671200	-1.49348900	1.63671900	C	0.30557500	6.05956500	-0.72536500
H	6.84583800	-2.36531400	2.47373800	C	-0.41991500	5.54671800	-1.80586300
C	6.93259800	0.98378100	1.46051600	C	-0.60872700	4.16893700	-1.91041900

C	-0.06891300	3.31689200	-0.94569000
H	1.36536300	5.62350600	1.09629000
H	0.45865700	7.13152000	-0.63531200
H	-0.82118700	6.21167700	-2.56472300
H	-1.14121300	3.75447400	-2.76032100
H	-0.16586700	2.23599300	-1.11497600
Se	1.36659700	2.61275700	1.49666000
C	-1.01534100	5.50674300	3.28955300
C	-1.28184100	4.17338200	3.00093900
C	-2.09792200	3.82365500	1.90474800
C	-2.64991300	4.85585500	1.12114500
C	-2.39980000	6.19179600	1.40285700
C	-1.57339900	6.49462200	2.48157400
H	-0.38397000	5.79407400	4.12325200
H	-0.84881200	3.40314400	3.62715400
H	-3.27866200	4.59811200	0.27696700
H	-2.81277800	6.99297900	0.80026300
F	-1.30602700	7.78350800	2.75372600
C	-2.43139700	2.45125700	1.56005100
H	-3.09777000	2.33882300	0.70910300
C	-2.08551300	1.31505300	2.23538900
H	-1.52318100	1.35307400	3.16316100
H	-2.61468800	0.39166400	2.03087300
H	-0.24657000	-0.17861700	1.76063000

### 38-ts-S

B3LYP-D3 SCF energy: -4539.828928 a.u.

B3LYP-D3 enthalpy: -4537.923725 a.u.

B3LYP-D3 free energy: -4538.169015 a.u.

M06 SCF energy in solution: -4538.804658 a.u.

Imaginary frequency: -254.87 cm<sup>-1</sup>

#### Cartesian coordinates

ATOM	X	Y	Z
C	-0.38556700	2.19918100	3.52823600
C	0.00414800	1.23505400	2.57248000
C	0.70728100	1.65948500	1.43099000
C	0.97201600	3.02531600	1.24195200
C	0.57315900	3.95854500	2.19399200
C	-0.09596100	3.55294300	3.34538100
C	-0.36641400	-0.18277200	2.86865900
C	-1.37433000	-0.89516700	2.18121000
C	0.25631100	-0.78862900	3.98596000
C	-1.78296700	-2.15091000	2.66321500
C	-0.13845700	-2.05203200	4.43370200
C	-1.17793700	-2.71057600	3.78230800
P	1.30173400	0.42495000	0.18994000
P	-1.95150100	-0.30543500	0.52518600
C	2.33316300	-0.68884900	1.21306600
C	2.10730900	-2.06272600	1.14690300
C	3.33742200	-0.21064600	2.06124200
C	2.90262400	-2.97873300	1.84346800
C	4.19103600	-1.08683400	2.73301200
C	3.98716800	-2.48647100	2.60357000
C	2.32568800	1.46804600	-0.91741900
C	3.54527100	2.01467300	-0.52164000
C	1.79892600	1.82390100	-2.16302200
C	4.23196600	2.92932400	-1.32833700
C	2.47335900	2.69298900	-3.02183800
C	3.68767800	3.27851800	-2.58538500
C	-2.36918100	1.46413400	0.68861700

C	-2.04547300	2.34830300	-0.33908100
C	-3.20030500	1.88945800	1.72809400
C	-2.54900800	3.65240100	-0.35323700
C	-3.73283400	3.18112000	1.74607100
C	-3.39924400	4.07287900	0.69688500
C	-3.62580200	-0.99100500	0.11980100
C	-4.54515300	-0.11621000	-0.47422400
C	-3.97179900	-2.35086000	0.16993500
C	-5.78108400	-0.54537300	-0.96770300
C	-5.21129200	-2.81790300	-0.27938500
C	-6.13502100	-1.90639400	-0.84811700
H	1.49500000	3.36546100	0.35935000
H	0.78899500	5.01164800	2.03770300
H	-2.59759100	-2.68248100	2.19759600
H	-1.51274600	-3.67716100	4.14733500
H	1.31928000	-2.44338700	0.50520600
H	3.45696700	0.85686400	2.19419100
H	3.97555200	1.74254700	0.43244000
H	0.87044000	1.37161900	-2.48297900
H	-1.38368600	2.01887900	-1.13452500
H	-3.44536200	1.19828300	2.52929400
H	-4.30439900	0.93391200	-0.56521000
H	-3.26737400	-3.08431400	0.54244600
N	-7.39348500	-2.42658600	-1.28969400
C	-8.57481200	-2.03592000	-0.53373100
H	-8.34868300	-2.07744900	0.53630300
H	-8.95696200	-1.02546600	-0.76179400
H	-9.38161700	-2.75017500	-0.73725700
C	-7.57201900	-2.58357000	-2.72555500
H	-6.67228000	-3.03668700	-3.15486500
H	-8.41347900	-3.26161800	-2.91101800
H	-7.77207700	-1.64337500	-3.26952600
N	-3.88184200	5.42038300	0.64661600
N	4.32082100	4.19927600	-3.48520100
N	4.92889100	-3.34260400	3.26493600
C	-3.37390400	6.35379500	1.63962600
H	-3.47082000	7.37714700	1.25585500
H	-3.88598600	6.31420000	2.61701200
H	-2.31082100	6.15389600	1.80784500
C	-5.26080300	5.61130700	0.22601700
H	-5.46694900	4.97356900	-0.64017600
H	-6.01310100	5.38134500	1.00172500
H	-5.40442000	6.65499200	-0.07889500
C	5.44623600	3.68440600	-4.24907200
H	5.67001500	4.37613200	-5.06984800
H	6.37115300	3.54632800	-3.66056700
H	5.17930700	2.71686800	-4.68499700
C	4.42630700	5.59441700	-3.08302300
H	5.30436100	5.83126100	-2.45878900
H	4.48001800	6.22361500	-3.98085200
H	3.52949800	5.87912100	-2.52448800
C	4.51549600	-3.89570300	4.54419100
H	3.75268400	-4.69199500	4.46924300
H	5.38947800	-4.31597200	5.05565600
H	4.10979700	-3.09851600	5.17653300
C	5.74279000	-4.22762900	2.44114600
H	5.98837000	-3.72358000	1.50177200
H	6.68180600	-4.44283100	2.96671900
H	5.27098900	-5.19274100	2.19321000
C	-6.67282700	0.50072300	-1.63036800
H	-7.59499700	0.01675500	-1.95383600

C	-5.99683400	1.08141300	-2.88864300	H	-2.77256900	5.48555700	-1.38120300
H	-5.07682200	1.62245600	-2.63391800	C	-0.67901900	5.03573700	-1.30090900
H	-5.73877400	0.28892200	-3.60047000	H	0.00564800	4.18545600	-1.40310800
H	-6.66735100	1.78657700	-3.39270000	H	-0.40560900	5.78135700	-2.05583900
C	-7.06072400	1.62223200	-0.64785300	H	-0.51988500	5.47608700	-0.31050900
H	-7.74519300	2.33042900	-1.12857800	C	-2.38460900	3.98276500	-2.86681000
H	-7.55670300	1.21568100	0.24024300	H	-1.74238800	3.11146600	-3.04671700
H	-6.18038700	2.18358700	-0.31288100	H	-3.42667900	3.66271100	-2.98538800
C	-5.54354900	-4.29716500	-0.13910800	H	-2.16270000	4.71497200	-3.65104600
H	-6.50838000	-4.44536500	-0.63063700	C	5.37641800	-0.54528500	3.52566300
C	-4.50808900	-5.19930500	-0.83335100	H	5.51763800	-1.19241500	4.39768400
H	-3.53436200	-5.16848700	-0.33039800	C	5.18381500	0.89595200	4.02458200
H	-4.84537100	-6.24167600	-0.82042900	H	5.22961300	1.62151500	3.20269200
H	-4.35267100	-4.90496000	-1.87747500	H	4.22328900	1.03169400	4.53342800
C	-5.70451300	-4.68116800	1.34392800	H	5.98432300	1.15654500	4.72490000
H	-4.76710800	-4.53523500	1.89670400	C	6.65987100	-0.63793500	2.67358200
H	-6.47616200	-4.07364100	1.82922900	H	6.54935800	-0.05717700	1.74990900
H	-5.98877300	-5.73523600	1.44017900	H	7.51965800	-0.24112800	3.22597700
C	1.92679000	2.98366700	-4.41854500	H	6.87784200	-1.67389100	2.40287500
H	2.79002200	3.01223100	-5.09265300	C	2.59894800	-4.46498700	1.67270700
C	1.24889000	4.36477200	-4.49718600	H	3.22393400	-5.02805600	2.36804700
H	0.36009800	4.39353400	-3.85991400	C	1.13712000	-4.79986400	2.02024400
H	1.92834400	5.15881000	-4.18052800	H	0.43393700	-4.29740900	1.34640600
H	0.93309900	4.57567300	-5.52581900	H	0.96875900	-5.87995400	1.93454900
C	0.96428700	1.90155800	-4.93851200	H	0.89118900	-4.49042400	3.04027600
H	0.74134300	2.08224300	-5.99553200	C	2.94091400	-4.92835600	0.24174000
H	1.38035700	0.89242100	-4.84124700	H	2.34099600	-4.39146900	-0.50213100
H	0.00660500	1.92170200	-4.40123800	H	3.99564400	-4.75056300	0.00702500
C	5.50325900	3.56466300	-0.77338000	H	2.74486900	-6.00108200	0.12692000
H	6.01879500	4.07294100	-1.59008300	Rh	-0.23178400	-0.88917900	-1.03169000
C	5.13712000	4.62244900	0.28831600	C	3.52784500	-1.14305000	-2.30442900
H	4.62071000	4.15319200	1.13527100	C	4.06892000	-0.34813100	-3.32524900
H	6.03760500	5.11579300	0.67209900	C	5.42550300	-0.02298400	-3.31947900
H	4.47393800	5.39100100	-0.12235100	C	6.25705000	-0.47997600	-2.29427100
C	6.49057600	2.53836800	-0.19126600	C	5.72087600	-1.26182900	-1.26936600
H	6.09515600	2.05657400	0.71055300	C	4.36716400	-1.59951200	-1.27792700
H	6.71732000	1.75150500	-0.91486700	H	3.43173100	0.00366900	-4.12904900
H	7.42463200	3.03678200	0.09123700	H	5.83792600	0.57814700	-4.12434700
H	-0.40401600	4.28302200	4.08488300	H	7.31609400	-0.23689400	-2.30116600
H	0.33858900	-2.51437900	5.28881700	H	6.35689900	-1.62189000	-0.46470500
O	1.23578200	-0.05537200	4.57665000	H	3.97142400	-2.23177100	-0.49590000
O	-1.07634200	1.72963000	4.60714400	Se	1.70111400	-1.82947400	-2.49095600
C	1.94932600	-0.62635300	5.66523100	C	0.15848700	-5.01909100	-3.98925100
H	2.46873200	-1.54155100	5.35653700	C	-0.51743900	-3.81873000	-3.81303900
H	2.68494700	0.12119700	5.96352700	C	-1.07479700	-3.48596500	-2.56254100
H	1.28708300	-0.84282700	6.51321000	C	-0.96769400	-4.41520900	-1.50246600
C	-0.93326100	2.42544700	5.84296000	C	-0.27962300	-5.60838000	-1.65997000
H	-1.49353100	3.36756700	5.84991400	C	0.28350500	-5.88681300	-2.90504200
H	-1.34653200	1.76357000	6.60640700	H	0.59699700	-5.29288300	-4.94233200
H	0.12430800	2.62288400	6.05560400	H	-0.60860800	-3.13262700	-4.64773900
C	-4.64999300	3.57554500	2.89946600	H	-1.39015700	-4.16392500	-0.53456300
H	-5.05546100	4.56681100	2.69358700	H	-0.16212100	-6.31609900	-0.84717900
C	-5.85011300	2.61984700	3.03485200	F	0.95314000	-7.03564400	-3.06790600
H	-5.53297200	1.60203500	3.28908000	C	-1.71685500	-2.21286700	-2.27897900
H	-6.52018400	2.96553800	3.83008900	H	-2.54406500	-2.27211100	-1.58393600
H	-6.42247300	2.56925500	2.10305000	C	-1.59698700	-0.99019800	-3.00457300
C	-3.86026300	3.66068100	4.21808200	H	-1.02387400	-0.98771700	-3.93080400
H	-3.42064100	2.69088800	4.47170300	H	-2.48949700	-0.36114400	-3.01230900
H	-3.04319600	4.38641100	4.13609800	H	-0.85698100	-0.08006400	-2.33063700
H	-4.51485600	3.97108100	5.04064100				
C	-2.14520500	4.59567200	-1.47595800				

39-S

B3LYP-D3 SCF energy: -4539.869343 a.u.  
 B3LYP-D3 enthalpy: -4537.955850 a.u.  
 B3LYP-D3 free energy: -4538.205307 a.u.  
 M06 SCF energy in solution: -4538.844233 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.19499800	-4.18487200	0.02465700
C	-0.26277800	-2.87723000	0.31512100
C	-1.05290800	-2.21987700	-0.65379000
C	-1.35936800	-2.84887500	-1.87127400
C	-0.89864800	-4.13563900	-2.12677600
C	-0.12365100	-4.80773100	-1.18535800
C	0.11429200	-2.29101300	1.64200100
C	0.97953200	-1.18446600	1.77722300
C	-0.35460700	-2.92401700	2.81692100
C	1.38020300	-0.74576700	3.04659000
C	0.03594800	-2.46838800	4.08058500
C	0.91136200	-1.39209800	4.18581400
P	-1.67215900	-0.50950100	-0.37200300
P	1.60934600	-0.36608600	0.24667500
C	-2.34560700	-0.55115600	1.32747200
C	-2.10016600	0.46416200	2.24496100
C	-3.17191200	-1.62339800	1.69259100
C	-2.64442400	0.42712900	3.53456800
C	-3.78192200	-1.67060800	2.94512600
C	-3.50119000	-0.63994800	3.88224000
C	-3.14075700	-0.30559300	-1.45695800
C	-4.44167700	-0.38120800	-0.95459400
C	-2.96452900	-0.01809400	-2.81406800
C	-5.55720900	-0.19862500	-1.77884700
C	-4.05029100	0.15603300	-3.67385600
C	-5.36498100	0.05692600	-3.15515500
C	2.48487400	-1.78571200	-0.54075500
C	2.43596300	-2.09313900	-1.90249000
C	3.32917400	-2.52817500	0.29124000
C	3.22501000	-3.11656100	-2.44017100
C	4.14431800	-3.54841300	-0.20547800
C	4.07516200	-3.85850400	-1.58213700
C	3.00844400	0.72235600	0.72664700
C	4.24478600	0.57932200	0.09203600
C	2.81472900	1.81648400	1.58551500
C	5.28628500	1.49454300	0.29276000
C	3.84782400	2.71657100	1.85978200
C	5.08748800	2.57234800	1.18095800
H	-1.98466200	-2.35064900	-2.60203900
H	-1.15045500	-4.62472700	-3.06317200
H	2.07765200	0.07387500	3.15320700
H	1.23275100	-1.05711200	5.16772800
H	-1.47409900	1.29836100	1.95680200
H	-3.34054200	-2.42363100	0.98265800
H	-4.60430000	-0.56018200	0.09899900
H	-1.96387400	0.08195800	-3.20689900
H	1.76396300	-1.55107900	-2.55044700
H	3.36951000	-2.29534400	1.35014700
H	4.40608800	-0.24686900	-0.58861400
H	1.84266900	1.96952600	2.04102000
N	6.09389300	3.55527800	1.45455100
C	7.15022100	3.15558900	2.37373000
H	6.71224300	2.63540400	3.23162800
H	7.91032600	2.49118800	1.92493300

H	7.66390800	4.05064500	2.74437300
C	6.51482300	4.43379300	0.37198400
H	5.65809400	4.65875800	-0.27033600
H	6.87765000	5.37874000	0.79596000
H	7.31627800	4.02756900	-0.26778900
N	4.84477300	-4.90871600	-2.18254900
N	-6.44837800	0.24403900	-4.07213900
N	-4.10483000	-0.76492300	5.17759600
C	4.57904200	-6.27607600	-1.76388600
H	4.88294500	-6.96253000	-2.56433400
H	5.09899400	-6.58973100	-0.84246800
H	3.50343200	-6.40111300	-1.60288200
C	6.23740700	-4.60308400	-2.47636800
H	6.30406200	-3.60961200	-2.93198900
H	6.90016200	-4.61575400	-1.59257500
H	6.62496200	-5.33406800	-3.19620200
C	-7.07955500	1.55537600	-4.07652700
H	-7.62948800	1.68978400	-5.01599100
H	-7.78812200	1.71778500	-3.24445100
H	-6.30995900	2.33115900	-4.01835300
C	-7.33162200	-0.88209900	-4.33377300
H	-8.14478800	-1.01333900	-3.59946800
H	-7.79580900	-0.75066400	-5.31944400
H	-6.74416700	-1.80491400	-4.35796700
C	-3.24624500	-1.30143100	6.22064600
H	-2.49834800	-0.58250300	6.60332700
H	-3.86198100	-1.62850500	7.06724000
H	-2.70432700	-2.17230500	5.83585600
C	-5.04581800	0.25703100	5.61794600
H	-5.59902500	0.63765700	4.75499300
H	-5.76655000	-0.19296400	6.31317500
H	-4.58491600	1.11798400	6.12998900
C	6.57441500	1.29840700	-0.49958300
H	7.32464800	1.99033100	-0.11526500
C	6.33986100	1.63558500	-1.98577800
H	5.60437200	0.95190200	-2.42789600
H	5.96360100	2.65710700	-2.10819000
H	7.27092900	1.54285400	-2.55623500
C	7.15397200	-0.11846300	-0.34180100
H	8.11729200	-0.19021100	-0.85899000
H	7.31255600	-0.36396600	0.71355500
H	6.49306400	-0.88089400	-0.76990000
C	3.65342000	3.85500900	2.85736400
H	4.60367300	3.97299100	3.38852300
C	3.37598900	5.18674100	2.13307900
H	2.47191600	5.11915800	1.52164900
H	3.23135000	5.99484800	2.85996800
H	4.21550300	5.46195200	1.49008100
C	2.56655000	3.56940600	3.90525200
H	1.56367300	3.55147200	3.46576400
H	2.72846100	2.60898600	4.40856700
H	2.57013200	4.35542500	4.66805000
C	-3.79198200	0.48401300	-5.13714000
H	-4.75928200	0.43515500	-5.64445300
C	-2.85090300	-0.53366600	-5.80629000
H	-1.84275600	-0.50839600	-5.37413400
H	-3.23497200	-1.55470400	-5.70215000
H	-2.75295500	-0.31504100	-6.87568000
C	-3.25329000	1.92052900	-5.28366200
H	-3.10043900	2.17182200	-6.33960800
H	-3.94680500	2.65073300	-4.85314800

H	-2.29347600	2.03804700	-4.76488900
C	-6.93812700	-0.29089600	-1.13726800
H	-7.67809900	0.04675800	-1.86477900
C	-7.26920500	-1.75177800	-0.77446500
H	-6.54567000	-2.14599000	-0.05080500
H	-8.26682400	-1.82423700	-0.32629100
H	-7.24247200	-2.39817100	-1.65820200
C	-7.07046200	0.62745600	0.09281700
H	-6.42060100	0.30769400	0.91561700
H	-6.81083000	1.66199100	-0.15590500
H	-8.10140700	0.61017800	0.46403300
H	0.23853900	-5.80543300	-1.40151400
H	-0.32822900	-2.95090300	4.97881500
O	-1.19012700	-3.98072100	2.63533800
O	0.96155100	-4.77691100	0.97832000
C	-1.52121500	-4.78448600	3.76197800
H	-2.15336400	-4.23707100	4.47247800
H	-2.08258700	-5.63274900	3.36872500
H	-0.61905500	-5.14620900	4.27081200
C	1.04671800	-6.19678600	0.97961500
H	1.67531200	-6.56705500	0.15971400
H	1.51024700	-6.46734100	1.92892200
H	0.05015300	-6.65000200	0.91007500
C	5.07850800	-4.26540800	0.76710900
H	5.74492000	-4.91008000	0.19180700
C	5.97779800	-3.27836000	1.53448000
H	5.39736400	-2.60688900	2.17729400
H	6.67586200	-3.82774600	2.17608500
H	6.56147000	-2.66102300	0.84568100
C	4.28956700	-5.16227600	1.73853200
H	3.52540400	-4.58925500	2.27565700
H	3.78435600	-5.96735900	1.19808700
H	4.96232100	-5.61769300	2.47428300
C	3.16899500	-3.44849000	-3.92805100
H	4.16792400	-3.78896700	-4.21565200
C	2.20230700	-4.61947400	-4.18962100
H	1.18100900	-4.34151100	-3.90840800
H	2.20496700	-4.89100500	-5.25175000
H	2.48931600	-5.50231700	-3.61126700
C	2.80596800	-2.24994200	-4.81787900
H	1.75279500	-1.96697600	-4.71214700
H	3.41933300	-1.37096600	-4.58645500
H	2.96421200	-2.50702500	-5.87071500
C	-4.76401200	-2.79118400	3.28357900
H	-4.53083300	-3.13684200	4.29798300
C	-4.68592800	-3.99609100	2.33130900
H	-5.09651900	-3.75117600	1.34352700
H	-3.66096100	-4.34650900	2.18565400
H	-5.28417600	-4.82207700	2.73057900
C	-6.21291000	-2.25957500	3.30412800
H	-6.48728600	-1.85532600	2.32258800
H	-6.91224200	-3.07028800	3.53996600
H	-6.34199800	-1.47311800	4.04867200
C	-2.31712100	1.57726600	4.48282200
H	-2.70172000	1.32895200	5.47272100
C	-0.80226500	1.79304400	4.64681100
H	-0.31832200	2.04289100	3.69681200
H	-0.61081000	2.61916400	5.34100100
H	-0.31530100	0.89384300	5.03391200
C	-3.01311500	2.87232800	4.01785100
H	-2.65124500	3.18527500	3.03194100

H	-4.09714700	2.73410800	3.94674400
H	-2.81733200	3.68880200	4.72266900
Rh	-0.02012200	1.07475300	-0.70725700
C	-1.26305500	4.26513200	0.04942200
C	-1.48982300	5.49108300	-0.59409200
C	-1.02450000	6.68165600	-0.03371000
C	-0.34129500	6.66560500	1.18396500
C	-0.12571300	5.45001300	1.83648600
C	-0.57197900	4.25502700	1.26908600
H	-2.03346100	5.51081700	-1.53359500
H	-1.19782200	7.62217300	-0.54933300
H	0.01282000	7.59261200	1.62531000
H	0.38693400	5.43234700	2.79319200
H	-0.39747700	3.31517500	1.78258300
Se	-2.03907100	2.64157000	-0.71556100
C	0.57886800	4.80617600	-2.88902200
C	0.42988200	3.43920800	-3.01408800
C	1.29956400	2.53813500	-2.34321000
C	2.33119000	3.09205400	-1.54631200
C	2.47171300	4.46834000	-1.38938000
C	1.58751300	5.30361500	-2.05657800
H	-0.08089100	5.50138700	-3.39480700
H	-0.38475200	3.05733000	-3.61580500
H	3.04716800	2.43561200	-1.07294600
H	3.24663600	4.89236000	-0.76320600
F	1.69556600	6.62853800	-1.90461600
C	1.17222600	1.07082100	-2.46999500
H	2.12342800	0.57718900	-2.27194000
C	0.49798200	0.48564600	-3.68889700
H	1.18964100	0.50734500	-4.54325900
H	0.21343500	-0.55685400	-3.52003300
H	-0.39919500	1.03310400	-3.97602000

#### cod

B3LYP-D3 SCF energy: -312.040162 a.u.

B3LYP-D3 enthalpy: -311.850482 a.u.

B3LYP-D3 free energy: -311.890286 a.u.

M06 SCF energy in solution: -311.846102 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z
C	-1.19541800	-1.24663100	-0.49962300
H	-1.79230800	-1.85358400	-1.18267300
C	0.03198700	-1.70210300	-0.22051200
H	0.33213300	-2.62325200	-0.72112000
C	1.09433300	-1.09412500	0.66984300
H	1.79155300	-1.88675900	0.96922000
H	0.66701200	-0.71328800	1.60031000
C	1.92102400	0.01210400	-0.02149200
H	2.73306000	0.32165100	0.65633400
H	2.42914000	-0.43025400	-0.89138800
C	1.19546400	1.24661000	-0.49955300
H	1.79247700	1.85362600	-1.18245200
C	-0.03193600	1.70214000	-0.22052300
H	-0.33195700	2.62331600	-0.72114300
C	-1.09440700	1.09418400	0.66971700
H	-1.79173100	1.88681700	0.96885700
H	-0.66721400	0.71356300	1.60034000
C	-1.92103100	-0.01220000	-0.02144900
H	-2.73292000	-0.32177500	0.65653800
H	-2.42934400	0.43005900	-0.89128000

**2-O**

B3LYP-D3 SCF energy: -307.465513 a.u.

B3LYP-D3 enthalpy: -307.354223 a.u.

B3LYP-D3 free energy: -307.389638 a.u.

M06 SCF energy in solution: -307.328761 a.u.

## Cartesian coordinates

ATOM	X	Y	Z
C	0.94151500	-0.02306000	0.00009300
C	0.26304900	1.20074300	0.00013300
C	-1.13329800	1.21914200	-0.00011900
C	-1.85804900	0.02662600	-0.00005200
C	-1.17093300	-1.19173800	0.00012100
C	0.22181900	-1.22375100	-0.00003600
H	0.82503400	2.13331500	0.00027400
H	-1.65210600	2.17415500	-0.00014300
H	-2.94386000	0.04452500	-0.00012800
H	-1.72414700	-2.12728800	0.00010100
H	0.76965600	-2.16075900	-0.00019500
H	2.68299100	0.78221000	-0.00003800
O	2.30722800	-0.11174200	-0.00008900

**3-O**

B3LYP-D3 SCF energy: -4504.443309 a.u.

B3LYP-D3 enthalpy: -4502.551580 a.u.

B3LYP-D3 free energy: -4502.799378 a.u.

M06 SCF energy in solution: -4503.327286 a.u.

## Cartesian coordinates

ATOM	X	Y	Z
C	-0.44126100	4.20437300	0.60901000
C	0.09527500	2.90220400	0.72873500
C	0.89153400	2.40098900	-0.32191800
C	1.16848400	3.20532600	-1.43781900
C	0.65158600	4.49508000	-1.51917500
C	-0.16095600	4.99825100	-0.50666900
C	-0.18399500	2.16375300	2.00166900
C	-1.01297300	1.02727600	2.07514200
C	0.36356200	2.67872600	3.20057300
C	-1.31076400	0.44624700	3.31768800
C	0.08976300	2.07297400	4.43072400
C	-0.75887700	0.96979300	4.48181900
P	1.46867200	0.64480800	-0.29142800
P	-1.60028600	0.25133300	0.51230800
C	2.40314500	0.51150400	1.26733800
C	2.25766000	-0.61841700	2.06723500
C	3.24629200	1.55103400	1.67699600
C	2.89918000	-0.70957900	3.30961500
C	3.93723800	1.48147000	2.88545100
C	3.74253500	0.34768700	3.71981000
C	2.73099900	0.51390400	-1.62312900
C	4.09144300	0.35531400	-1.36925400
C	2.27940400	0.40866700	-2.94957200
C	5.00475600	0.08710300	-2.40069700
C	3.14741000	0.10405300	-4.00058700
C	4.52783700	-0.08157000	-3.72127500
C	-2.57811500	1.52920800	-0.34412700
C	-2.40267100	1.67922900	-1.72344400
C	-3.51662100	2.31674400	0.32273100
C	-3.12619900	2.62915100	-2.44379000

C	-4.29384700	3.25178000	-0.37157000
C	-4.06510800	3.43771300	-1.75529200
C	-2.79117900	-1.06403300	0.99562300
C	-4.10687000	-1.08054700	0.52286700
C	-2.31116700	-2.18810400	1.68699100
C	-4.95196100	-2.17999900	0.74780200
C	-3.14102800	-3.26661900	1.99372400
C	-4.48733400	-3.25502300	1.53947300
H	1.79688800	2.83539700	-2.23858900
H	0.87788500	5.11422600	-2.38229400
H	-1.97443100	-0.40590200	3.38348300
H	-0.99013000	0.51572100	5.44126200
H	1.60535500	-1.41746400	1.72753600
H	3.34275000	2.42792400	1.04738500
H	4.45441100	0.42514400	-0.35039800
H	1.21881700	0.53891200	-3.15564600
H	-1.66509600	1.05611900	-2.21823200
H	-3.65165300	2.19713900	1.39409200
H	-4.48064100	-0.23274200	-0.04178700
H	-1.27183000	-2.21101700	2.00093500
N	-5.31551000	-4.36008300	1.90592200
C	-6.52315000	-4.09953900	2.67646900
H	-6.33857700	-3.26886500	3.36370400
H	-7.41488700	-3.85435400	2.07586600
H	-6.76193300	-4.98736000	3.27528800
C	-5.38353300	-5.46807100	0.96629100
H	-4.37185800	-5.74878000	0.65287100
H	-5.83309000	-6.33614700	1.46184000
H	-5.97346500	-5.25136800	0.05774700
N	-4.74142100	4.43865500	-2.52664500
N	5.37165300	-0.44649300	-4.81536700
N	4.40627700	0.36945300	4.99200600
C	-4.52787700	5.83224100	-2.16950800
H	-4.69311100	6.45979500	-3.05477700
H	-5.18435200	6.21199700	-1.36743600
H	-3.49001300	5.96541000	-1.84819500
C	-6.07498400	4.10975600	-3.00560100
H	-6.08232500	3.08479900	-3.39045800
H	-6.86386100	4.18848000	-2.23565500
H	-6.34253800	4.78415300	-3.82825700
C	6.04589400	-1.73521100	-4.77349400
H	6.24561200	-2.06729700	-5.79999500
H	7.00643700	-1.73950100	-4.23122800
H	5.38771900	-2.47283900	-4.30361100
C	6.09863100	0.63239900	-5.46759000
H	6.98338500	0.98113800	-4.90540500
H	6.43804500	0.29645300	-6.45456100
H	5.43109900	1.48820000	-5.61129000
C	3.59178500	0.79941000	6.11684100
H	2.88513400	0.03135600	6.48177400
H	4.24331900	1.08099100	6.95317300
H	3.00570000	1.67845800	5.82808800
C	5.39403000	-0.65339900	5.30199300
H	5.93322500	-0.92651700	4.39068300
H	6.12116800	-0.24528800	6.01628800
H	4.98058500	-1.57673800	5.74118700
C	-6.32285900	-2.17499200	0.08138400
H	-6.79613600	-3.14095800	0.26427200
C	-6.18871900	-2.02993600	-1.44818800
H	-5.77489400	-1.05449300	-1.72954000
H	-5.53566200	-2.80687300	-1.86310800

H	-7.17106700	-2.12125600	-1.92474400	H	-1.69449100	4.13908100	-5.22345200
C	-7.23527300	-1.08222500	0.66820400	H	-2.20537200	4.89534100	-3.70069300
H	-8.22232100	-1.10891300	0.19310100	C	-2.39395700	1.54737500	-4.64779900
H	-7.37111100	-1.21547400	1.74679800	H	-1.37916200	1.25992700	-4.34340400
H	-6.81124000	-0.08446100	0.50531500	H	-3.05671800	0.69787300	-4.44666200
C	-2.58173500	-4.42142600	2.81321900	H	-2.36949400	1.71366600	-5.73031100
H	-3.36412100	-5.18154100	2.87521700	C	4.90130500	2.59364000	3.29074100
C	-1.34423700	-5.05209200	2.14703400	H	4.74710500	2.78967900	4.35813100
H	-0.50698300	-4.34708000	2.09118400	C	4.68956600	3.90877300	2.52316800
H	-1.00551700	-5.91956700	2.72506200	H	5.02073400	3.82191300	1.48073600
H	-1.56464600	-5.38480600	1.12637600	H	3.64019100	4.21563200	2.51236700
C	-2.27020300	-3.96005900	4.24980400	H	5.28310900	4.70634800	2.98298100
H	-1.50617200	-3.17436700	4.25900700	C	6.36254500	2.12959000	3.11905500
H	-3.16833900	-3.56490700	4.73733800	H	6.56584800	1.88923000	2.06784600
H	-1.89707700	-4.79775200	4.85017200	H	7.05508600	2.92379900	3.42161900
C	2.57322800	-0.05401400	-5.40115200	H	6.57505200	1.24474700	3.72204900
H	3.40181900	-0.34162600	-6.05343300	C	2.67022200	-1.95546800	4.15890200
C	1.98277100	1.27237400	-5.91557700	H	2.99704500	-1.74012100	5.17802700
H	1.13214300	1.59792600	-5.30322700	C	1.18528200	-2.35105900	4.24252600
H	2.73138200	2.07249900	-5.90192800	H	0.80828600	-2.70371200	3.27590600
H	1.62567200	1.15828500	-6.94521600	H	1.05257000	-3.16989400	4.95847100
C	1.52009500	-1.17915200	-5.44744600	H	0.56396400	-1.50679400	4.55659400
H	1.17133900	-1.33572200	-6.47413900	C	3.50687700	-3.13359500	3.62292400
H	1.93453400	-2.12723500	-5.08348000	H	3.20279900	-3.38649400	2.60168800
H	0.64154800	-0.93468600	-4.83625400	H	4.57455000	-2.89265000	3.60366100
C	6.47956700	-0.03868400	-2.03283200	H	3.36847200	-4.02324700	4.24916700
H	7.05996900	-0.09711700	-2.95535100	Rh	-0.13040700	-0.83374700	-0.77050100
C	6.98174500	1.20056800	-1.26693200	C	-1.82937700	-3.37143500	-2.14378300
H	6.49619900	1.30012500	-0.28937800	C	-2.54279500	-4.35237800	-1.45608900
H	8.06055100	1.12321300	-1.09211900	C	-2.44950400	-5.68084600	-1.87746200
H	6.79131200	2.11924900	-1.83229800	C	-1.64557700	-6.02063000	-2.96685000
C	6.73981000	-1.32762900	-1.22801100	C	-0.94572900	-5.01968300	-3.64783000
H	6.16623500	-1.33005500	-0.29350200	C	-1.03898400	-3.68735600	-3.24644600
H	6.45427200	-2.21725600	-1.80041600	H	-3.15135500	-4.07782100	-0.60108800
H	7.80188300	-1.41501400	-0.97297900	H	-3.00719300	-6.44841300	-1.34783400
H	-0.56874600	5.99878400	-0.58834100	H	-1.56942200	-7.05477900	-3.28817900
H	0.51960700	2.45963400	5.34634500	H	-0.32604700	-5.27547600	-4.50243400
O	1.15213100	3.78042800	3.07127300	H	-0.50079300	-2.89984200	-3.75921900
O	-1.23710900	4.61570000	1.63456600	H	-2.65040600	-1.91660900	-1.14815700
C	1.57817200	4.45075100	4.25110200	C	1.97512800	-3.11366700	-1.17867600
H	2.28473400	3.83952000	4.82721300	C	1.26578300	-4.03123200	-0.40376600
H	2.08561900	5.35527800	3.91338400	C	1.97704500	-4.94829600	0.36891100
H	0.72485400	4.72425300	4.88441400	C	3.37610400	-4.95026100	0.36462000
C	-1.39837400	6.01415200	1.83724700	C	4.06549900	-4.02375800	-0.41947800
H	-2.00054600	6.47726800	1.04638000	C	3.36799400	-3.09855700	-1.19955600
H	-1.92675000	6.11901300	2.78616000	H	0.18198900	-4.02812900	-0.42300100
H	-0.42391500	6.51522500	1.89486400	H	1.43146600	-5.66706900	0.97322800
C	-5.37200200	4.00904600	0.39771300	H	3.92257100	-5.66685300	0.96994500
H	-5.95479100	4.59676400	-0.31330300	H	5.15155900	-4.01125200	-0.42685200
C	-6.35715400	3.03907700	1.07866900	H	3.89771400	-2.36766100	-1.80301700
H	-5.86701400	2.43262300	1.84885100	H	1.84193900	-1.65048900	-2.47181600
H	-7.16715000	3.59664700	1.56243800	O	-1.87968200	-2.04164800	-1.73478000
H	-6.80379400	2.35661500	0.34671600	O	1.23950100	-2.20539000	-1.93710300
C	-4.75710800	4.98641800	1.41527500				
H	-4.09680000	4.46593000	2.11787400	<b>4-ts-O</b>			
H	-4.16226900	5.75030800	0.90506000	B3LYP-D3 SCF energy: -4504.394013 a.u.			
H	-5.54147000	5.49277800	1.98955400	B3LYP-D3 enthalpy: -4502.508076 a.u.			
C	-2.86756400	2.82441800	-3.93387200	B3LYP-D3 free energy: -4502.751636 a.u.			
H	-3.81009500	3.13733400	-4.39327000	M06 SCF energy in solution: -4503.269259 a.u.			
C	-1.85291900	3.96362200	-4.15265500	Imaginary frequency: -1153.43 cm <sup>-1</sup>			
H	-0.88941400	3.70763400	-3.69764100				



Cartesian coordinates							
ATOM	X	Y	Z				
C	-0.20804900	0.00575400	3.98789100	N	-3.83884100	3.96098400	3.53579500
C	0.19725400	-0.36873600	2.68872700	N	5.55412400	4.39025900	-1.22719900
C	0.95405900	0.54392400	1.92658000	N	4.40841500	-5.17091200	0.93232500
C	1.28954300	1.79591300	2.46462500	C	-3.45123700	4.02965900	4.93579100
C	0.87665900	2.14302900	3.74828700	H	-3.42147500	5.08126300	5.24959500
C	0.13013500	1.25407400	4.51603900	H	-4.12404100	3.49688400	5.62941100
C	-0.19688100	-1.72882200	2.21450800	H	-2.44624100	3.61240100	5.05160300
C	-1.12004800	-1.94056800	1.17098100	C	-5.16255100	4.47815000	3.22495700
C	0.33482800	-2.85287000	2.88985200	H	-5.29229000	4.52446700	2.13895100
C	-1.51449500	-3.24516200	0.83185500	H	-5.98891400	3.87277600	3.63972000
C	-0.04924300	-4.14858500	2.53207100	H	-5.25970100	5.49517600	3.62417500
C	-0.98353400	-4.33321800	1.51567700	C	6.41330300	4.13587900	-2.37439900
P	1.50701200	0.10116500	0.21903200	H	6.64527900	5.08921900	-2.86665600
P	-1.69143100	-0.53484900	0.11747500	H	7.37250500	3.64657200	-2.13273600
C	2.37028700	-1.49025300	0.42776300	H	5.87983300	3.50172900	-3.08715400
C	2.12157300	-2.53579800	-0.45878400	C	6.12687700	5.21749100	-0.17753000
C	3.27673200	-1.67865100	1.47701200	H	6.95133800	4.73129300	0.37514100
C	2.76313400	-3.77223100	-0.32924900	H	6.51742800	6.14377700	-0.61605500
C	3.95948600	-2.88566100	1.62865000	H	5.34917900	5.48597100	0.54453600
C	3.69875200	-3.94327600	0.71588000	C	3.66299700	-6.22534900	1.60142200
C	2.76556500	1.36714400	-0.18471800	H	2.92278200	-6.73502500	0.95802100
C	4.13118800	1.09694500	-0.12539300	H	4.36194100	-6.98341600	1.97460700
C	2.34563100	2.65796800	-0.53584200	H	3.12643100	-5.80641000	2.45948200
C	5.08346000	2.08379100	-0.40548100	C	5.33918100	-5.62883200	-0.09113400
C	3.26111700	3.65754100	-0.86515200	H	5.82513900	-4.76503000	-0.55336000
C	4.64854600	3.36092800	-0.82327100	H	6.11666500	-6.24349700	0.38031500
C	-2.31579200	0.78346900	1.19887700	H	4.88182000	-6.23036600	-0.89427400
C	-2.05173900	2.11467500	0.86441700	C	-6.93907800	-0.87427000	-0.78421000
C	-3.12358900	0.48936300	2.29938900	H	-7.63371000	-1.13090100	-1.58582600
C	-2.55305000	3.16024100	1.64120000	C	-7.05809000	0.64484800	-0.56048300
C	-3.70183800	1.51304600	3.05908900	H	-6.45003400	0.98578300	0.28525600
C	-3.37695900	2.85477700	2.75329400	H	-6.73714200	1.20313100	-1.44606900
C	-3.13749000	-1.17664300	-0.80087600	H	-8.09877600	0.91171600	-0.34550700
C	-4.44865700	-0.83944900	-0.46048000	C	-7.36900500	-1.64854400	0.47737400
C	-2.91549100	-1.99609900	-1.91343600	H	-8.38898700	-1.37448100	0.77049300
C	-5.53690200	-1.29289200	-1.21534300	H	-7.33990700	-2.73032100	0.31041300
C	-3.97160900	-2.48130600	-2.68534100	H	-6.70366000	-1.41971800	1.31758200
C	-5.29949700	-2.12309600	-2.33699700	C	-3.66184300	-3.33646000	-3.90536200
H	1.88347900	2.49774100	1.89409700	H	-4.61854200	-3.71066600	-4.27946500
H	1.13887000	3.11613900	4.15242800	C	-3.01503200	-2.48028400	-5.01232000
H	-2.23689300	-3.41466800	0.04385300	H	-2.06761800	-2.04466400	-4.67364800
H	-1.29824900	-5.33936700	1.25422800	H	-2.81654100	-3.08816100	-5.90241600
H	1.39693100	-2.39378600	-1.25560600	H	-3.66854400	-1.65082300	-5.30502700
H	3.43995500	-0.87274800	2.18250400	C	-2.77759700	-4.54674700	-3.55463300
H	4.47298000	0.10620700	0.14792700	H	-1.77833000	-4.24211100	-3.21867900
H	1.28390900	2.89235400	-0.55102900	H	-3.22888600	-5.15237900	-2.76048400
H	-1.43284000	2.32331300	-0.00134000	H	-2.64411300	-5.18528600	-4.43505500
H	-3.31646100	-0.54694700	2.56182300	C	2.75375300	5.04727800	-1.22638400
H	-4.63277700	-0.19280200	0.38826900	H	3.62294800	5.62065200	-1.55934700
H	-1.89918000	-2.24571800	-2.20323600	C	2.16009800	5.74502100	0.01240200
N	-6.34914600	-2.61299100	-3.17677900	H	1.27492300	5.21473100	0.37971100
C	-7.30335000	-3.55896500	-2.61884100	H	2.88599600	5.79051300	0.83228000
H	-6.78350000	-4.23608500	-1.93443400	H	1.85691400	6.77015300	-0.23007800
H	-8.14493500	-3.09988200	-2.07251000	C	1.73741800	5.02306300	-2.38188600
H	-7.72723000	-4.16094400	-3.43247500	H	1.40926000	6.04142100	-2.61943000
C	-6.87800000	-1.68296700	-4.16258600	H	2.18297000	4.58995600	-3.28207400
H	-6.05209400	-1.14012100	-4.63318800	H	0.84216300	4.43965200	-2.13295500
H	-7.40478400	-2.24317800	-4.94436500	C	6.55315900	1.73944200	-0.18409300
H	-7.58228200	-0.93835200	-3.74874300	H	7.14851700	2.63268800	-0.37785100
				C	6.80404300	1.34992400	1.28676900
				H	6.26538000	0.43433800	1.55851900

H	7.87165100	1.16913700	1.45593600
H	6.47844900	2.14416600	1.96772800
C	7.04165000	0.63638600	-1.13923000
H	6.49113500	-0.29879700	-0.98023300
H	6.89984300	0.92846000	-2.18362100
H	8.10557600	0.43135700	-0.97428200
H	-0.19228200	1.53083200	5.51341600
H	0.36482500	-5.01019100	3.04086400
O	1.22349300	-2.58455200	3.88475600
O	-0.95822400	-0.90654300	4.66809400
C	1.67752500	-3.66075800	4.69657300
H	2.30143600	-4.35766500	4.12298000
H	2.28220100	-3.20745400	5.48278000
H	0.83745500	-4.20272300	5.14856800
C	-0.82747600	-0.94727800	6.08696100
H	-1.34330500	-0.11022600	6.57083500
H	-1.29899400	-1.87974100	6.40294500
H	0.22984100	-0.94804900	6.37754100
C	-4.67487400	1.13891000	4.17273100
H	-5.14544500	2.05453600	4.53460900
C	-5.80931600	0.23591400	3.65270900
H	-5.43401400	-0.74112900	3.32715600
H	-6.54589100	0.05714500	4.44408000
H	-6.32626700	0.69835900	2.80456700
C	-3.94771200	0.48039800	5.35797400
H	-3.43726600	-0.43445600	5.04094900
H	-3.19289100	1.15588000	5.77488800
H	-4.65619100	0.22558600	6.15453900
C	-2.15889200	4.60253000	1.34383000
H	-3.00476400	5.24131300	1.61443700
C	-0.97607700	5.00804700	2.24602300
H	-0.11380300	4.35751900	2.06148300
H	-0.67471100	6.04345300	2.04904700
H	-1.24393300	4.92220000	3.30294000
C	-1.82961300	4.85839200	-0.13346500
H	-0.90912800	4.35009500	-0.44450000
H	-2.63242300	4.51847200	-0.79509600
H	-1.67333600	5.92979500	-0.30076700
C	4.99810700	-3.04652200	2.73537800
H	4.88313300	-4.05539200	3.14763800
C	4.84179400	-2.03395100	3.88216200
H	5.14917200	-1.02664300	3.57417500
H	3.80985100	-1.97006900	4.23957000
H	5.48466700	-2.32196000	4.72071800
C	6.42445800	-2.95009700	2.15469300
H	6.58244800	-1.97140000	1.68497900
H	7.16939800	-3.06501900	2.95060300
H	6.60450800	-3.72438800	1.40655300
C	2.45151200	-4.85517000	-1.35797800
H	2.88503400	-5.79463200	-1.01206300
C	0.94089400	-5.10100900	-1.52408400
H	0.42389100	-4.22453500	-1.93247500
H	0.76985600	-5.93254900	-2.21680000
H	0.47228900	-5.34319400	-0.56622600
C	3.10175000	-4.50628100	-2.71198600
H	2.68727100	-3.57445500	-3.11629100
H	4.18424200	-4.37386900	-2.61154700
H	2.92057000	-5.30040300	-3.44519200
Rh	-0.06055600	0.01167300	-1.42210600
C	2.37500100	0.81147000	-3.42904200
C	2.89555200	1.87438200	-4.17947700

C	4.21650100	1.83173900	-4.62290500
C	5.03203900	0.73898100	-4.31252900
C	4.51225600	-0.31528400	-3.55664300
C	3.19077600	-0.28299000	-3.11581800
H	2.24500600	2.70593300	-4.42743700
H	4.60698400	2.65135000	-5.22017700
H	6.05940200	0.70656000	-4.66309900
H	5.13622500	-1.16949700	-3.30903200
H	2.78134200	-1.09682800	-2.52972200
H	0.50803500	1.45097300	-1.91638700
C	-2.21153800	1.39248800	-3.32252400
C	-3.58671300	1.23170000	-3.18018500
C	-4.40173800	2.36539200	-3.19706200
C	-3.85141200	3.63805500	-3.36492700
C	-2.46947500	3.77708400	-3.52008000
C	-1.64003300	2.65571700	-3.49421200
H	-4.00300900	0.23924700	-3.06920200
H	-5.47645700	2.24713500	-3.09427900
H	-4.49353800	4.51346500	-3.38441500
H	-2.02957900	4.76098900	-3.65534400
H	-0.56468400	2.75168300	-3.60668200
H	-0.57055900	0.43614800	-3.77375400
O	-1.40806200	0.24465800	-3.28659900
O	1.04914900	0.82803700	-3.10597700

### 5-O

B3LYP-D3 SCF energy: -4504.425165 a.u.

B3LYP-D3 enthalpy: -4502.538956 a.u.

B3LYP-D3 free energy: -4502.784313 a.u.

M06 SCF energy in solution: -4503.303880 a.u.

### Cartesian coordinates

ATOM	X	Y	Z
C	-0.02104700	-2.46019700	3.22227000
C	0.37682300	-1.94181000	1.97041800
C	1.06928200	-0.71319000	1.94186100
C	1.34702300	-0.03055000	3.13572500
C	0.94381300	-0.56409000	4.35683400
C	0.26191800	-1.77628400	4.40781500
C	0.04923800	-2.75872600	0.76084000
C	-0.91489500	-2.37198500	-0.19248500
C	0.67528600	-4.01819200	0.61447500
C	-1.25459300	-3.22955500	-1.25052600
C	0.34939800	-4.85718000	-0.45637300
C	-0.62470800	-4.46363300	-1.37096900
P	1.58964700	0.03241700	0.34137600
P	-1.64322300	-0.68472800	-0.12274400
C	2.52209800	-1.27132800	-0.51417200
C	2.29205800	-1.53954900	-1.86193600
C	3.47175300	-2.02091000	0.18973900
C	2.98508000	-2.55796500	-2.52717300
C	4.22178800	-3.00821900	-0.44806700
C	3.96954600	-3.28393000	-1.81889000
C	2.73612300	1.37949400	0.77044800
C	4.11974200	1.20960300	0.71887500
C	2.21555900	2.60276700	1.21096800
C	4.99155300	2.23052700	1.11094600
C	3.05179900	3.65185000	1.59111400
C	4.45633100	3.47410700	1.51630000
C	-2.37498900	-0.49077200	1.53252300
C	-2.23273600	0.70423600	2.23777900

C	-3.16761100	-1.51034200	2.07122500	H	-6.26981300	1.12628100	0.53678700
C	-2.85841200	0.90306700	3.46966900	H	-6.54382300	2.19448900	-0.84739000
C	-3.82973600	-1.34328600	3.29204000	H	-7.91974100	1.41160400	-0.03845900
C	-3.64889100	-0.13692300	4.01229400	C	-7.28957700	-1.21913200	-0.65815700
C	-3.02513800	-0.61582200	-1.31215400	H	-8.32745800	-1.09247500	-0.32920600
C	-4.33973600	-0.38648100	-0.90452800	H	-7.25265600	-2.06195200	-1.35729300
C	-2.72708200	-0.62030100	-2.68345700	H	-6.69048900	-1.48637600	0.21910300
C	-5.35122000	-0.11795700	-1.83587800	C	-3.33265600	-0.28793700	-5.11501400
C	-3.70334600	-0.34814600	-3.63865700	H	-4.24763000	-0.46412800	-5.68693600
C	-5.01892500	-0.04320500	-3.20557900	C	-2.83532200	1.12619300	-5.47228500
H	1.88618100	0.90826100	3.11666100	H	-1.93477500	1.36925100	-4.89570800
H	1.16336300	-0.02990900	5.27619700	H	-2.59243000	1.19418600	-6.53907100
H	-2.01268100	-2.94344900	-1.96846100	H	-3.59773200	1.87622100	-5.24209100
H	-0.89328100	-5.12905200	-2.18623400	C	-2.29819000	-1.34777200	-5.52701100
H	1.55861300	-0.95536000	-2.40871100	H	-1.30677400	-1.14215000	-5.10572900
H	3.62018700	-1.82675000	1.24521900	H	-2.59892800	-2.35254600	-5.20826100
H	4.53578600	0.27171200	0.37179800	H	-2.18580200	-1.35557800	-6.61664300
H	1.14013800	2.74949600	1.24365300	C	2.43279400	4.96163100	2.06024800
H	-1.60326100	1.49109100	1.83717400	H	3.25952100	5.61780900	2.34385300
H	-3.27757100	-2.44455700	1.52827400	C	1.53433500	4.75192700	3.29288600
H	-4.58652100	-0.39558800	0.15092300	H	0.65292300	4.14521000	3.05217400
H	-1.70504200	-0.78832800	-3.00907500	H	2.07520800	4.24831200	4.10263900
N	-5.94900100	0.37288200	-4.21089400	H	1.17454600	5.71541500	3.67167700
C	-6.90082700	-0.61874400	-4.68711200	C	1.65580700	5.65387600	0.92596700
H	-6.38522000	-1.57078000	-4.85114900	H	1.24845300	6.61152700	1.26999400
H	-7.74518800	-0.80443100	-3.99917000	H	2.30536700	5.84276400	0.06618100
H	-7.31778900	-0.28826000	-5.64613300	H	0.81658600	5.03631000	0.58101400
C	-6.44008200	1.74255100	-4.13545000	C	6.48747400	1.93103000	1.11397900
H	-5.63254700	2.40022500	-3.80017000	H	7.00889500	2.79354600	1.53156500
H	-6.75208700	2.06492700	-5.13695800	C	6.81084500	0.73163300	2.02692800
H	-7.29870600	1.88782800	-3.45713700	H	6.36143400	-0.19548900	1.65103200
N	-4.22555700	0.08808200	5.30245600	H	7.89425300	0.57515000	2.07900400
N	5.27714300	4.59820400	1.84289800	H	6.43882400	0.89600500	3.04436500
N	4.74351900	-4.33218600	-2.41628300	C	7.02690700	1.70334100	-0.30935700
C	-3.76797600	-0.74392000	6.40387600	H	6.54823500	0.83545500	-0.77895900
H	-3.92841800	-0.20936200	7.34858700	H	6.83335500	2.57076000	-0.94692900
H	-4.27057300	-1.72321700	6.48695400	H	8.10730700	1.52045700	-0.28515100
H	-2.69344500	-0.92279600	6.29438900	H	-0.05249600	-2.18415900	5.36172800
C	-5.62094200	0.49706300	5.34090700	H	0.83800100	-5.81609000	-0.57658700
H	-5.79725100	1.25910200	4.57460300	O	1.58787600	-4.34406700	1.56925500
H	-6.34011300	-0.32492300	5.17433600	O	-0.70315300	-3.63889900	3.19354800
H	-5.84139900	0.94158400	6.31884400	C	2.13639100	-5.65720200	1.56273500
C	6.11592100	5.15636800	0.79214500	H	2.77702300	-5.81750400	0.68644000
H	6.28427200	6.22163300	0.99591100	H	2.74370700	-5.73143700	2.46540400
H	7.10512900	4.67801600	0.68837100	H	1.34790500	-6.41957400	1.58917700
H	5.59480800	5.06687900	-0.16485400	C	-0.54008500	-4.52648200	4.29656600
C	5.81804400	4.65118800	3.19103200	H	-1.06708700	-4.17490100	5.19081800
H	6.67965300	3.97935400	3.35814000	H	-0.97911800	-5.47516900	3.98307300
H	6.14405800	5.67486800	3.41143700	H	0.52315600	-4.66470100	4.52658900
H	5.03662600	4.38213800	3.90972000	C	-4.74049600	-2.46271900	3.78695200
C	4.08934200	-5.62711500	-2.51549700	H	-5.25123100	-2.11519800	4.68608600
H	3.33713400	-5.69233200	-3.32279200	C	-5.83727600	-2.79150600	2.75680100
H	4.84324700	-6.40287800	-2.69523600	H	-5.41796400	-3.18115600	1.82213700
H	3.58482900	-5.85571000	-1.57037500	H	-6.51824400	-3.55158500	3.15590900
C	5.63494300	-4.00307000	-3.52101300	H	-6.42688200	-1.90028200	2.51586300
H	6.04751500	-3.00183300	-3.36887300	C	-3.93476500	-3.71655800	4.16867900
H	6.46929900	-4.71602500	-3.53273500	H	-3.34837200	-4.08687700	3.32129800
H	5.16325400	-4.02722100	-4.51736900	H	-3.23685900	-3.49197900	4.98175300
C	-6.77341100	0.07307200	-1.31927200	H	-4.60373700	-4.51712500	4.50434100
H	-7.42438000	0.27679200	-2.17004600	C	-2.64507700	2.22125800	4.20067600
C	-6.88162300	1.27380700	-0.36185000	H	-3.33342100	2.23226000	5.04946000

C	-1.21296300	2.30070100	4.76107300
H	-0.46931500	2.23508300	3.95825600
H	-1.05635400	3.24615200	5.29296300
H	-1.01911300	1.47667000	5.45612800
C	-2.95898500	3.43519200	3.30677800
H	-2.26148100	3.52026300	2.46415800
H	-3.97289100	3.37314800	2.89422400
H	-2.88394500	4.36206300	3.88614400
C	5.32599800	-3.74194400	0.30779700
H	5.28883700	-4.79466100	0.00586900
C	5.18327500	-3.67069500	1.83710900
H	5.41911900	-2.66854900	2.21675100
H	4.17206800	-3.92124900	2.17058100
H	5.88774300	-4.36469800	2.30760900
C	6.70902700	-3.19539300	-0.10501300
H	6.78753000	-2.12837400	0.13808000
H	7.50458100	-3.72269900	0.43405300
H	6.88403500	-3.31855400	-1.17553600
C	2.65979700	-2.81203700	-3.99636600
H	3.16049600	-3.73094800	-4.30422300
C	1.15451100	-3.03034700	-4.23175600
H	0.56870700	-2.13724800	-3.98645400
H	0.96742500	-3.26487400	-5.28561400
H	0.77419300	-3.85207300	-3.61869500
C	3.19180200	-1.66681900	-4.88020200
H	2.69354400	-0.72015200	-4.63992700
H	4.26860100	-1.52264700	-4.74161600
H	3.00929000	-1.88141500	-5.93927100
Rh	-0.10369500	0.85463900	-0.91979300
C	2.21883000	2.48283200	-2.36693400
C	2.31129100	3.86970300	-2.15637900
C	3.38130100	1.76446200	-2.69648600
C	3.53519100	4.52210500	-2.28781900
H	1.41074400	4.41603200	-1.89203700
C	4.59984800	2.42637300	-2.83355100
H	3.31263600	0.69348200	-2.84611700
C	4.68728800	3.80633000	-2.63039400
H	3.58939100	5.59651900	-2.13032700
H	5.48783000	1.85948000	-3.09944900
H	5.63781800	4.31922300	-2.74653300
H	-0.47887100	1.66030800	0.31752800
C	-2.48683700	2.92596200	-2.05246900
C	-2.84985500	3.82429800	-3.05765800
C	-3.91370200	4.70097600	-2.83640600
C	-4.61314800	4.67434300	-1.62658400
C	-4.23560300	3.76939900	-0.63195300
C	-3.17171000	2.89058100	-0.83982300
H	-2.31077900	3.82399700	-3.99990400
H	-4.19518500	5.40386400	-3.61516100
H	-5.43982600	5.35790900	-1.45892800
H	-4.76506200	3.74464400	0.31595800
H	-2.87609300	2.18566900	-0.07346900
H	-0.64767100	2.42737400	-2.68358800
O	-1.45809100	2.02030500	-2.27912500
O	1.01853900	1.87316700	-2.30443900

Cartesian coordinates

ATOM	X	Y	Z
C	-1.37211000	-4.16468400	-0.08198600
C	-0.62462800	-2.99919900	-0.36004200
C	0.14621200	-2.43334400	0.67817600
C	0.17476500	-3.03294700	1.94775800
C	-0.57083200	-4.18278600	2.19332700
C	-1.34752100	-4.75060500	1.18802400
C	-0.68187200	-2.48548100	-1.76688900
C	-1.41496200	-1.34165200	-2.13705800
C	-0.04618900	-3.23724800	-2.77926700
C	-1.52929400	-0.96733600	-3.48233000
C	-0.13019200	-2.83805700	-4.11945100
C	-0.88327300	-1.71696200	-4.46214500
P	1.16740000	-0.94334000	0.35270500
P	-1.94040100	-0.19477000	-0.80534800
C	2.39149900	-1.49062300	-0.87192700
C	2.80638200	-0.67697700	-1.92106100
C	2.96691300	-2.75779900	-0.70217100
C	3.76369200	-1.11948400	-2.84276800
C	3.97504700	-3.20347400	-1.55496900
C	4.37924900	-2.37447900	-2.63689300
C	2.08090400	-0.50287600	1.86391500
C	3.46093200	-0.33044800	1.77758000
C	1.42445500	-0.21965900	3.07327400
C	4.21169600	0.10041600	2.87614200
C	2.13874100	0.21438700	4.19291000
C	3.54303800	0.40549300	4.08108500
C	-3.06047700	-1.11895000	0.28457500
C	-2.96458300	-0.98548400	1.66980900
C	-4.08879400	-1.88807800	-0.26603500
C	-3.89051900	-1.59869100	2.51774100
C	-5.03897300	-2.51262800	0.54780900
C	-4.92547700	-2.38332700	1.95326800
C	-2.92912400	1.17654600	-1.49411900
C	-4.18842200	1.47076000	-0.97325300
C	-2.30785100	2.10941200	-2.34364500
C	-4.83376400	2.68008600	-1.26264300
C	-2.91460200	3.32880000	-2.64906300
C	-4.17768400	3.63156100	-2.07427200
H	0.79099600	-2.62160700	2.73634000
H	-0.54529600	-4.64038900	3.17755300
H	-2.11125100	-0.09761900	-3.76351700
H	-0.96345600	-1.42663200	-5.50569100
H	2.38252000	0.31221600	-2.03765100
H	2.63035400	-3.39047100	0.11025300
H	3.96630300	-0.53055800	0.84071300
H	0.34879100	-0.34881300	3.14080800
H	-2.14420900	-0.41358800	2.09208400
H	-4.15316100	-1.99700300	-1.34469100
H	-4.67569200	0.76091100	-0.31503800
H	-1.33032600	1.88487700	-2.75605500
N	-4.72066300	4.92625100	-2.35398700
C	-5.74112400	4.99410900	-3.39028500
H	-5.43271100	4.38665300	-4.24734300
H	-6.73746600	4.64391100	-3.06638600
H	-5.84405600	6.03213200	-3.72825100
C	-4.89072500	5.85119300	-1.24263800
H	-4.05615400	5.73654400	-0.54417100
H	-4.87188800	6.87873600	-1.62679300

7-O

B3LYP-D3 SCF energy: -4605.826796 a.u.

B3LYP-D3 enthalpy: -4603.915702 a.u.

B3LYP-D3 free energy: -4604.166499 a.u.

M06 SCF energy in solution: -4604.683358 a.u.

H	-5.82808900	5.72581400	-0.67432900	H	5.98510600	-1.42402200	1.25422600
N	-5.81899900	-3.03255200	2.86413700	H	7.42393600	-1.06696000	2.21703700
N	4.21663700	0.91393200	5.23891800	H	6.06612900	-1.94875500	2.94468400
N	5.42873200	-2.87544600	-3.47430900	C	6.10691800	1.33669600	1.74162300
C	-5.79058000	-4.48553700	2.92243300	H	5.71127900	1.14993300	0.73684300
H	-6.15175800	-4.81335400	3.90533300	H	5.71041300	2.29932100	2.08292300
H	-6.40366000	-4.99242700	2.15724800	H	7.19653600	1.42458700	1.66382500
H	-4.75703900	-4.82854800	2.80999900	H	-1.92624200	-5.64437300	1.39020700
C	-7.11623100	-2.40791600	3.07289800	H	0.37045200	-3.40125400	-4.89704300
H	-6.98447900	-1.32719400	3.18992000	O	0.62659600	-4.34169500	-2.36195700
H	-7.83903300	-2.57550700	2.25441500	O	-2.10424000	-4.65925200	-1.11547400
H	-7.56075800	-2.79764100	3.99649900	C	1.33694700	-5.10461600	-3.33044600
C	4.84426600	2.22417000	5.13393700	H	2.11673900	-4.50027200	-3.80842100
H	4.93561500	2.65700700	6.13781400	H	1.80229500	-5.92430400	-2.78304500
H	5.84877900	2.22256700	4.67857400	H	0.66286200	-5.51328000	-4.09368200
H	4.20603700	2.88511800	4.53918600	C	-2.41000900	-6.05155100	-1.11623300
C	4.92811900	-0.05716100	6.05898500	H	-3.16446600	-6.30594900	-0.36339900
H	5.89643100	-0.38145000	5.63880800	H	-2.81573800	-6.26512300	-2.10626400
H	5.11977700	0.37712700	7.04741600	H	-1.50450000	-6.64702000	-0.94818500
H	4.30557200	-0.94770100	6.19394000	C	-6.15881500	-3.30399300	-0.11987800
C	5.01904300	-3.55008000	-4.69559100	H	-6.87293800	-3.60457400	0.64819900
H	4.64270500	-2.87026900	-5.48107000	C	-6.93534500	-2.44719900	-1.13760400
H	5.87258700	-4.10078200	-5.10822300	H	-6.30545000	-2.13974500	-1.97993100
H	4.23050100	-4.27622600	-4.47116600	H	-7.77746800	-3.01664400	-1.54637600
C	6.65848000	-2.10060400	-3.58151900	H	-7.33355400	-1.54120900	-0.66765000
H	6.86955400	-1.62255400	-2.62081700	C	-5.61031500	-4.58633900	-0.77194700
H	7.48829300	-2.78104100	-3.81176800	H	-4.83945700	-4.35369100	-1.51482200
H	6.64473700	-1.31676100	-4.35582800	H	-5.15939200	-5.23983800	-0.01760000
C	-6.21029800	2.91514300	-0.65061800	H	-6.41338400	-5.14258100	-1.26859400
H	-6.61023000	3.84960000	-1.04644200	C	-3.74582200	-1.44006300	4.02424300
C	-6.11074500	3.05913200	0.88095900	H	-4.67095800	-1.80712400	4.47537400
H	-5.73328800	2.13664000	1.33952300	C	-2.59820300	-2.32707300	4.54135100
H	-5.43325700	3.87351200	1.15984300	H	-1.64784100	-2.05817500	4.06817300
H	-7.09548500	3.26978900	1.31321900	H	-2.48157300	-2.22167400	5.62599900
C	-7.20239400	1.80241600	-1.03897200	H	-2.79187500	-3.38138300	4.31510500
H	-8.19936400	2.03106400	-0.64593100	C	-3.56182700	0.02975300	4.44048300
H	-7.27799800	1.70074400	-2.12699000	H	-2.63204900	0.46036800	4.04914000
H	-6.90061100	0.83055300	-0.63177500	H	-4.39040700	0.64992500	4.07955400
C	-2.19750100	4.35151900	-3.52258200	H	-3.52302700	0.11393500	5.53209100
H	-2.96889200	4.95392800	-4.01013900	C	4.67080600	-4.53560400	-1.29205400
C	-1.36728900	5.30879400	-2.64195400	H	4.87491900	-5.00118700	-2.26196900
H	-0.57162700	4.77034400	-2.11555600	C	3.83543800	-5.51883300	-0.45553500
H	-0.89435300	6.08327100	-3.25686200	H	3.76489500	-5.20043800	0.59179800
H	-2.00267400	5.80605400	-1.90186400	H	2.81435700	-5.62480800	-0.83696000
C	-1.32559500	3.72011400	-4.62000100	H	4.31032600	-6.50566700	-0.45908400
H	-0.45115200	3.19993700	-4.21245700	C	6.03189400	-4.29246500	-0.60713200
H	-1.89470100	3.00303400	-5.22280100	H	5.88900400	-3.80508400	0.36533800
H	-0.94934200	4.50163100	-5.28895800	H	6.55200700	-5.24234300	-0.43659200
C	1.43998300	0.48657500	5.52379600	H	6.67433400	-3.65690300	-1.22116500
H	2.15086900	0.21890600	6.31083700	C	4.08204700	-0.21112600	-4.02514600
C	0.17250500	-0.35299300	5.73122600	H	4.67851600	-0.77923900	-4.74200200
H	-0.63989700	-0.04126500	5.06624900	C	2.79859600	0.23138800	-4.75800100
H	0.35620200	-1.41961300	5.56005300	H	2.20958500	0.92782900	-4.15063400
H	-0.19303100	-0.23178900	6.75666500	H	3.05988900	0.75079500	-5.68689600
C	1.12597300	1.98414800	5.70657100	H	2.16350400	-0.62684300	-5.00599500
H	0.70265300	2.16476400	6.70124700	C	4.89878000	1.01586900	-3.57646100
H	2.02755100	2.59369900	5.60640100	H	4.33741800	1.61783200	-2.85568800
H	0.39375400	2.32972700	4.96736600	H	5.84145700	0.71736700	-3.10539200
C	5.72474700	0.20223700	2.71039600	H	5.13319600	1.65603900	-4.43444100
H	6.16358600	0.43397700	3.68167900	Rh	-0.00842900	0.89798100	-0.13650000
C	6.33128100	-1.13986500	2.25474500	C	2.33547000	2.66179400	-0.82074000

C	3.63953400	3.16095300	-0.59874600	C	-5.18840300	-1.41931400	-1.03449900
C	4.22686200	4.04994400	-1.49319500	C	-3.64396700	-2.21431200	-2.76493700
C	3.55263700	4.45576800	-2.65178200	C	-4.96656500	-1.98539700	-2.31059600
C	2.27392200	3.95394800	-2.89563900	C	2.72004400	-1.49236000	-0.38638500
C	1.66948100	3.07367100	-1.99511600	C	2.22270000	-2.09447300	-1.54757700
H	4.15125600	2.84986200	0.30386700	C	3.77381300	-2.09555000	0.30032100
H	5.22549100	4.42760000	-1.28727100	C	2.73037700	-3.30388600	-2.01726900
H	4.01790600	5.14584400	-3.34886900	C	4.35213700	-3.28227500	-0.16929600
H	1.73059900	4.25622800	-3.78757100	C	3.79830000	-3.91059500	-1.30883300
H	0.66041500	2.71494000	-2.17719200	C	3.22830900	1.39050100	-0.06541400
H	0.44714300	0.50659400	-1.54488900	C	4.51982700	1.11823500	-0.51235200
C	1.27898700	5.82512500	0.68231200	C	2.87009900	2.71971500	0.20513400
C	0.29578500	4.86800200	0.90005300	C	5.46194800	2.14293800	-0.68827200
C	0.51519500	3.79181700	1.77962700	C	3.79810400	3.75645500	0.11335400
C	1.75145400	3.70626800	2.44508200	C	5.11278400	3.46531600	-0.33768200
C	2.74133000	4.66059900	2.24365800	H	-1.73127900	-3.62410200	-0.44899300
C	2.49247700	5.70118100	1.35453800	H	-0.55871500	-5.69976000	0.15855200
H	1.13092900	6.65095100	-0.00436700	H	2.75626900	1.79715900	2.40279800
H	-0.65119400	4.96194400	0.37803500	H	2.19840300	1.81204100	4.78795000
H	1.94905700	2.86019600	3.09406600	H	-1.09999000	1.91208800	1.34417100
H	3.70619600	4.59951100	2.73569600	H	-2.83094400	-1.79825500	2.57003800
F	3.45447600	6.61223600	1.13421800	H	-4.26225700	-0.62386600	0.72825700
C	-0.46760500	2.73179700	1.98655300	H	-1.56095500	-1.99040700	-2.31309700
H	-0.26316300	2.07359800	2.82928300	H	1.40664900	-1.61951700	-2.08549000
C	-1.58908600	2.48600400	1.25778900	H	4.15566600	-1.63475400	1.20653700
H	-1.88936400	3.11193500	0.42009500	H	4.80403300	0.09787000	-0.74296500
H	-2.32502600	1.76485500	1.59465300	H	1.85971500	2.94246700	0.53696200
O	1.80717200	1.86017400	0.10169900	N	6.03139500	4.55962000	-0.41329600

### 8-ts-O

B3LYP-D3 SCF energy: -4605.818059 a.u.

B3LYP-D3 enthalpy: -4603.909043 a.u.

B3LYP-D3 free energy: -4604.157207 a.u.

M06 SCF energy in solution: -4604.667683 a.u.

Imaginary frequency: -247.12 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z		X	Y	Z
C	1.16549500	-3.52696800	2.11229100	N	4.25843400	-5.17327000	-1.80100900
C	0.51827100	-2.32080700	1.76970300	N	-6.03435100	-2.34068500	-3.19787900
C	-0.52991000	-2.35846700	0.82851700	N	-3.37721800	1.77788300	5.38189000
C	-0.91244200	-3.58255600	0.25799800	C	4.14366600	-6.33391600	-0.93129600
C	-0.25460000	-4.75906000	0.60804900	H	4.04929200	-7.23701700	-1.54808700
C	0.78895800	-4.73918900	1.52924100	H	4.99721700	-6.48661400	-0.24908600
C	0.93787500	-1.09692200	2.52217200	H	3.23744200	-6.24021400	-0.32490700
C	1.68542400	-0.03631700	1.97097900	C	5.42180800	-5.15612600	-2.67483000
C	0.62853400	-1.06217900	3.90431000	H	5.33405900	-4.32905600	-3.38661500
C	2.14568300	0.99952600	2.80200100	H	6.38248000	-5.04329000	-2.14068200
C	1.05719800	-0.00579700	4.71179100	H	5.46311600	-6.09285200	-3.24381900
C	1.83392600	1.00687600	4.15635400	C	-6.79004600	-1.24923700	-3.79318900
P	-1.31889900	-0.77934000	0.28688600	H	-7.26635700	-1.60182100	-4.71681400
P	1.97010400	0.07855200	0.14695100	H	-7.58253800	-0.83097200	-3.14730100
C	-1.93101000	-0.00297000	1.81633000	H	-6.10402500	-0.43617700	-4.04681200
C	-1.68477500	1.34534100	2.05831800	C	-6.78880300	-3.54341800	-2.88314200
C	-2.65697100	-0.74488200	2.75571700	H	-7.53370100	-3.41995200	-2.07677900
C	-2.13857800	1.97950900	3.21871700	H	-7.32261500	-3.87929100	-3.78071400
C	-3.15152000	-0.14935400	3.91644100	H	-6.09707900	-4.33765400	-2.58397900
C	-2.88340200	1.22669600	4.15307100	C	-2.40071700	1.89766000	6.45279000
C	-2.78175700	-1.27590700	-0.68505200	H	-1.69110500	2.73591200	6.32557300
C	-4.08837600	-1.06888100	-0.24434400	H	-2.92219900	2.04090600	7.40682100
C	-2.57463100	-1.83819800	-1.95086100	H	-1.81628000	0.97332100	6.51939800
				C	-4.36668400	2.84532900	5.32604300
				H	-5.02796300	2.68352500	4.47023100

H	-4.97802700	2.81675400	6.23720500	H	4.74350500	-3.62050000	2.56850900
H	-3.94553600	3.86127600	5.24151100	H	4.46835900	-5.21005300	1.84752500
C	6.83735600	1.77348500	-1.23349400	H	6.08105800	-4.78711600	2.45594000
H	7.37298900	2.69671300	-1.46128400	C	2.10942600	-3.98627700	-3.23150400
C	6.74072700	0.97856900	-2.54966900	H	2.91426500	-4.49399900	-3.77176700
H	6.28092200	-0.00529800	-2.39981300	C	1.11233400	-5.06886000	-2.77297300
H	6.14670800	1.51798800	-3.29565300	H	0.30727500	-4.62081700	-2.18087800
H	7.74190600	0.81336900	-2.96334000	H	0.66526300	-5.57323300	-3.63742000
C	7.65650500	0.99998300	-0.18248900	H	1.60933300	-5.82076000	-2.15433700
H	8.65529800	0.76463500	-0.56765400	C	1.42966400	-3.01264700	-4.20783400
H	7.77334300	1.58031300	0.73872300	H	0.51795500	-2.57221500	-3.78447000
H	7.16500000	0.05553800	0.07605300	H	2.09812700	-2.19380500	-4.49902800
C	3.41899300	5.15378800	0.58760500	H	1.12863300	-3.54589300	-5.11561100
H	4.20911400	5.82949100	0.25166700	C	-4.00629100	-0.95482400	4.89152900
C	2.08211700	5.65512600	0.02090200	H	-3.70654600	-0.66719900	5.90573200
H	1.23243700	5.07669200	0.40617000	C	-3.84019600	-2.47673300	4.75048800
H	1.91839800	6.69830900	0.31409300	H	-4.31109200	-2.84941700	3.83238800
H	2.06161000	5.60278400	-1.07254900	H	-2.78896600	-2.77819900	4.72832000
C	3.40301500	5.18609100	2.12946200	H	-4.32907600	-2.98247000	5.58992800
H	2.63507000	4.50910600	2.52649400	C	-5.49600500	-0.58503500	4.73316800
H	4.37093500	4.87823600	2.54003000	H	-5.84119700	-0.81174600	3.71686900
H	3.18311800	6.19616900	2.49430500	H	-6.10999100	-1.16284000	5.43379300
C	-3.35901200	-2.87783200	-4.10611700	H	-5.66758900	0.47563000	4.92620300
H	-4.32809600	-3.12973900	-4.54443600	C	-1.84370400	3.46828600	3.38163400
C	-2.56256500	-4.18273600	-3.92008500	H	-2.08496900	3.75965100	4.40509900
H	-1.56143900	-3.99304500	-3.51730500	C	-0.35910000	3.81362300	3.16249100
H	-3.07549200	-4.86598600	-3.23334700	H	-0.04374000	3.62729800	2.12857600
H	-2.43842500	-4.69616300	-4.88066400	H	-0.18499300	4.87572800	3.36878600
C	-2.63789800	-1.92313300	-5.07502800	H	0.28715600	3.22046000	3.81493600
H	-2.38587200	-2.43990600	-6.00838700	C	-2.73526400	4.29328800	2.43081700
H	-3.27682000	-1.06984600	-5.32353700	H	-2.50956300	4.05480600	1.38348200
H	-1.70966700	-1.53007300	-4.64216400	H	-3.79725500	4.08625200	2.59972000
C	-6.58139600	-1.20911300	-0.44927400	H	-2.56848500	5.36709300	2.57490500
H	-7.31964700	-1.48952600	-1.20133900	Rh	0.12267300	0.49100100	-1.14398300
C	-6.80170600	-2.12811600	0.76846400	C	-0.86545600	5.42111000	-1.99619700
H	-6.09622100	-1.89331900	1.57479500	C	-0.27123800	4.17835800	-2.15952900
H	-7.81615100	-2.00513700	1.16494500	C	-0.51936800	3.39874000	-3.30646900
H	-6.66351800	-3.18143400	0.50018600	C	-1.39993100	3.90137500	-4.28351500
C	-6.83823500	0.26475900	-0.08702500	C	-2.00594300	5.14471800	-4.13500400
H	-6.16138900	0.60949200	0.70390200	C	-1.73078600	5.88298400	-2.98841600
H	-6.68789500	0.91416700	-0.95445000	H	-0.67838500	6.03369300	-1.12115700
H	-7.86505400	0.39324100	0.27448400	H	0.38830200	3.80178300	-1.38829900
H	1.30010100	-5.65706300	1.79726800	H	-1.61457000	3.30625300	-5.16567900
H	0.80880800	0.02551500	5.76526600	H	-2.68675100	5.54389200	-4.87839000
O	-0.09240600	-2.11578200	4.37720200	F	-2.31370700	7.08045400	-2.82954400
O	2.16908800	-3.43009200	3.03221200	C	0.02092000	2.05299300	-3.44894600
C	-0.32981100	-2.19836600	5.77716600	C	1.15842300	1.56612900	-2.67217500
H	-0.98435200	-1.38637000	6.11937000	C	-2.56271500	1.50290700	-2.50580400
H	-0.83180100	-3.15304300	5.93839800	C	-3.45879700	1.44841400	-3.58693700
H	0.60936000	-2.18023500	6.34447000	C	-4.71225600	2.04926900	-3.49170500
C	2.33889300	-4.51820800	3.93720800	C	-5.08967900	2.71938200	-2.32363600
H	2.81193100	-5.38325200	3.45868000	C	-4.20024500	2.77677200	-1.24797100
H	2.99875500	-4.15086200	4.72556400	C	-2.94357800	2.18115700	-1.33799600
H	1.37505800	-4.81604500	4.36675200	H	-3.14954600	0.93068800	-4.48773500
C	5.57156400	-3.83859300	0.55890800	H	-5.39416000	2.00338600	-4.33679800
H	5.97616700	-4.66072600	-0.03360700	H	-6.06445800	3.19308000	-2.25449200
C	6.68975500	-2.78530300	0.67238700	H	-4.48045600	3.29196500	-0.33299400
H	6.39521200	-1.94624200	1.31304800	H	-2.24863300	2.23313400	-0.51012800
H	7.58919900	-3.23242800	1.11030800	H	-0.02194300	1.75592600	-0.32022400
H	6.95396400	-2.38268500	-0.31179200	H	1.78822700	2.34405800	-2.24495600
C	5.19503600	-4.39666300	1.94236300	H	-0.15912100	1.59810100	-4.41905000

H	1.76456500	0.82769900	-3.20658100
O	-1.34162500	0.93204900	-2.65259100

**9-O**

B3LYP-D3 SCF energy: -4605.828610 a.u.

B3LYP-D3 enthalpy: -4603.917587 a.u.

B3LYP-D3 free energy: -4604.164809 a.u.

M06 SCF energy in solution: -4604.679357 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.94611400	-3.64335000	2.15441900
C	0.37410800	-2.41468800	1.76930500
C	-0.62100700	-2.41818500	0.77219200
C	-1.00368200	-3.61950800	0.15901700
C	-0.40618300	-4.81923600	0.53995500
C	0.56405600	-4.83919000	1.53936500
C	0.79678600	-1.18556300	2.51177100
C	1.56538200	-0.13838200	1.95928600
C	0.42084500	-1.09913000	3.87579100
C	1.95046700	0.94875800	2.76315200
C	0.78897500	-0.00120900	4.65710900
C	1.56369300	1.01025300	4.09597200
P	-1.34072500	-0.81682100	0.22769400
P	1.95818400	-0.03912300	0.15305700
C	-2.07393200	-0.08804700	1.72883100
C	-1.91752400	1.27520100	1.96369700
C	-2.81168000	-0.85731700	2.63629500
C	-2.46741800	1.89765100	3.08887900
C	-3.41522000	-0.27251200	3.75013400
C	-3.23293200	1.11878900	3.98385500
C	-2.74562000	-1.24407800	-0.86506600
C	-4.07426600	-1.22201800	-0.44084500
C	-2.47256700	-1.51403000	-2.21216500
C	-5.12979600	-1.44980900	-1.33036700
C	-3.49650600	-1.71427800	-3.13991300
C	-4.84312400	-1.65516500	-2.69902800
C	2.57063300	-1.65797300	-0.40573600
C	2.10046300	-2.14416400	-1.63014300
C	3.51448800	-2.39759800	0.30965100
C	2.52282400	-3.37206100	-2.13571500
C	4.01778100	-3.60258600	-0.19860400
C	3.48247700	-4.11418600	-1.40362800
C	3.34789300	1.14690200	0.02167900
C	4.67068700	0.72833500	-0.13029800
C	3.07921300	2.51971200	0.09782400
C	5.72305300	1.65115200	-0.20695600
C	4.10061600	3.46877000	0.06488100
C	5.44084700	3.03136100	-0.09205300
H	-1.77280400	-3.61958400	-0.60496500
H	-0.70345300	-5.74680300	0.05939900
H	2.55534800	1.74745500	2.35528700
H	1.86911400	1.85467300	4.70711400
H	-1.32605200	1.86350500	1.27266600
H	-2.90971400	-1.92246700	2.46229900
H	-4.30204000	-1.01504900	0.59823200
H	-1.44030400	-1.55034100	-2.55578300
H	1.37200000	-1.56245700	-2.18824200
H	3.86769900	-2.03261500	1.26965500
H	4.89654700	-0.32852600	-0.20705300
H	2.05247300	2.85930600	0.18195100

N	6.45600800	4.04003900	-0.13658500
C	7.41433700	4.09653400	0.95658900
H	6.90311100	3.87501500	1.89836900
H	8.26780100	3.40348200	0.85939500
H	7.82117100	5.11346100	1.02355300
C	6.97289100	4.40006600	-1.44790500
H	6.14750800	4.45406300	-2.16402100
H	7.44090500	5.39063200	-1.39346400
H	7.72393000	3.69505400	-1.84811600
N	3.85121400	-5.38884500	-1.93798500
N	-5.86552500	-1.79228200	-3.69000700
N	-3.83543500	1.65737500	5.16846800
C	3.58506000	-6.57608100	-1.14083200
H	3.43110400	-7.43168000	-1.81112900
H	4.38877400	-6.84850900	-0.43578000
H	2.66622800	-6.42447000	-0.56613500
C	5.04982900	-5.43917600	-2.76130300
H	5.07273100	-4.57254400	-3.42972600
H	5.99079400	-5.44548800	-2.18220000
H	5.03013100	-6.34585000	-3.37819700
C	-6.73958600	-0.65286900	-3.92456500
H	-7.13688600	-0.71165000	-4.94601500
H	-7.60134200	-0.58188400	-3.23812400
H	-6.15911300	0.27019900	-3.83641000
C	-6.46955600	-3.10591700	-3.84219000
H	-7.21481200	-3.35409400	-3.06468500
H	-6.97035500	-3.16496000	-4.81619900
H	-5.68831400	-3.87245900	-3.81595800
C	-2.94675500	1.81160500	6.30951300
H	-2.25531500	2.67041300	6.22918100
H	-3.54280000	1.94396200	7.22040900
H	-2.34201400	0.90557400	6.42748700
C	-4.85113800	2.69255800	5.03355400
H	-5.44359000	2.50508700	4.13359300
H	-5.52543000	2.64824500	5.89845900
H	-4.45773600	3.72106900	4.97257400
C	7.13848000	1.11562600	-0.39841600
H	7.79986500	1.96073800	-0.59480500
C	7.24269700	0.17642000	-1.61494400
H	6.65761700	-0.74007300	-1.47532600
H	6.88435800	0.66783600	-2.52615500
H	8.28567500	-0.12036300	-1.77300200
C	7.63847100	0.42019300	0.88239700
H	8.66753200	0.06571600	0.75294600
H	7.61614400	1.10171300	1.73935700
H	7.01334800	-0.44614500	1.12549800
C	3.74396600	4.94603900	0.15664300
H	4.67782400	5.48391400	0.34093100
C	3.16179200	5.44021700	-1.18177300
H	2.23631300	4.90812800	-1.42598200
H	2.92699000	6.50951300	-1.13069200
H	3.86717600	5.28571100	-2.00568900
C	2.77296000	5.24921900	1.31229200
H	1.78064500	4.81528900	1.13914300
H	3.15171300	4.86353900	2.26585600
H	2.63644600	6.33182800	1.41276000
C	-3.14703100	-1.99572900	-4.59455300
H	-4.08962100	-1.98981600	-5.14820200
C	-2.51219300	-3.39130700	-4.74232700
H	-1.56462100	-3.45754400	-4.19679600
H	-3.17480400	-4.17312500	-4.35383600



H	-2.30743100	-3.61213900	-5.79645100
C	-2.24294500	-0.90535000	-5.19607900
H	-2.04469900	-1.11648100	-6.25318100
H	-2.72065800	0.07604100	-5.12229600
H	-1.27436900	-0.84410200	-4.68455700
C	-6.54731200	-1.48453900	-0.76679600
H	-7.22983400	-1.76707000	-1.56977900
C	-6.68274700	-2.55672400	0.33223700
H	-6.06137000	-2.32245400	1.20492000
H	-7.72196400	-2.62122100	0.67412200
H	-6.38173700	-3.54288600	-0.03799000
C	-6.98839700	-0.10393100	-0.24713400
H	-6.33918900	0.23653500	0.56923900
H	-6.94943800	0.64564800	-1.04354700
H	-8.01404800	-0.14700200	0.13677500
H	1.02192400	-5.77551400	1.83837800
H	0.48530800	0.06969200	5.69401400
O	-0.31423600	-2.13973200	4.35618500
O	1.89070100	-3.58474200	3.13826300
C	-0.61611600	-2.16842200	5.74574000
H	-1.29755400	-1.35360400	6.02268000
H	-1.11128000	-3.12368900	5.92372300
H	0.29480400	-2.11201300	6.35489500
C	1.94116600	-4.66792900	4.06445200
H	2.41059100	-5.55835100	3.63094000
H	2.55324700	-4.31936100	4.89867700
H	0.93464100	-4.91691000	4.42052500
C	5.14191100	-4.30756300	0.55395100
H	5.51511700	-5.11615800	-0.07684400
C	6.32951200	-3.36097500	0.81095300
H	6.06255200	-2.56003900	1.50967300
H	7.16687600	-3.91346600	1.25166600
H	6.67825900	-2.89661400	-0.11808800
C	4.64373900	-4.92515600	1.87171500
H	4.25265800	-4.15011100	2.53739600
H	3.83801600	-5.64373500	1.68764400
H	5.45886200	-5.44751700	2.38554100
C	1.90479000	-3.93658600	-3.40906300
H	2.66308300	-4.55202000	-3.90108400
C	0.73163400	-4.86682000	-3.04078100
H	-0.04470300	-4.31234800	-2.50119600
H	0.28275000	-5.30086100	-3.94164100
H	1.07082300	-5.68312600	-2.39637300
C	1.45375700	-2.85873700	-4.40691700
H	0.59764400	-2.28266400	-4.03503100
H	2.26177200	-2.15381900	-4.63440500
H	1.13414000	-3.32699600	-5.34377900
C	-4.30491500	-1.10525600	4.66944700
H	-4.09836100	-0.79556100	5.70006100
C	-4.06631600	-2.62009400	4.56138900
H	-4.44813600	-3.02085800	3.61412500
H	-3.00557800	-2.87878200	4.62496800
H	-4.59863900	-3.13755100	5.36650800
C	-5.79187400	-0.80083900	4.38937400
H	-6.04632000	-1.05670800	3.35302500
H	-6.43505200	-1.39397300	5.04982000
H	-6.02091300	0.25448200	4.54987800
C	-2.23246400	3.39618400	3.25823000
H	-2.54059200	3.68373100	4.26487800
C	-0.74700500	3.78190800	3.12234200
H	-0.36695600	3.60986700	2.10812500

H	-0.61337000	4.84685600	3.34405300
H	-0.12214900	3.20286300	3.80827400
C	-3.09224700	4.18956300	2.25312300
H	-2.81922800	3.93833100	1.22044200
H	-4.15772800	3.96923800	2.37650900
H	-2.95007500	5.26842900	2.38688100
Rh	0.15783800	0.60013900	-1.05874200
C	-0.65392800	5.53904000	-0.71616400
C	-0.62935000	4.22745600	-1.18471300
C	-0.24783500	3.93535400	-2.50248400
C	0.08781800	4.99571700	-3.35320400
C	0.07763900	6.31511600	-2.90018900
C	-0.28773600	6.56441400	-1.58242200
H	-0.95297000	5.77342500	0.29976700
H	-0.93089000	3.42667900	-0.52133300
H	0.37260700	4.79136000	-4.38236400
H	0.34508400	7.14321900	-3.54743600
F	-0.29191000	7.83238900	-1.13171800
C	-0.11545000	2.51866600	-3.00943700
C	1.11520700	1.77686600	-2.48929800
C	-2.53186900	2.05085300	-2.60908200
C	-3.05334400	2.46117500	-3.83636100
C	-4.39358700	2.84577800	-3.91059600
C	-5.20244600	2.81986300	-2.77114600
C	-4.66192200	2.41065300	-1.55002900
C	-3.32335000	2.02940400	-1.46409600
H	-2.42412900	2.47778300	-4.71945100
H	-4.80361900	3.16621100	-4.86391800
H	-6.24294800	3.12423400	-2.83400100
H	-5.27623100	2.39286200	-0.65560900
H	-2.89535800	1.71785000	-0.51990900
H	0.20274500	1.76866600	-0.08986300
H	1.91606400	2.44431600	-2.17815800
H	-0.18398700	2.51566900	-4.10360400
H	1.50420100	1.05959400	-3.22761200
O	-1.20652900	1.63551200	-2.50717400

## 2-S

B3LYP-D3 SCF energy: -630.432938 a.u.

B3LYP-D3 enthalpy: -630.327072 a.u.

B3LYP-D3 free energy: -630.363450 a.u.

M06 SCF energy in solution: -630.291818 a.u.

## Cartesian coordinates

ATOM	X	Y	Z
C	0.49915100	-0.00004000	-0.00815000
C	-0.20303900	1.21154900	-0.01006500
C	-1.59931600	1.20876700	0.00446700
C	-2.29886900	0.00004600	0.01325200
C	-1.59940100	-1.20870600	0.00463000
C	-0.20310400	-1.21157300	-0.00969900
H	0.34519700	2.14848800	-0.02348200
H	-2.13920700	2.15188900	0.00602600
H	-3.38547600	0.00008500	0.02210900
H	-2.13934500	-2.15179600	0.00637500
H	0.34509700	-2.14853600	-0.02259200
H	2.53030300	0.00484700	1.25782100
S	2.30443100	-0.00032700	-0.07580400

## 3-S

B3LYP-D3 SCF energy: -5150.384776 a.u.

B3LYP-D3 enthalpy: -5148.501680 a.u.  
 B3LYP-D3 free energy: -5148.752167 a.u.  
 M06 SCF energy in solution: -5149.275623 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.29125800	-4.28491000	0.96491800
C	0.19288200	-3.11272200	0.34717000
C	1.05280000	-2.26766100	1.07488500
C	1.44270800	-2.61325300	2.37767200
C	0.96233500	-3.78281400	2.96214100
C	0.08934900	-4.61723400	2.26868800
C	-0.16898000	-2.88002500	-1.08511800
C	-1.02861700	-1.85160900	-1.51504100
C	0.37156900	-3.76323400	-2.04823300
C	-1.36891700	-1.73834200	-2.87255900
C	0.03888900	-3.63529900	-3.40046300
C	-0.84195500	-2.63201700	-3.79863500
P	1.60999100	-0.69369800	0.29777300
P	-1.55638400	-0.53696100	-0.33024800
C	2.59842200	-1.22353300	-1.13904700
C	2.41813500	-0.58858700	-2.36481300
C	3.55239100	-2.24114300	-1.02001700
C	3.18614800	-0.93437400	-3.48414900
C	4.34875700	-2.60627000	-2.10507300
C	4.17216200	-1.93523000	-3.34604800
C	2.78997800	0.08919000	1.46101600
C	4.07118200	0.46652500	1.05435700
C	2.32147600	0.52837400	2.70657200
C	4.87709000	1.29314700	1.85011200
C	3.11376900	1.30686400	3.55314600
C	4.39273600	1.72748400	3.10573800
C	-2.39770800	-1.39201500	1.04232200
C	-2.09006800	-1.01136700	2.35191100
C	-3.35160000	-2.38761400	0.82494300
C	-2.72241300	-1.60088700	3.44702600
C	-4.02697900	-2.98773900	1.89454700
C	-3.68776400	-2.61181900	3.21561000
C	-2.82792600	0.41862100	-1.24267600
C	-4.20684700	0.26469500	-1.09676600
C	-2.35010400	1.37798200	-2.14541200
C	-5.10624100	1.02861300	-1.85686600
C	-3.20721800	2.12433500	-2.95055300
C	-4.60496700	1.91928900	-2.83716900
H	2.12919200	-1.98580200	2.93196600
H	1.26841200	-4.04585100	3.97040400
H	-2.03806100	-0.95608900	-3.20781900
H	-1.11021800	-2.54157100	-4.84719100
H	1.64451900	0.16772600	-2.45572000
H	3.66811800	-2.74694600	-0.06770600
H	4.44796800	0.12698600	0.09509000
H	1.31325300	0.26918500	3.01621000
H	-1.30692700	-0.27666000	2.50764600
H	-3.56989500	-2.70440500	-0.19079200
H	-4.59565400	-0.44245900	-0.37192200
H	-1.27634500	1.52092500	-2.23789700
N	-5.45031400	2.62072500	-3.75037200
C	-6.33208100	1.85841100	-4.62016700
H	-5.85715700	0.90548200	-4.87019900
H	-7.32833800	1.64354100	-4.19820700
H	-6.48368400	2.41627500	-5.55339000

C	-5.92991700	3.93271600	-3.35558600
H	-5.10835000	4.51274600	-2.92531000
H	-6.29818900	4.46701800	-4.23955500
H	-6.75138200	3.90213600	-2.61480700
N	-4.26655400	-3.22730200	4.37259600
N	5.13404600	2.59824800	3.96838400
N	5.02902800	-2.33972900	-4.42388200
C	-4.00930300	-4.64111400	4.59543500
H	-4.08183200	-4.85553500	5.66949200
H	-4.70064800	-5.32531900	4.07368400
H	-2.99082800	-4.87618700	4.27063300
C	-5.57715300	-2.75055200	4.78557600
H	-5.60087100	-1.65713800	4.73312200
H	-6.41307100	-3.13779800	4.17528300
H	-5.75908300	-3.04521000	5.82632300
C	5.34022900	3.97125400	3.53202500
H	5.51005700	4.60600000	4.41101400
H	6.19503800	4.11565900	2.84862900
H	4.44115100	4.33016700	3.02235300
C	6.22703900	2.00058700	4.72051200
H	7.14111000	1.81767600	4.12760300
H	6.49580500	2.66174800	5.55318500
H	5.89966000	1.04364100	5.13949500
C	4.43578300	-3.22176500	-5.41636000
H	3.73995100	-2.71987800	-6.11291000
H	5.23173000	-3.68411400	-6.01248100
H	3.88430400	-4.02202800	-4.91025300
C	5.98180400	-1.36855800	-4.94382600
H	6.36589300	-0.76063100	-4.11961200
H	6.82800800	-1.90172400	-5.39557900
H	5.57505700	-0.68345800	-5.70725800
C	-6.59815300	0.88256500	-1.57341100
H	-7.12801700	1.64878700	-2.14318300
C	-6.91660100	1.13902600	-0.08712700
H	-6.46777300	0.37886700	0.56295700
H	-6.54566600	2.11884300	0.23575600
H	-7.99978000	1.11521100	0.07723400
C	-7.12868800	-0.49345100	-2.01725300
H	-8.20755400	-0.56866400	-1.83930400
H	-6.94513300	-0.66680100	-3.08260400
H	-6.64036900	-1.29863600	-1.45651500
C	-2.59982000	3.11510700	-3.93368700
H	-3.42454600	3.59891800	-4.46308000
C	-1.78606600	4.19908000	-3.19935700
H	-0.92172800	3.76578200	-2.67977500
H	-1.40728900	4.93921400	-3.91424200
H	-2.39188800	4.71909000	-2.45109000
C	-1.73544500	2.39322100	-4.98497800
H	-0.87541600	1.89324200	-4.52247200
H	-2.31682800	1.63469500	-5.52093400
H	-1.34767900	3.10830900	-5.71976600
C	2.56786500	1.69943500	4.92024000
H	3.37761200	2.20591000	5.45172100
C	2.15281100	0.46085500	5.73648200
H	1.30380900	-0.06329800	5.28222800
H	2.98003400	-0.25268700	5.82358100
H	1.85104100	0.75691400	6.74755500
C	1.39773900	2.69332100	4.79382500
H	0.98489700	2.92977100	5.78113900
H	1.72588500	3.63176900	4.33542400
H	0.58568200	2.28968200	4.17724800

C	6.23018700	1.71875900	1.29158100	H	3.11842400	1.81833200	-5.61105600
H	6.76662100	2.26905100	2.06552100	Rh	0.08156500	0.95350600	0.09043200
C	7.10594200	0.51123700	0.90755000	C	-2.29113600	3.84319800	0.69629400
H	6.66537500	-0.06844000	0.08802500	C	-3.59829700	3.63505300	0.24628300
H	8.09368500	0.85072300	0.57625000	C	-4.33896300	4.71973100	-0.22293000
H	7.24407900	-0.16313200	1.75968500	C	-3.76863000	5.99396500	-0.28427700
C	6.03848600	2.67039600	0.09326700	C	-2.45236700	6.18492600	0.14336600
H	5.54034300	2.15719500	-0.73920200	C	-1.71308800	5.11544000	0.65018400
H	5.42819300	3.53788600	0.36968300	H	-4.03570900	2.64231800	0.25616200
H	7.00523800	3.03463100	-0.27229000	H	-5.36278900	4.56158100	-0.54688000
H	-0.28279000	-5.52112900	2.73693300	H	-4.34840800	6.83315500	-0.65748900
H	0.45323500	-4.30850000	-4.14070500	H	-2.00068600	7.17207100	0.10438200
O	1.21731700	-4.71580800	-1.56821500	H	-0.70860200	5.27570400	1.02397300
O	-1.13325800	-5.04820100	0.21435400	H	-2.36578000	1.73911400	1.75696600
C	1.79795600	-5.63066000	-2.48757500	C	1.74816100	4.19018500	0.03541000
H	2.44324100	-5.11233200	-3.20906200	C	1.52885100	5.34383200	-0.72253200
H	2.40393300	-6.31139700	-1.88840300	C	1.51656100	6.58970400	-0.08919700
H	1.03180500	-6.20469900	-3.02439000	C	1.72729300	6.67840500	1.28815900
C	-1.19964800	-6.44188400	0.49648000	C	1.94411100	5.51751000	2.03872500
H	-1.72451100	-6.64703600	1.43696000	C	1.94736000	4.26743700	1.41861200
H	-1.76580400	-6.88557800	-0.32417800	H	1.36834500	5.26854300	-1.79361700
H	-0.19409400	-6.87854900	0.53453400	H	1.34609100	7.48807200	-0.67528400
C	-5.10546400	-4.02026200	1.58339300	H	1.72027000	7.64755000	1.77819500
H	-5.63215500	-4.25663100	2.50956700	H	2.10185600	5.58555300	3.11127000
C	-6.15696500	-3.46545000	0.60330900	H	2.09540400	3.36099400	1.99595200
H	-5.72975200	-3.28409200	-0.38959700	H	2.92974300	2.17130900	-0.41284500
H	-6.97713200	-4.18162400	0.48045600	S	-1.31265500	2.49555400	1.38622600
H	-6.57939900	-2.52165500	0.96666300	S	1.70483000	2.59479600	-0.80083400
C	-4.48710000	-5.32481200	1.04864200				
H	-3.88962200	-5.13697300	0.14994000				
H	-3.82729900	-5.77568800	1.79655600	<b>4-ts-S</b>			
H	-5.26920700	-6.05158900	0.80047100	B3LYP-D3 SCF energy: -5150.360713 a.u.			
C	-2.32916900	-1.20001700	4.86357800	B3LYP-D3 enthalpy: -5148.480714 a.u.			
H	-3.18319400	-1.41418800	5.51187200	B3LYP-D3 free energy: -5148.724923 a.u.			
C	-1.15586600	-2.07186200	5.35068700	M06 SCF energy in solution: -5149.253230 a.u.			
H	-0.27704900	-1.92497400	4.71274400	Imaginary frequency: -714.45 cm <sup>-1</sup>			
H	-0.88259000	-1.81512900	6.38099700				
H	-1.41829300	-3.13416400	5.31786100	Cartesian coordinates			
C	-1.98778900	0.29263300	5.00055000	ATOM X Y Z			
H	-1.06493800	0.55613800	4.47041400	C -0.07237700 -1.19742700 3.65986400			
H	-2.79168200	0.92887000	4.61212600	C -0.37728800 -0.44539800 2.50276700			
H	-1.83242100	0.54724100	6.05460400	C -1.18727800 -1.03063700 1.50724400			
C	5.42514800	-3.67438500	-1.94546100	C -1.68488300 -2.32982800 1.69899000			
H	5.48891600	-4.21637600	-2.89461800	C -1.38223800 -3.04477900 2.85406700			
C	5.12644600	-4.68785700	-0.82866200	C -0.57234200 -2.48814900 3.83809800			
H	5.24916800	-4.24424500	0.16689500	C 0.17250500 0.94222500 2.44824800			
H	4.10561500	-5.07764400	-0.89276100	C 1.16873000 1.34504300 1.53764200			
H	5.82457100	-5.52937000	-0.89316300	C -0.26864100 1.86606300 3.42745100			
C	6.79828700	-3.01479900	-1.70419000	C 1.72419800 2.63223900 1.63708400			
H	6.78305300	-2.42590800	-0.77829600	C 0.26891100 3.15327100 3.49482800			
H	7.58058700	-3.77666400	-1.60681000	C 1.27653200 3.52014500 2.60772500			
H	7.07064600	-2.35164400	-2.52913700	P -1.60782600 -0.11618400 -0.05787300			
C	2.91812100	-0.19426700	-4.79082600	P 1.67370700 0.24340500 0.13165900			
H	3.55856700	-0.61403000	-5.56721600	C -2.22260600 1.49185400 0.54912500			
C	1.46478700	-0.38150500	-5.26301100	C -1.75639600 2.67361100 -0.02340000			
H	0.74636900	0.02194000	-4.54089200	C -3.13254200 1.55705700 1.61033500			
H	1.30608900	0.13273400	-6.21792400	C -2.18133300 3.92613200 0.43183500			
H	1.23044100	-1.44228500	-5.39636600	C -3.61254700 2.78202100 2.07276500			
C	3.27065000	1.30014600	-4.65726600	C -3.12692200 3.97865900 1.48191500			
H	2.64146900	1.79074300	-3.90453000	C -3.05480400 -1.07179900 -0.67118300			
H	4.31654700	1.43403100	-4.35885600	C -4.37050500 -0.70775000 -0.38297200			

C	-5.44923000	-1.53908300	-0.71091200	H	-5.05618200	6.70517300	1.82629800
C	-3.87393700	-3.10964100	-1.73818800	H	-3.77168400	6.82648900	0.60806200
C	-5.20328300	-2.73940200	-1.41349700	C	7.02710500	0.55632700	-0.06029800
C	2.09825000	-1.38220300	0.84924100	H	7.82159500	1.04094500	-0.63047500
C	1.63502500	-2.53957800	0.21585100	C	7.17389400	-0.95774700	-0.28632000
C	2.90766700	-1.49798300	1.98192500	H	6.43854700	-1.53338300	0.28679800
C	1.97355700	-3.80921100	0.68362200	H	7.04458600	-1.21369700	-1.34069600
C	3.29994900	-2.75378000	2.46334200	H	8.16914300	-1.28757400	0.03224900
C	2.80993700	-3.91543900	1.82267600	C	7.24021900	0.91001400	1.42603700
C	3.25398400	0.99834800	-0.43141300	H	8.21908800	0.55702200	1.77069400
C	4.51070700	0.47553500	-0.12397200	H	7.18769200	1.99103000	1.59134200
C	3.18143200	2.18642500	-1.17087900	H	6.47246000	0.43796600	2.04811800
C	5.68818100	1.11617900	-0.53285900	C	4.18672600	4.17122900	-2.35190600
C	4.32907000	2.85123200	-1.60669500	H	5.18293000	4.43613000	-2.71572000
C	5.59821700	2.30757300	-1.28984500	C	3.23981700	4.07651200	-3.56028100
H	-2.32517000	-2.78720100	0.95729500	H	2.20843900	3.85479600	-3.26064500
H	-1.77807500	-4.04750900	2.98379500	H	3.22738000	5.02784900	-4.10387200
H	2.51415200	2.94635900	0.96981600	H	3.55404900	3.29137000	-4.25664400
H	1.71666900	4.51107600	2.67484800	C	3.72959000	5.27725400	-1.37999900
H	-1.02217700	2.61683200	-0.82104500	H	2.73833400	5.05403300	-0.96565700
H	-3.45254500	0.63904500	2.08800200	H	4.42908400	5.38127000	-0.54270100
H	-4.57316900	0.22919900	0.11975300	H	3.66818100	6.24318000	-1.89452000
H	-1.80599300	-2.58868000	-1.55435700	C	-3.56683400	-4.41350600	-2.46287600
H	0.97415400	-2.43015800	-0.63588300	H	-4.52094100	-4.79460400	-2.83672100
H	3.23905900	-0.60116600	2.49692000	C	-2.99591900	-5.45271500	-1.47878400
H	4.58446800	-0.44284300	0.44458600	H	-2.03874500	-5.11675400	-1.06492800
H	2.21004600	2.61809500	-1.39670900	H	-3.68012300	-5.62768000	-0.64085000
N	6.74918000	3.01065500	-1.77430800	H	-2.82449500	-6.41095600	-1.98306600
C	7.57598000	3.72754000	-0.81553300	C	-2.62053600	-4.22172400	-3.66067400
H	6.93409300	4.18329200	-0.05533500	H	-2.48171000	-5.17343600	-4.18601700
H	8.32721000	3.10566100	-0.29926400	H	-3.02006200	-3.49572800	-4.37666400
H	8.11128600	4.53366700	-1.33289000	H	-1.62900900	-3.86878800	-3.35319300
C	7.44670700	2.42177000	-2.90477500	C	-6.83631700	-1.15260500	-0.20194700
H	6.71835100	2.11153200	-3.66135600	H	-7.54733500	-1.91109700	-0.53103700
H	8.10061500	3.17667300	-3.35729900	C	-6.85611600	-1.15823900	1.33978800
H	8.07048400	1.54415600	-2.65476900	H	-6.19569900	-0.38351200	1.74563100
N	3.11041500	-5.24038800	2.27707500	H	-7.86827500	-0.96184400	1.71150200
N	-6.25102300	-3.62481600	-1.82737200	H	-6.52447200	-2.12363300	1.73770600
N	-3.61153400	5.20966000	2.03594700	C	-7.32560900	0.19730800	-0.75152500
C	2.65777400	-5.64334900	3.59930200	H	-6.64192800	1.01372900	-0.49131100
H	2.49317100	-6.72879000	3.60868600	H	-7.40643700	0.17019400	-1.84147100
H	3.35768400	-5.40771700	4.41906300	H	-8.31147100	0.43920500	-0.33824500
H	1.70400400	-5.15354700	3.81803400	H	-0.32959000	-3.05095000	4.73236500
C	4.38127600	-5.80417400	1.85025600	H	-0.07792300	3.86215800	4.23612800
H	4.54628600	-5.57550900	0.79216600	O	-1.22818800	1.41948200	4.28500200
H	5.25305900	-5.43028500	2.41737200	O	0.74632700	-0.59602100	4.57094100
H	4.35188300	-6.89488700	1.96270300	C	-1.53912600	2.21531300	5.42254700
C	-7.16329000	-3.14416800	-2.85251100	H	-2.05624400	3.14008900	5.13670200
H	-7.68286500	-4.00073800	-3.29867500	H	-2.20843100	1.61127600	6.03643000
H	-7.93196400	-2.43495500	-2.49776200	H	-0.63650500	2.45917100	5.99659800
H	-6.58840300	-2.65053300	-3.64229600	C	0.53154900	-0.89216300	5.94813000
C	-6.82578800	-4.49506100	-0.81288900	H	0.91312100	-1.88289300	6.22024500
H	-7.55790300	-4.00235200	-0.14844500	H	1.08872300	-0.13717800	6.50645800
H	-7.33184500	-5.33648600	-1.30171900	H	-0.53455200	-0.82620300	6.19565400
H	-6.02455900	-4.90009600	-0.18689300	C	4.23742100	-2.82333300	3.66505800
C	-2.73561000	5.85551600	3.00008600	H	4.58701000	-3.85244500	3.76289600
H	-1.87339800	6.37926800	2.54791700	C	5.48834000	-1.94665000	3.47853200
H	-3.30898600	6.59013300	3.57838700	H	5.23562800	-0.88073100	3.45921600
H	-2.34167200	5.10586100	3.69453000	H	6.18642500	-2.10070900	4.30896900
C	-4.37856100	6.11642100	1.19450000	H	6.01000400	-2.18787800	2.54622300
H	-4.98833800	5.53640500	0.49610000	C	3.50128500	-2.44665300	4.96325300

H	3.11571800	-1.42423700	4.90327900
H	2.65022600	-3.11315900	5.13823200
H	4.17479800	-2.51683400	5.82525100
C	1.40814600	-5.06238700	0.02032200
H	2.17272800	-5.84230400	0.08921800
C	0.17691400	-5.56558700	0.79863900
H	-0.61582800	-4.81095000	0.78734200
H	-0.21616200	-6.48448700	0.34840500
H	0.43109300	-5.77498600	1.84097600
C	1.05835500	-4.87968400	-1.46448700
H	0.23331800	-4.17217600	-1.61222600
H	1.91608100	-4.52390700	-2.04547600
H	0.73728300	-5.83526800	-1.89233700
C	-4.67707500	2.82803000	3.16536800
H	-4.43342900	3.66607600	3.82765500
C	-4.75728700	1.54845300	4.01417100
H	-5.21168700	0.72159400	3.45562400
H	-3.77309900	1.21464600	4.35180000
H	-5.38862500	1.72511700	4.89160600
C	-6.05951500	3.12112400	2.54508700
H	-6.33870200	2.32733300	1.84065200
H	-6.82845700	3.16454700	3.32525200
H	-6.06346300	4.07314800	2.00994800
C	-1.64017700	5.17663400	-0.25652000
H	-1.85156800	6.03581500	0.38307400
C	-0.11489400	5.14262200	-0.46299500
H	0.18450700	4.36711900	-1.17872800
H	0.23034600	6.10158600	-0.86500200
H	0.40940300	4.94815500	0.47605800
C	-2.35425800	5.40303000	-1.60474900
H	-2.13606400	4.58367900	-2.29991200
H	-3.44047500	5.45808200	-1.48162500
H	-2.01613000	6.33542700	-2.07122200
Rh	0.09028000	0.14473000	-1.63727300
C	-2.92248000	0.42183600	-3.45850000
C	-4.02186200	-0.31851900	-3.91586600
C	-5.29679700	0.24401800	-3.87622400
C	-5.48774400	1.53226700	-3.36931100
C	-4.39517900	2.26464700	-2.90048900
C	-3.11611300	1.71700400	-2.95852400
H	-3.87491700	-1.32270400	-4.29721500
H	-6.14651700	-0.32772900	-4.23785500
H	-6.48405000	1.96290700	-3.34077900
H	-4.53093700	3.26681000	-2.50390000
H	-2.25887100	2.28807100	-2.62847400
H	-0.59208800	-1.15773000	-2.36310700
C	3.22837500	-0.56603600	-3.33296200
C	4.46408700	-0.07053300	-3.75528100
C	5.57873900	-0.91011800	-3.73463400
C	5.45720800	-2.22695300	-3.28567900
C	4.22057500	-2.70713000	-2.84728800
C	3.09964400	-1.87839500	-2.87333400
H	4.55177400	0.95710600	-4.09084200
H	6.54202400	-0.53076000	-4.06259600
H	6.32751900	-2.87655400	-3.27011000
H	4.12737400	-3.72634300	-2.48373000
H	2.13501100	-2.23837200	-2.53842400
H	1.19743300	-0.02799400	-4.48695200
S	1.79875200	0.53163300	-3.41201600
S	-1.27042500	-0.20513600	-3.68354400

## 5-S

B3LYP-D3 SCF energy: -5150.378630 a.u.

B3LYP-D3 enthalpy: -5148.496084 a.u.

B3LYP-D3 free energy: -5148.744810 a.u.

M06 SCF energy in solution: -5149.268479 a.u.

### Cartesian coordinates

ATOM	X	Y	Z
C	0.05573500	1.51119700	3.52950300
C	0.36877900	0.66756300	2.44120200
C	1.18847900	1.17060200	1.40921800
C	1.68585800	2.48082700	1.48985500
C	1.37959100	3.28507100	2.58411900
C	0.56216600	2.81057300	3.60478100
C	-0.15751800	-0.72941000	2.49595300
C	-1.14580500	-1.22069700	1.61981600
C	0.31120500	-1.57299500	3.53198900
C	-1.65454100	-2.51942300	1.79077500
C	-0.18499100	-2.87123800	3.67803100
C	-1.17609200	-3.32856600	2.81409800
P	1.64532800	0.12051800	-0.04687800
P	-1.71330700	-0.20289900	0.18216800
C	2.35608200	-1.37537300	0.71446000
C	2.00092400	-2.64440200	0.26301600
C	3.25270500	-1.25120500	1.78351000
C	2.53650100	-3.80005100	0.84527200
C	3.84756400	-2.37343400	2.35803700
C	3.48623200	-3.66188500	1.88195000
C	2.98436700	1.08580400	-0.83146100
C	4.31337300	0.96903600	-0.42429100
C	2.64031800	2.09565900	-1.73561100
C	5.29516700	1.85906300	-0.87270900
C	3.59477900	2.98605300	-2.22914400
C	4.94003000	2.86224400	-1.80297300
C	-2.24801200	1.40271400	0.87037500
C	-1.84451200	2.59964400	0.27373800
C	-3.08957800	1.45338400	1.98732200
C	-2.28117800	3.83850400	0.74617600
C	-3.56757000	2.67225400	2.48179100
C	-3.14407700	3.87570600	1.86804000
C	-3.20458500	-1.09052200	-0.41238700
C	-4.51071000	-0.69733700	-0.12862700
C	-2.99375300	-2.27041800	-1.14369500
C	-5.60818200	-1.46071400	-0.55613200
C	-4.05633200	-3.04338500	-1.60902100
C	-5.38112700	-2.62088800	-1.32909500
H	2.32550500	2.87300400	0.71023900
H	1.77836200	4.29340500	2.63728300
H	-2.42932000	-2.89875400	1.13885300
H	-1.57945100	-4.32872200	2.94251700
H	1.30107300	-2.74179700	-0.55944000
H	3.47725400	-0.26623200	2.17377200
H	4.59834400	0.18727800	0.26801100
H	1.61215500	2.18491000	-2.07043100
H	-1.14731600	2.57016600	-0.55580400
H	-3.37539700	0.52989200	2.48183900
H	-4.68890300	0.20518700	0.44354700
H	-1.97846100	-2.60005700	-1.33985700
N	-6.43983500	-3.42971500	-1.85919100
C	-7.11824900	-4.32487400	-0.93303200
H	-6.37931200	-4.79846100	-0.27863800

H	-7.87288800	-3.83239200	-0.29522600	H	3.49981700	2.85223000	-4.99932100
H	-7.62502600	-5.11504500	-1.50045300	H	1.83257000	2.78754100	-4.40287000
C	-7.27819000	-2.84959600	-2.89624000	C	6.68821800	1.75387300	-0.25763900
H	-6.65547400	-2.26958900	-3.58277500	H	7.31751600	2.53087500	-0.69305500
H	-7.75207600	-3.65736800	-3.46748200	C	6.62690400	2.02797800	1.25860600
H	-8.08140300	-2.18693000	-2.52767900	H	6.04248600	1.26016000	1.77898300
N	-3.53982300	5.16700300	2.34177700	H	7.63495200	2.02732100	1.68871400
N	5.89167700	3.77685500	-2.35716900	H	6.16456500	2.99915100	1.46750000
N	4.11590800	-4.78312500	2.51799400	C	7.35991500	0.40051200	-0.54575400
C	-3.08741800	5.58742000	3.65785300	H	6.77494000	-0.43345900	-0.13991600
H	-3.03880700	6.68347000	3.68918800	H	7.46433700	0.23451000	-1.62127400
H	-3.72832300	5.25984000	4.49445400	H	8.35592300	0.36501700	-0.08987200
H	-2.07880600	5.19881300	3.83079300	H	0.31936200	3.44462800	4.44999900
C	-4.84872000	5.64756500	1.92981600	H	0.18462400	-3.52193200	4.46056300
H	-4.99544700	5.43610200	0.86535500	O	1.25178400	-1.04043500	4.36011100
H	-5.69250700	5.19869100	2.48440900	O	-0.76688300	0.98509500	4.48107300
H	-4.89695200	6.73425000	2.06986100	C	1.63375600	-1.78183100	5.51274300
C	6.95747600	3.23217500	-3.18461800	H	2.18608300	-2.68934500	5.23829300
H	7.30048500	4.00544600	-3.88367100	H	2.29020000	-1.12650500	6.08614300
H	7.84030400	2.87351500	-2.62726700	H	0.76194300	-2.04919300	6.12277700
H	6.56486800	2.39433300	-3.76682700	C	-0.55895400	1.39157800	5.83062900
C	6.24340600	4.92934900	-1.54335200	H	-0.91853100	2.41050900	6.01511100
H	6.94102800	4.70308600	-0.71662600	H	-1.14011900	0.70054700	6.44398300
H	6.71153000	5.69220400	-2.17720000	H	0.50292800	1.32206200	6.09475800
H	5.33475000	5.36014900	-1.10953300	C	-4.52886700	2.65835200	3.66645400
C	3.32264100	-5.47347500	3.52228500	H	-4.93494100	3.66429700	3.78555900
H	2.52858900	-6.12026900	3.10668900	C	-5.72543300	1.72007300	3.42731300
H	3.97979100	-6.10092800	4.13637100	H	-5.41452300	0.66996000	3.39860900
H	2.84427700	-4.73827200	4.17860000	H	-6.45507900	1.82116400	4.23842900
C	4.97791400	-5.64013800	1.71415100	H	-6.23128100	1.94894700	2.48278600
H	5.50802300	-5.03134700	0.97624900	C	-3.79900500	2.28886200	4.97033300
H	5.72475900	-6.11087600	2.36623300	H	-3.33534500	1.30029600	4.89036300
H	4.45360300	-6.44572500	1.17345200	H	-3.00550500	3.00985200	5.19035100
C	-7.00063700	-1.06277100	-0.07455500	H	-4.49771700	2.27991800	5.81484400
H	-7.73564800	-1.66840900	-0.60573200	C	-1.79275200	5.11823000	0.07573900
C	-7.34440600	0.40987500	-0.35292500	H	-2.40851700	5.93330000	0.46399400
H	-6.66968400	1.09547500	0.17249200	C	-0.33391300	5.41634400	0.46664900
H	-7.27775200	0.63365600	-1.42078700	H	0.33628800	4.62003800	0.12419100
H	-8.36381200	0.62765300	-0.01517000	H	-0.00081600	6.35896200	0.01680000
C	-7.14181900	-1.38958700	1.42607000	H	-0.22845000	5.49525000	1.55336000
H	-8.15302100	-1.15473900	1.77788600	C	-1.94547300	5.08921300	-1.45409600
H	-6.94811700	-2.44979900	1.62120200	H	-1.31334400	4.32198900	-1.91805500
H	-6.43320700	-0.80381200	2.02100800	H	-2.98215300	4.89858200	-1.75114800
C	-3.79091800	-4.30963800	-2.41577200	H	-1.64553200	6.05234300	-1.88155400
H	-4.61906400	-4.99566300	-2.21478600	C	4.90438400	-2.20894300	3.44670100
C	-3.81261000	-4.00196400	-3.92622200	H	4.74391300	-3.00375500	4.18363700
H	-3.01982900	-3.29066800	-4.18808600	C	4.84429500	-0.85445200	4.17247000
H	-3.65104900	-4.91673900	-4.50783200	H	5.21681300	-0.04112200	3.53777100
H	-4.77583600	-3.57846700	-4.22695600	H	3.82802500	-0.59249000	4.47839700
C	-2.47977700	-5.01530300	-2.03252300	H	5.48228600	-0.88180800	5.06228700
H	-1.59631100	-4.44677500	-2.34853700	C	6.31538700	-2.41060100	2.85535200
H	-2.40781800	-5.17906100	-0.95113300	H	6.51598600	-1.66004600	2.08032300
H	-2.42442500	-5.99067500	-2.52757100	H	7.07714400	-2.29998500	3.63595300
C	3.15938800	4.06355500	-3.21270300	H	6.42477900	-3.40216100	2.41150600
H	4.03849300	4.67995400	-3.41774000	C	2.08480300	-5.15303500	0.30170300
C	2.06453000	4.96604800	-2.61454000	H	2.50976900	-5.93639100	0.93021200
H	1.13840000	4.40940500	-2.42448700	C	0.55580200	-5.31928600	0.36040700
H	2.38546000	5.40721800	-1.66386500	H	0.04053100	-4.57995900	-0.26237600
H	1.82086700	5.78248700	-3.30401000	H	0.27034100	-6.31313800	-0.00301700
C	2.69909900	3.44608100	-4.54587400	H	0.18750500	-5.20388400	1.38365100
H	2.41221500	4.23042100	-5.25576600	C	2.60326300	-5.37131900	-1.13312100

H	2.16590800	-4.64312900	-1.82642700	C	2.01735500	-0.70430900	2.84721800
H	3.69320300	-5.27169800	-1.18314700	C	4.78741100	-1.05604700	2.57160500
H	2.33622000	-6.37265500	-1.48964000	C	2.81507100	-0.70493200	3.99094000
Rh	-0.08251100	-0.29228900	-1.51860100	C	4.21830900	-0.86967600	3.84983300
C	3.04866300	-1.10924300	-3.22675200	C	-2.52366800	-1.81544000	0.24973800
C	3.59179100	-0.16492400	-4.11215600	C	-2.22124600	-2.11861400	1.57841500
C	3.91217100	-1.94900900	-2.50708800	C	-3.40885800	-2.63572900	-0.45620700
C	4.97182500	-0.06865200	-4.27922600	C	-2.79680100	-3.21641600	2.22240300
H	2.92698400	0.48104700	-4.67482800	C	-4.01014300	-3.74211400	0.15301600
C	5.29273600	-1.84892500	-2.68008000	C	-3.68472300	-4.04649500	1.49770200
H	3.50635500	-2.68212600	-1.82228300	C	-3.21780700	0.85098000	-0.72441600
C	5.82766900	-0.91481500	-3.56976600	C	-4.51631900	0.53434000	-0.32320300
H	5.37677400	0.65666000	-4.98012400	C	-2.96273000	2.13352900	-1.23434900
H	5.95136200	-2.50912000	-2.12198000	C	-5.55950100	1.46464000	-0.42372400
H	6.90201700	-0.85293300	-3.71747000	C	-3.99080900	3.05782900	-1.43187100
H	-0.25897700	1.22505500	-1.59830000	C	-5.30467900	2.72630200	-1.00767000
C	-3.23363000	0.42850900	-3.35566200	H	1.71363800	-3.12916300	1.72616800
C	-4.39329500	-0.16157200	-3.86633800	H	0.90303000	-5.43644100	1.43760800
C	-5.59832100	0.54158800	-3.81502400	H	-2.30243800	0.83850000	-3.18809000
C	-5.64422000	1.81686600	-3.24998500	H	-1.18944700	0.50695200	-5.35350800
C	-4.48379600	2.39106700	-2.72604000	H	2.00019400	1.62794500	-1.64316700
C	-3.27385600	1.70117200	-2.78037400	H	3.27341900	-2.45216700	-1.32539600
H	-4.35152400	-1.15269300	-4.30395900	H	4.40594900	-1.06723400	0.45929400
H	-6.50003600	0.09196100	-4.21977900	H	0.94271300	-0.58073400	2.94597800
H	-6.58309600	2.36149000	-3.21363800	H	-1.50256000	-1.50644500	2.11458900
H	-4.51881900	3.37591500	-2.27153500	H	-3.63365900	-2.40791900	-1.49415300
H	-2.37341400	2.14412300	-2.37555500	H	-4.72572100	-0.44428200	0.09197900
H	-1.02790900	0.32988600	-4.30141900	H	-1.95152600	2.40413100	-1.52118200
S	-1.69608500	-0.50513700	-3.48009400	N	-6.32114300	3.71379100	-1.19818800
S	1.27558900	-1.30685500	-3.17941000	C	-7.42427400	3.41539000	-2.09919200
				H	-7.05475400	2.82335200	-2.94162900
				H	-8.26278900	2.86776500	-1.63656900
				H	-7.82499000	4.35637000	-2.49699600
				C	-6.65567200	4.54326600	-0.05042400
				H	-5.74083000	4.82240800	0.48075800
				H	-7.14298700	5.46328000	-0.39537500
				H	-7.33225300	4.05436400	0.67374900
				N	-4.20874300	-5.19122500	2.17891700
				N	4.99660300	-0.82124200	5.05060500
				N	5.16119100	0.06608400	-4.64980400
				C	-3.79788000	-6.50518600	1.71073900
				H	-3.88364700	-7.22439300	2.53508200
				H	-4.38443400	-6.90020800	0.86306000
				H	-2.74741100	-6.46365700	1.40520700
				C	-5.56141300	-5.08833200	2.70346500
				H	-5.68941700	-4.11572700	3.18989200
				H	-6.35455000	-5.19418100	1.94162800
				H	-5.71710200	-5.86834300	3.45844600
				C	5.98162700	0.24314200	5.18767100
				H	6.14050600	0.44745700	6.25413400
				H	6.96615900	0.02192100	4.74195500
				H	5.59757000	1.15445800	4.72038900
				C	5.37543500	-2.10172900	5.62946300
				H	6.20694100	-2.60458100	5.10353900
				H	5.68019300	-1.95216100	6.67223600
				H	4.51361800	-2.77725100	5.62058100
				C	4.61400400	-0.13661300	-5.98168300
				H	3.99331700	0.70162500	-6.34644800
				H	5.43600300	-0.28087300	-6.69287800
				H	3.99713000	-1.04153900	-5.99396100
				C	6.19833300	1.08699600	-4.56027800

#### 7-S

B3LYP-D3 SCF energy: -4928.809006 a.u.

B3LYP-D3 enthalpy: -4926.900674 a.u.

B3LYP-D3 free energy: -4927.151574 a.u.

M06 SCF energy in solution: -4927.671924 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z
C	-0.38575000	-4.06792000	-1.39008900
C	0.06586400	-2.73935700	-1.24707800
C	0.82835700	-2.40431800	-0.11034900
C	1.12023800	-3.37999300	0.85636900
C	0.66662400	-4.68578500	0.68970800
C	-0.08442500	-5.03701600	-0.42833600
C	-0.27243600	-1.78087100	-2.34185500
C	-1.21606800	-0.74664400	-2.18881600
C	0.32723600	-1.97745400	-3.60732400
C	-1.55432900	0.06309600	-3.28421300
C	0.01772400	-1.13627400	-4.68097800
C	-0.93101400	-0.13054700	-4.51292800
P	1.50376100	-0.70531300	0.10653200
P	-1.82075700	-0.31151400	-0.49685400
C	2.54198000	-0.42981500	-1.35786600
C	2.59273500	0.79906800	-2.00806200
C	3.33718800	-1.48964000	-1.81781700
C	3.39603100	0.98807800	-3.13844100
C	4.21714300	-1.31465700	-2.88511300
C	4.24255600	-0.06245200	-3.55669000
C	2.58516100	-0.81593900	1.56942600
C	3.96048400	-0.98694800	1.44362600

H	6.52372700	1.18197800	-3.52058300	C	-4.28552300	-5.34611900	-1.77986000
H	7.06173000	0.77118300	-5.15982400	H	-3.76366300	-4.66491000	-2.45990800
H	5.89491500	2.08600400	-4.91330500	H	-3.54089000	-6.03147000	-1.36101000
C	-6.93547300	1.06144900	0.09571800	H	-5.00378400	-5.93564200	-2.36099600
H	-7.57008000	1.94923400	0.10568000	C	-2.44389200	-3.49721500	3.67653000
C	-6.87413300	0.54183500	1.54509000	H	-3.09845600	-4.30574500	4.01130100
H	-6.31900100	-0.40072900	1.61872300	C	-0.99232200	-3.99287400	3.80389000
H	-6.39182800	1.26953000	2.20715600	H	-0.28218100	-3.24709400	3.42832300
H	-7.88663900	0.35635400	1.92062400	H	-0.74656600	-4.20029700	4.85188800
C	-7.59014000	0.02243000	-0.83462200	H	-0.84148000	-4.91115700	3.22684000
H	-8.58821100	-0.24758800	-0.47101600	C	-2.69541700	-2.27106800	4.57262200
H	-7.69052100	0.40718200	-1.85482800	H	-2.03058300	-1.43625900	4.32018900
H	-6.98852100	-0.89214300	-0.87983100	H	-3.72838800	-1.91693400	4.48122100
C	-3.69220200	4.38562600	-2.11659400	H	-2.51265900	-2.52319000	5.62321700
H	-4.66071300	4.81505200	-2.38675300	C	5.17242700	-2.43647900	-3.28412000
C	-2.98930100	5.36834200	-1.16383900	H	5.21383600	-2.46476800	-4.37869300
H	-2.00851300	4.98976500	-0.85977300	C	4.74312000	-3.82545500	-2.78271800
H	-2.83450500	6.33631400	-1.65482000	H	4.87784200	-3.92049000	-1.69782500
H	-3.58322200	5.54183700	-0.25939200	H	3.69348400	-4.04218400	-3.00421900
C	-2.87074800	4.20118900	-3.40594300	H	5.36363300	-4.59687000	-3.25091900
H	-1.85728600	3.83303300	-3.20177400	C	6.59806600	-2.12650600	-2.78089300
H	-3.35413800	3.49329900	-4.08887800	H	6.61078500	-2.05280000	-1.68627900
H	-2.76907000	5.15947000	-3.92760500	H	7.28921400	-2.92600900	-3.07234800
C	2.20432700	-0.43505100	5.36085500	H	6.96929200	-1.18671700	-3.19411300
H	2.80757200	-0.96636300	6.10246200	C	3.29665400	2.32841600	-3.85977300
C	0.75130300	-0.91013300	5.50191700	H	3.86940100	2.26330600	-4.78637600
H	0.06174100	-0.31901000	4.88564200	C	1.83994900	2.63960700	-4.26017800
H	0.63580300	-1.96126000	5.21898800	H	1.21136800	2.81958200	-3.38171300
H	0.42082600	-0.79885800	6.54009400	H	1.80595400	3.54468700	-4.87734100
C	2.31348500	1.07084500	5.67570400	H	1.39894800	1.81293900	-4.82807500
H	1.87271300	1.29698600	6.65365800	C	3.89078300	3.46886200	-3.00984900
H	3.35756900	1.39496200	5.68548500	H	3.34470200	3.58923100	-2.06849900
H	1.78696000	1.65642700	4.91232500	H	4.94202700	3.27625600	-2.76995400
C	6.26973000	-1.33615500	2.34874900	H	3.83152200	4.41996200	-3.55097000
H	6.75449500	-1.42771600	3.32156400	Rh	-0.07207300	0.84769800	0.58879600
C	6.47629700	-2.67917300	1.62084600	C	1.66677700	3.76227100	0.28384900
H	6.04702300	-2.66252300	0.61204100	C	2.56274800	4.80213200	0.60435800
H	7.54567300	-2.89675400	1.52148300	C	2.53641000	6.01021000	-0.08853500
H	6.00859600	-3.50360900	2.17061300	C	1.62147100	6.21819000	-1.12524100
C	6.95302700	-0.18272200	1.59028100	C	0.73016100	5.19801000	-1.45357800
H	6.52651000	-0.05924300	0.58758100	C	0.74469800	3.98974100	-0.75315500
H	6.83388200	0.76691800	2.12254800	H	3.28079700	4.65505200	1.40596300
H	8.02475400	-0.38116000	1.47591500	H	3.23602400	6.79554600	0.18478300
H	-0.43641600	-6.05515300	-0.55039800	H	1.60590000	7.15986900	-1.66560900
H	0.49466500	-1.26617200	-5.64431300	H	0.01198100	5.33721100	-2.25716100
O	1.19959200	-3.01759800	-3.69578800	H	0.02660900	3.21970200	-1.01393100
O	-1.13012000	-4.32983900	-2.49958100	H	0.24659200	1.24026000	-0.84516100
C	1.79273800	-3.29450800	-4.95886900	C	-1.09172000	5.87505700	1.76983700
H	2.44191800	-2.47047900	-5.27814000	C	-1.44371400	4.54126700	1.92882800
H	2.39645400	-4.19092500	-4.81637200	C	-0.73311600	3.70550400	2.80914400
H	1.03177700	-3.48570000	-5.72574200	C	0.33289500	4.25566100	3.54446300
C	-1.03177500	-5.63119700	-3.07377800	C	0.69620900	5.58995300	3.39847800
H	-1.56497100	-6.38357000	-2.48186400	C	-0.01550500	6.37570600	2.49887300
H	-1.50287200	-5.55934200	-4.05561600	H	-1.61415800	6.52549400	1.07834100
H	0.01879100	-5.92469200	-3.18562100	H	-2.26736300	4.14281700	1.34595400
C	-4.99987600	-4.57374100	-0.65666900	H	0.89613300	3.62262200	4.22238700
H	-5.45489000	-5.30848600	0.00896300	H	1.52566500	6.02170900	3.94733300
C	-6.14784500	-3.71050600	-1.21144700	F	0.34627400	7.65728300	2.32362000
H	-5.78864500	-2.96177100	-1.92675800	C	-1.02180900	2.28174200	2.95441700
H	-6.87902300	-4.33921800	-1.73180900	H	-0.39683400	1.76510700	3.68188400
H	-6.66696900	-3.18373800	-0.40325700	C	-1.97496600	1.55106900	2.31586000



H	-2.68929200	1.99803700	1.63215200
H	-2.19223700	0.53499500	2.62946500
S	1.82280100	2.25375500	1.21626700

### 8-ts-S

B3LYP-D3 SCF energy: -4928.798445 a.u.

B3LYP-D3 enthalpy: -4926.891845 a.u.

B3LYP-D3 free energy: -4927.143863 a.u.

M06 SCF energy in solution: -4927.658010 a.u.

Imaginary frequency: -142.17 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z
C	-1.93198000	-4.10472000	0.02308700
C	-1.03364400	-3.06178200	-0.27927100
C	0.00169600	-2.77461900	0.63270000
C	0.12237000	-3.51928300	1.81611300
C	-0.78693900	-4.53582300	2.09995500
C	-1.81747900	-4.83173900	1.21122600
C	-1.17287600	-2.39659300	-1.61276500
C	-1.64091700	-1.08063100	-1.80243700
C	-0.85624400	-3.17559200	-2.75290100
C	-1.79449000	-0.57300600	-3.10376800
C	-0.97897800	-2.64773900	-4.04068200
C	-1.46128900	-1.35188800	-4.20549100
P	1.14223000	-1.37698600	0.27397700
P	-1.89081100	0.05973600	-0.36728300
C	1.97016000	-1.81199600	-1.28422500
C	2.17656200	-0.83547900	-2.25398900
C	2.43442800	-3.11419400	-1.50358900
C	2.80155000	-1.13624400	-3.46958800
C	3.10576700	-3.44600000	-2.67989000
C	3.27878800	-2.44901300	-3.67897900
C	2.43480800	-1.38023200	1.55964200
C	3.78099600	-1.37211100	1.20192300
C	2.08126000	-1.04096800	2.87409700
C	4.78018800	-1.01704500	2.11690600
C	3.04663200	-0.69020100	3.81811000
C	4.41218200	-0.66699000	3.43370000
C	-2.94488400	-0.78992500	0.84859800
C	-2.57464400	-0.71732900	2.19555900
C	-4.11224700	-1.46853700	0.49503800
C	-3.32898600	-1.33365700	3.19254500
C	-4.92703500	-2.05660700	1.47111600
C	-4.50806300	-2.02650100	2.82171800
C	-2.85731400	1.46786700	-1.03003700
C	-4.20565200	1.67089000	-0.73638800
C	-2.20183200	2.39467500	-1.85170400
C	-4.90639000	2.77424400	-1.24463700
C	-2.87636100	3.46975400	-2.42781100
C	-4.24790000	3.66518100	-2.12286600
H	0.93290400	-3.32122100	2.50678300
H	-0.68876800	-5.10534000	3.01943700
H	-2.17926600	0.42501600	-3.26411200
H	-1.58162100	-0.94758600	-5.20655300
H	1.83106900	0.17415600	-2.06862900
H	2.26773000	-3.86712500	-0.74210900
H	4.06136700	-1.59989700	0.17981700
H	1.03050200	-1.00782500	3.15715800
H	-1.66399300	-0.19030700	2.46565300
H	-4.39543500	-1.53665400	-0.55116300

H	-4.72389800	0.97485800	-0.08705900
H	-1.14485400	2.26432600	-2.06431800
N	-4.89701200	4.78726400	-2.72774900
C	-6.00481500	4.54933700	-3.64015900
H	-5.81282900	3.63639800	-4.21157300
H	-6.99084500	4.44876600	-3.15592300
H	-6.06977000	5.38464800	-4.34911100
C	-4.98455900	5.99744200	-1.92556500
H	-4.02683300	6.17460200	-1.42512900
H	-5.19011000	6.85334500	-2.57975100
H	-5.77198600	5.96740300	-1.15081500
N	-5.21888100	-2.69078200	3.87160200
N	5.36060800	-0.23100300	4.41564400
N	3.93517400	-2.85746400	-4.88711500
C	-5.35082800	-4.13773100	3.80198800
H	-5.44999700	-4.53888100	4.81889400
H	-6.21665200	-4.49546200	3.21897400
H	-4.44436700	-4.55977800	3.35693500
C	-6.34748900	-1.98284200	4.45656600
H	-6.08307700	-0.93089200	4.60498600
H	-7.26666700	-2.01818800	3.84449900
H	-6.58093500	-2.41731800	5.43621300
C	5.91971000	1.10064200	4.23753600
H	6.31477300	1.45811600	5.19668500
H	6.73528500	1.16084200	3.49535400
H	5.12551200	1.78390600	3.91910900
C	6.25719700	-1.23257500	4.97186300
H	7.10676800	-1.50423800	4.32061600
H	6.66983600	-0.85971600	5.91739600
H	5.69161400	-2.14491400	5.18571400
C	3.06145700	-3.18246600	-6.00271000
H	2.62319700	-2.30024700	-6.50461400
H	3.62460500	-3.75029200	-6.75317600
H	2.23592500	-3.81110400	-5.65106200
C	5.19498200	-2.22591100	-5.25410400
H	5.76314800	-1.99534400	-4.34867900
H	5.78621900	-2.92834400	-5.85579100
H	5.09241700	-1.29501400	-5.83643500
C	-6.36342500	2.95652700	-0.83166200
H	-6.68755400	3.94707300	-1.15614900
C	-6.54229800	2.90963400	0.69789800
H	-6.31747300	1.91712600	1.10588800
H	-5.88902100	3.63441500	1.19612500
H	-7.57944500	3.14506100	0.96185100
C	-7.26517400	1.91432200	-1.52094400
H	-8.31509100	2.06988800	-1.24731600
H	-7.18345600	1.97365800	-2.61119700
H	-6.98592600	0.89901900	-1.21765000
C	-2.12349900	4.38531200	-3.38415200
H	-2.84167800	5.12872200	-3.73970300
C	-0.97223800	5.12515500	-2.67966100
H	-0.20222200	4.42742800	-2.32673300
H	-0.48659000	5.82671900	-3.36797400
H	-1.33587700	5.69532300	-1.81681000
C	-1.60272700	3.60356500	-4.60553200
H	-0.86318400	2.84556500	-4.31579400
H	-2.42101700	3.09225400	-5.12468500
H	-1.11965200	4.28210200	-5.31812400
C	2.60466000	-0.25103500	5.20660400
H	3.51434300	-0.11585700	5.79738000
C	1.72516800	-1.30298000	5.90358300

H	0.77964100	-1.46532300	5.37365600	C	1.64117400	0.74310800	-4.74233500
H	2.24116700	-2.26723000	5.96993400	H	1.31868300	1.30473800	-3.85734700
H	1.47793800	-0.97898300	6.92114000	H	1.77149100	1.46465000	-5.55694700
C	1.88937000	1.11332900	5.13093800	H	0.83175400	0.05710400	-5.00970700
H	1.62167000	1.46896900	6.13266100	C	4.07405300	0.95736600	-4.06006700
H	2.52712300	1.86477900	4.65167100	H	3.82267300	1.43887100	-3.10842100
H	0.96464200	1.04027100	4.54403600	H	5.02932100	0.43802700	-3.93222500
C	6.21353600	-0.94812000	1.60225200	H	4.21196400	1.74616300	-4.80916800
H	6.87004000	-0.68355500	2.43206000	Rh	0.13284700	0.78320800	0.51980100
C	6.69187100	-2.30797600	1.05922200	C	1.47657300	6.55719300	0.49463900
H	6.10134000	-2.62658100	0.19166000	C	0.83676800	5.33256700	0.64277900
H	7.73866800	-2.24402000	0.74126300	C	0.98910900	4.57098000	1.81811800
H	6.61347900	-3.08878700	1.82373900	C	1.81219300	5.07802900	2.84670900
C	6.35166100	0.15841900	0.53617600	C	2.44965600	6.30396500	2.71737900
H	5.74546600	-0.06335700	-0.35008800	C	2.27490900	7.02326500	1.53472500
H	6.02146800	1.12774600	0.92545000	H	1.37639600	7.14664400	-0.40972200
H	7.39548200	0.25183800	0.21475900	H	0.21848000	4.96276300	-0.16343800
H	-2.52128500	-5.62560800	1.43535400	H	1.95594900	4.49067300	3.75005200
H	-0.71443500	-3.23578500	-4.91051900	H	3.07977500	6.71041500	3.50094000
O	-0.43495800	-4.44629700	-2.50429600	F	2.90105200	8.20211000	1.39676000
O	-2.90442600	-4.34680800	-0.90286400	C	0.37298300	3.26511800	1.97974200
C	-0.19253100	-5.30580600	-3.61098400	C	-0.66345700	2.70550900	1.14278900
H	0.66501000	-4.95992100	-4.20206900	C	2.87049200	2.96681700	0.03289800
H	0.03797000	-6.28294200	-3.18514300	C	3.94426600	3.78958600	0.42462000
H	-1.07683800	-5.38954300	-4.25529800	C	4.47238400	4.73196800	-0.45445500
C	-3.30584300	-5.70148300	-1.09405600	C	3.94112700	4.87751300	-1.73944700
H	-3.94070100	-6.06306700	-0.27716300	C	2.87988000	4.06401900	-2.13951100
H	-3.88558800	-5.71354000	-2.01899400	C	2.34906900	3.11619900	-1.26397800
H	-2.42892000	-6.35155100	-1.19594900	H	4.35046400	3.69388100	1.42687300
C	-6.24724500	-2.68712800	1.03977300	H	5.29697300	5.36149500	-0.13200100
H	-6.81323200	-2.93923500	1.93814500	H	4.35518400	5.61329200	-2.42249800
C	-7.10923700	-1.69422200	0.23695200	H	2.46112000	4.15948800	-3.13771100
H	-6.65084500	-1.44857800	-0.72779600	H	1.52320800	2.49225900	-1.58388700
H	-8.09453200	-2.12700500	0.03065200	H	0.39194200	1.15376100	-0.92231400
H	-7.25589700	-0.75903600	0.78901000	H	-0.98520100	3.30776000	0.29731900
C	-6.02080500	-3.98541200	0.24597300	H	0.44356900	2.86245800	2.98838500
H	-5.42737500	-3.79460800	-0.65369700	H	-1.52294200	2.35014100	1.72348200
H	-5.47968800	-4.72094000	0.85007900	S	2.25306900	1.83316900	1.24521400
H	-6.97807000	-4.42646300	-0.05472100				
C	-2.85616500	-1.31569700	4.64132100	<b>9-S</b>			
H	-3.74391400	-1.36245000	5.27807900	B3LYP-D3 SCF energy:	-4928.803923 a.u.		
C	-2.01923800	-2.57661100	4.93309700	B3LYP-D3 enthalpy:	-4926.895731 a.u.		
H	-1.13235100	-2.60739700	4.28995600	B3LYP-D3 free energy:	-4927.150074 a.u.		
H	-1.68885800	-2.58980700	5.97828100	M06 SCF energy in solution:	-4927.667200 a.u.		
H	-2.60205000	-3.48289700	4.74352200				
C	-2.07308400	-0.04766800	5.01516400	Cartesian coordinates			
H	-1.09903400	-0.00384900	4.51328700	ATOM	X	Y	Z
H	-2.62767200	0.86232800	4.75803900	C	-0.40598800	-4.40018800	0.54145900
H	-1.87304200	-0.03418100	6.09181000	C	0.09627800	-3.18044000	0.04465800
C	3.69621600	-4.84120000	-2.86303500	C	1.00176400	-2.44809300	0.84034000
H	3.54176300	-5.13176100	-3.90800100	C	1.37438900	-2.93201700	2.10336900
C	3.05621900	-5.91085200	-1.96330700	C	0.85199000	-4.13293200	2.57888100
H	3.35256100	-5.78505700	-0.91477900	C	-0.03867400	-4.87180400	1.80462800
H	1.96335800	-5.88441700	-2.00231800	C	-0.29782800	-2.79705900	-1.34894800
H	3.39080800	-6.90621300	-2.27451200	C	-1.18854700	-1.75165500	-1.66877900
C	5.21941200	-4.80585300	-2.61757400	C	0.21604100	-3.59092200	-2.40374500
H	5.43298000	-4.48118600	-1.59118500	C	-1.54808600	-1.51626400	-3.00676200
H	5.65383600	-5.80319200	-2.75349000	C	-0.12382200	-3.32874400	-3.73352600
H	5.71828600	-4.12073500	-3.30634800	C	-1.01467800	-2.29864400	-4.02379800
C	2.95912500	-0.01575100	-4.49294000	P	1.59707000	-0.80470100	0.25189900
H	3.24878700	-0.45985300	-5.44712700	P	-1.78127400	-0.56537200	-0.38520800

C	2.44549200	-1.14210600	-1.32253600	H	7.38547200	0.12336000	4.38382400
C	2.24508400	-0.28422300	-2.40025900	H	6.88792700	1.03750800	5.82486300
C	3.28808200	-2.24971100	-1.47232300	H	5.91956800	-0.34278500	5.27568500
C	2.83064900	-0.52692500	-3.64750000	C	3.49919300	-2.70176700	-5.98263600
C	3.93225800	-2.50359800	-2.68315200	H	2.76120600	-2.06700700	-6.50698100
C	3.68666300	-1.64171400	-3.78729300	H	4.14028800	-3.16761000	-6.74079600
C	2.89281300	-0.28536800	1.43494600	H	2.94854500	-3.49651500	-5.46760800
C	4.24362600	-0.22287700	1.09803400	C	5.27666200	-1.04997300	-5.61100100
C	2.48685500	0.20270800	2.68421900	H	5.82186600	-0.53849100	-4.81293300
C	5.19400200	0.30932700	1.97978200	H	6.00371200	-1.60894300	-6.21432800
C	3.39619100	0.75733400	3.58505800	H	4.82785800	-0.28084200	-6.26175200
C	4.76784300	0.81613900	3.22790200	C	-6.98665100	0.53049800	-0.86826500
C	-2.43465500	-1.51322000	1.02194700	H	-7.64769400	1.30708400	-1.25665800
C	-2.07240600	-1.09209700	2.30582600	C	-7.11054400	0.56825500	0.66702800
C	-3.30322100	-2.59498800	0.87548500	H	-6.53588600	-0.23472200	1.14356200
C	-2.52861100	-1.75109700	3.44513700	H	-6.75328500	1.52230500	1.07006800
C	-3.83736600	-3.24446200	1.99618500	H	-8.15815400	0.44193500	0.96266200
C	-3.40996200	-2.84972600	3.28529000	C	-7.47114700	-0.82178300	-1.42594200
C	-3.18834500	0.33214200	-1.13613800	H	-8.50356600	-1.02016600	-1.11586500
C	-4.51618600	0.08602500	-0.78652700	H	-7.43321500	-0.83819200	-2.52028000
C	-2.91341200	1.34746700	-2.06004200	H	-6.84584100	-1.64220500	-1.05528700
C	-5.56668200	0.83411900	-1.33585300	C	-3.55579600	3.17067800	-3.66319600
C	-3.92950500	2.09137800	-2.65638700	H	-4.49318700	3.59154800	-4.03637600
C	-5.27602800	1.83120200	-2.29535900	C	-2.75151500	4.30315800	-2.99575200
H	2.07939200	-2.37883200	2.71266500	H	-1.77900000	3.94648600	-2.63277500
H	1.14399500	-4.49733900	3.55948400	H	-2.55770500	5.11132800	-3.71066200
H	-2.24605800	-0.72829600	-3.25792400	H	-3.29468200	4.72664700	-2.14291100
H	-1.29773300	-2.10904300	-5.05529600	C	-2.78495200	2.58463000	-4.86078000
H	1.59879800	0.57605900	-2.27503000	H	-1.82097300	2.15814100	-4.55414100
H	3.43096900	-2.91683700	-0.63039100	H	-3.36043700	1.79184000	-5.35143800
H	4.56991800	-0.58659900	0.13009500	H	-2.57979000	3.36475800	-5.60301100
H	1.43305100	0.16428100	2.95773400	C	2.89135400	1.30398800	4.91311100
H	-1.40216400	-0.24318800	2.41446700	H	3.75526300	1.74432000	5.41774200
H	-3.57512200	-2.93285000	-0.12007700	C	2.33622000	0.17854200	5.80510000
H	-4.74606800	-0.68291800	-0.05841000	H	1.47010400	-0.30981800	5.34378400
H	-1.88252900	1.56560300	-2.32099100	H	3.09490600	-0.59072900	5.98782900
N	-6.28636600	2.62349500	-2.92782100	H	2.01584900	0.57722500	6.77480700
C	-7.24855500	1.95828300	-3.79299100	C	1.84478600	2.41593700	4.70715800
H	-6.74555900	1.15847500	-4.34475100	H	1.55307400	2.84993400	5.67062700
H	-8.11626400	1.51980800	-3.27130500	H	2.23603000	3.21592400	4.06909600
H	-7.63366500	2.68210300	-4.52241800	H	0.93368300	2.02843800	4.23364100
C	-6.79009800	3.75945300	-2.17149000	C	6.65195500	0.31989500	1.53204200
H	-5.95206300	4.28770700	-1.70504300	H	7.26201100	0.71476600	2.34537600
H	-7.29342500	4.45514500	-2.85373300	C	7.16044800	-1.10485900	1.23858900
H	-7.50684900	3.48982100	-1.37486500	H	6.62105200	-1.56064100	0.39960500
N	-3.81496500	-3.52556400	4.47988800	H	8.22414300	-1.08283100	0.97581200
N	5.66515300	1.41387700	4.17168300	H	7.03626700	-1.75664000	2.11042200
N	4.32531700	-1.98414400	-5.02539300	C	6.85267500	1.24284000	0.31463100
C	-3.45954100	-4.92822100	4.63024400	H	6.28483200	0.88594700	-0.55284200
H	-3.37320800	-5.16430300	5.69876300	H	6.52186800	2.26387200	0.53439700
H	-4.18210900	-5.63744100	4.19181500	H	7.91071800	1.27838800	0.03070000
H	-2.48548500	-5.10389600	4.16323200	H	-0.44250500	-5.80689600	2.17655300
C	-5.09139300	-3.13525300	5.05938800	H	0.28841700	-3.92282400	-4.53951600
H	-5.19165400	-2.04565800	5.02583700	O	1.04230800	-4.60827200	-2.03369100
H	-5.96826700	-3.57215300	4.54852700	O	-1.26923000	-5.07232400	-0.27575500
H	-5.12528000	-3.44903400	6.10981400	C	1.47105100	-5.52643300	-3.03175800
C	6.24933000	2.69891000	3.81945300	H	2.14496900	-5.04624300	-3.75260300
H	6.58579900	3.20287500	4.73406600	H	2.01540500	-6.30960000	-2.50286500
H	7.11211400	2.64345000	3.13280300	H	0.61797400	-5.96950200	-3.56095100
H	5.48452300	3.32520800	3.34925000	C	-1.20337500	-6.49656000	-0.26783000
C	6.51264000	0.51307100	4.93762300	H	-1.66615400	-6.92603800	0.62798200

H	-1.76489100	-6.82677000	-1.14404100
H	-0.16303700	-6.83403000	-0.34386900
C	-4.88105600	-4.33539400	1.77919600
H	-5.29914200	-4.60415300	2.75077900
C	-6.05332400	-3.82721400	0.91772700
H	-5.73673400	-3.60919700	-0.10870300
H	-6.84147700	-4.58648400	0.86308800
H	-6.48825400	-2.91320400	1.33763700
C	-4.25748500	-5.60152400	1.16675500
H	-3.79654700	-5.37976500	0.19916200
H	-3.47836000	-6.00729300	1.82056100
H	-5.01939500	-6.37567400	1.02035800
C	-2.03535600	-1.33800400	4.82701700
H	-2.84222500	-1.53405700	5.53901400
C	-0.83888900	-2.21918300	5.23737600
H	-0.01163200	-2.09733500	4.52899400
H	-0.48139400	-1.94629400	6.23708700
H	-1.11981900	-3.27613500	5.24794600
C	-1.66825200	0.15077300	4.92991500
H	-0.76998300	0.39212100	4.34799200
H	-2.48246100	0.79619400	4.58018000
H	-1.44745700	0.41093500	5.97044500
C	4.91785700	-3.66316800	-2.80393900
H	4.75034400	-4.13952600	-3.77671600
C	4.75946900	-4.73027000	-1.70848600
H	5.11180000	-4.36276600	-0.73676500
H	3.71997800	-5.04631500	-1.58402900
H	5.36301400	-5.60966600	-1.95740800
C	6.36799300	-3.13561000	-2.79661700
H	6.57990000	-2.61415500	-1.85462100
H	7.07805700	-3.96575000	-2.88878300
H	6.54580000	-2.44277200	-3.62131000
C	2.52796000	0.44537600	-4.78437900
H	2.86813600	-0.00206500	-5.71997600
C	1.01941300	0.71314100	-4.94815300
H	0.60133300	1.24454900	-4.08437900
H	0.84176900	1.33658800	-5.83194200
H	0.45945600	-0.21955100	-5.06060000
C	3.29399300	1.76804300	-4.58267200
H	2.97412100	2.26616400	-3.65971500
H	4.37336500	1.59844100	-4.51470800
H	3.10813400	2.45422300	-5.41763500
Rh	-0.14004400	0.88470500	0.30558900
C	-1.25775000	6.98769300	0.51618700
C	-1.18860200	5.59668000	0.46960300
C	-0.72583800	4.86075900	1.57025700
C	-0.32227100	5.55457600	2.72296600
C	-0.38225000	6.94422300	2.78591300
C	-0.85145200	7.64027900	1.67479400
H	-1.61287900	7.56846600	-0.32822600
H	-1.48980100	5.08745200	-0.43813000
H	0.05029100	4.99789400	3.57991500
H	-0.07963900	7.49212700	3.67183900
F	-0.91146400	8.98318100	1.72449200
C	-0.57364400	3.37111900	1.52187800
C	-1.44185500	2.51499200	0.62332200
C	1.48328900	3.96241700	-0.44507400
C	2.09362900	5.19317800	-0.16259500
C	2.29043600	6.12427900	-1.18249200
C	1.88746400	5.83376000	-2.48751900
C	1.28651500	4.60546000	-2.77148000

C	1.08393400	3.67105600	-1.75526100
H	2.39370600	5.42618700	0.85403700
H	2.75581000	7.07844100	-0.95374500
H	2.04329800	6.55968700	-3.28015300
H	0.97406600	4.36742300	-3.78422300
H	0.61183200	2.72303100	-1.97866900
H	-0.07994000	1.20226900	-1.17128500
H	-1.70179900	3.00429200	-0.31417200
H	-0.55941900	2.97306300	2.54265700
H	-2.36444500	2.19487900	1.12157700
S	1.22899800	2.85684800	0.94646200

### 8-ts-Regio

B3LYP-D3 SCF energy: -4539.842243 a.u.

B3LYP-D3 enthalpy: -4537.934128 a.u.

B3LYP-D3 free energy: -4538.182793 a.u.

M06 SCF energy in solution: -4538.806615 a.u

Imaginary frequency: -151.32 cm<sup>-1</sup>

### Cartesian coordinates

ATOM	X	Y	Z
C	0.56416400	-2.48350900	3.28046100
C	0.04447000	-1.51277400	2.39896800
C	-0.73533800	-1.94112900	1.30695300
C	-1.01396100	-3.30554200	1.13366000
C	-0.51348600	-4.24141900	2.03506100
C	0.28604500	-3.84101100	3.10122700
C	0.22028000	-0.07633700	2.77541000
C	1.00089700	0.85644800	2.06495900
C	-0.43576700	0.34840500	3.96021500
C	1.13014400	2.16976300	2.54924800
C	-0.32763700	1.66566800	4.41028300
C	0.46832700	2.56432400	3.70518800
P	-1.47002100	-0.68010600	0.18316600
P	1.72613800	0.43927900	0.40589800
C	-2.62200900	0.20926000	1.28644100
C	-2.79345000	1.59034500	1.24717300
C	-3.37116300	-0.55337400	2.19287000
C	-3.68144500	2.23265600	2.12311900
C	-4.29515700	0.04144400	3.04873000
C	-4.45371200	1.45174400	3.01166600
C	-2.52205100	-1.59771700	-0.98945600
C	-3.88178000	-1.30673600	-1.09670100
C	-1.93966000	-2.47962200	-1.91036100
C	-4.67703400	-1.88507600	-2.09225000
C	-2.70941000	-3.11262000	-2.88906400
C	-4.09376600	-2.81170200	-2.98353900
C	2.60712200	-1.14490800	0.63265600
C	2.42124300	-2.22188300	-0.24606400
C	3.46921700	-1.28488200	1.72365000
C	3.04648400	-3.45241900	-0.01361100
C	4.17019900	-2.47446200	1.94646400
C	3.91451900	-3.57790600	1.10326600
C	2.99820100	1.73328400	0.12392000
C	4.37131500	1.48209000	0.12025000
C	2.55642700	3.02456900	-0.19591200
C	5.29604100	2.48237700	-0.21792800
C	3.44116800	4.05946000	-0.49141200
C	4.83302900	3.78852300	-0.50295200
H	-1.64005300	-3.63889100	0.31594000

H	-0.74120000	-5.29414400	1.89911400	H	1.80041700	6.43142200	-2.43502200
H	1.75687600	2.88747300	2.03922900	H	2.76432700	5.04425900	-2.97621200
H	0.57490800	3.58371900	4.06471600	C	1.97438700	5.97055400	0.30376400
H	-2.23128300	2.18211700	0.53476300	H	1.07557500	5.35309100	0.43277100
H	-3.22603200	-1.62608700	2.22462300	H	2.50314400	5.99540500	1.26303200
H	-4.32925400	-0.59621000	-0.41221800	H	1.64268800	6.98930200	0.07255900
H	-0.87491500	-2.69664900	-1.84996500	C	-2.04815900	-4.11326400	-3.82575400
H	1.76115700	-2.10217000	-1.10007700	H	-2.82832600	-4.47516700	-4.49995700
H	3.60310100	-0.45297300	2.40903900	C	-1.48834300	-5.31937200	-3.04850300
H	4.73325200	0.48404500	0.33818000	H	-0.68871800	-5.02055500	-2.36018500
H	1.49092400	3.23067900	-0.21667000	H	-2.27288000	-5.80891400	-2.46064200
N	5.70688700	4.87373900	-0.82153000	H	-1.06917100	-6.05986700	-3.73951200
C	6.66602300	5.31975600	0.17787200	C	-0.94949600	-3.44569500	-4.67048900
H	6.22245900	5.22394000	1.17319200	H	-0.51612800	-4.16298900	-5.37724400
H	7.62456000	4.77390000	0.17616500	H	-1.34618700	-2.59862600	-5.24248000
H	6.89074900	6.38042500	0.00833000	H	-0.13874200	-3.07451100	-4.03486500
C	6.13723900	4.98174300	-2.20696600	C	-6.13051100	-1.43366200	-2.18445400
H	5.28617800	4.79897300	-2.87079400	H	-6.61204900	-1.97324100	-3.00069800
H	6.50346600	5.99784500	-2.39629300	C	-6.91020400	-1.75737900	-0.89611300
H	6.94140500	4.27570300	-2.48286100	H	-6.50241000	-1.21712300	-0.03347700
N	4.49138700	-4.86710300	1.33408100	H	-7.96151400	-1.46688500	-1.00224400
N	-4.83982200	-3.47359200	-4.01146100	H	-6.87257000	-2.82878400	-0.66983500
N	-5.42410100	2.01478400	3.90667500	C	-6.21081900	0.06877400	-2.52354000
C	4.17906000	-5.55179900	2.57765400	H	-5.77013500	0.68358000	-1.72997200
H	4.23842500	-6.63609900	2.41622500	H	-5.67234000	0.29010500	-3.45179000
H	4.84629800	-5.30617400	3.42168600	H	-7.25552700	0.37637400	-2.64774700
H	3.15388900	-5.30833500	2.87360000	H	0.67805400	-4.57675400	3.79422600
C	5.82395300	-5.10297900	0.80085800	H	-0.84604600	1.99330900	5.30252200
H	5.89700900	-4.67810100	-0.20547800	O	-1.16325600	-0.60106400	4.61028800
H	6.63524600	-4.66790800	1.41205200	O	1.32438900	-2.01315100	4.30829700
H	6.00201500	-6.18292000	0.72844000	C	-1.78706500	-0.25361600	5.83949600
C	-5.16323600	-2.68868300	-5.19353100	H	-2.56296400	0.50553600	5.68679900
H	-5.42479400	-3.36564600	-6.01581300	H	-2.25087700	-1.16880200	6.20848600
H	-6.00231600	-1.98329600	-5.05815800	H	-1.05529800	0.10645000	6.57359600
H	-4.28403300	-2.11061500	-5.49610400	C	1.26656600	-2.71485700	5.54678500
C	-5.83880800	-4.44615300	-3.59464100	H	1.80816800	-3.66741400	5.50832700
H	-6.79590300	-4.01250000	-3.25561600	H	1.75101900	-2.06758100	6.27985800
H	-6.05781900	-5.11607200	-4.43512900	H	0.22505800	-2.89547800	5.83772500
H	-5.43449500	-5.05113700	-2.77708600	C	5.20024000	-2.52236100	3.07125100
C	-4.91735100	2.58607500	5.14305000	H	5.75156800	-3.46029100	2.98575300
H	-4.41382000	3.56219500	5.01981500	C	6.23249800	-1.38857500	2.92921100
H	-5.74841600	2.72429000	5.84505900	H	5.77415500	-0.40499300	3.08289800
H	-4.20231700	1.89607900	5.60302600	H	7.02672100	-1.50042000	3.67584800
C	-6.57495300	2.70350200	3.33800900	H	6.69471400	-1.39619100	1.93572700
H	-6.86789800	2.21182200	2.40613400	C	4.54095200	-2.49094600	4.46052500
H	-7.41706100	2.63269000	4.03859600	H	3.92674700	-1.59336100	4.58598700
H	-6.41152400	3.77217800	3.12114000	H	3.88970300	-3.35817600	4.60060000
C	6.77468500	2.11353700	-0.28835600	H	5.30350400	-2.50397700	5.24782200
H	7.31040400	2.95002400	-0.73986800	C	2.76295400	-4.68316300	-0.87544100
C	7.02163100	0.89399000	-1.19683100	H	3.65511500	-5.31287300	-0.83858900
H	6.55114300	-0.01481900	-0.80402900	C	1.61450100	-5.50695200	-0.26443400
H	6.62917800	1.07154900	-2.20469200	H	0.67388200	-4.95041500	-0.31686200
H	8.09635200	0.69853200	-1.28131700	H	1.48759900	-6.44818000	-0.81204200
C	7.35804200	1.88605900	1.11827100	H	1.80801400	-5.74139100	0.78617400
H	8.42820000	1.65672600	1.06066200	C	2.47152400	-4.38353300	-2.34817200
H	7.23199700	2.77257000	1.74856900	H	1.58958100	-3.74629800	-2.47723100
H	6.86033800	1.04714200	1.61490500	H	3.31772400	-3.89930200	-2.83746100
C	2.88096100	5.43623600	-0.82052000	H	2.26929600	-5.31963900	-2.88104600
H	3.73726200	6.10934900	-0.91515100	C	-5.14725400	-0.81952900	3.97630800
C	2.12967300	5.42126100	-2.16636200	H	-5.25487800	-0.27623400	4.92145900
H	1.23527900	4.78771800	-2.11766700	C	-4.53258000	-2.19673100	4.27904200

H	-4.59344900	-2.86501500	3.41133700	C	7.50188300	-0.46528700	-2.15487400
H	-3.47846100	-2.12560500	4.56476000	C	5.79592000	0.66514700	1.02723100
H	-5.08375800	-2.67841800	5.09383800	C	4.77608900	1.62375400	1.20254800
C	-6.56248100	-0.99986100	3.38977000	C	6.71010000	0.44114400	2.08541900
H	-6.51264700	-1.51755700	2.42375400	C	4.70763700	2.34322000	2.40881000
H	-7.18399800	-1.60166800	4.06321900	C	6.61270000	1.14481600	3.28653600
H	-7.05615600	-0.03698100	3.24034600	C	5.61361300	2.10437600	3.43317400
C	-3.79076300	3.75232000	2.06130900	P	3.50052400	-1.40846100	0.06466000
H	-4.36248300	4.08879900	2.92797900	P	3.37664200	1.82009200	-0.01589400
C	-2.41324800	4.43581400	2.15156600	C	4.00195800	-1.82207400	1.78497300
H	-1.79038800	4.21326500	1.27935400	C	3.21719000	-1.31900900	2.81914300
H	-2.53695600	5.52401400	2.19577000	C	5.14415100	-2.56713700	2.09771800
H	-1.86953200	4.10979100	3.04416400	C	3.56863100	-1.49940200	4.16116400
C	-4.54981100	4.19006600	0.79447900	C	5.48974300	-2.84111000	3.42121600
H	-4.02650700	3.86207100	-0.10718600	C	4.70344100	-2.28140800	4.46377700
H	-5.55878900	3.76510200	0.77164700	C	3.04445000	-3.02388800	-0.70868800
H	-4.63663200	5.28148800	0.75183100	C	3.57380500	-4.23931400	-0.27201800
Rh	-0.01311200	0.59418100	-1.17259200	C	2.16986000	-3.03098800	-1.79904100
C	2.30166500	-1.71642600	-4.42376500	C	3.28512300	-5.44545800	-0.91829200
C	1.49795500	-0.67068700	-3.97168700	C	1.82223800	-4.21845000	-2.45045300
C	2.05323600	0.41071100	-3.25627400	C	2.41945800	-5.43257400	-2.03546500
C	3.43519800	0.39170900	-2.97898500	C	4.14123600	2.03777500	-1.67564300
C	4.24061300	-0.65568500	-3.40889900	C	3.48276800	1.41531400	-2.73940900
C	3.66021900	-1.68837700	-4.13776500	C	5.28206200	2.80117800	-1.93672100
H	1.89248400	-2.54700600	-4.98682600	C	3.95052100	1.51516000	-4.04962800
H	0.43550300	-0.68666400	-4.19984100	C	5.75506800	2.97018900	-3.24491000
H	3.88216800	1.22057800	-2.44264900	C	5.10421400	2.29201700	-4.30186000
H	5.30511400	-0.67682600	-3.20328100	C	2.72201100	3.49880400	0.40111900
F	4.43757100	-2.71004400	-4.55359500	C	3.08049700	4.65325900	-0.29761900
C	1.24441600	1.57716400	-2.85188400	C	1.83298000	3.62092000	1.47519000
C	0.17419900	2.01680900	-3.64431500	C	2.59512900	5.91518800	0.06736600
C	-2.45090400	3.18573300	-2.32826000	C	1.32673100	4.85949700	1.87555200
C	-3.61183500	3.72635300	-2.89854600	C	1.73367900	6.02395200	1.18209000
C	-3.90136000	5.08378300	-2.74513400	H	4.75659100	-2.44209100	-2.37416700
C	-3.03709200	5.91809500	-2.03183100	H	6.82868800	-1.91747300	-3.59222800
C	-1.88349000	5.38119400	-1.45958400	H	3.94013500	3.09164000	2.55373600
C	-1.59542200	4.02148900	-1.59851700	H	5.54168100	2.66732800	4.36015600
H	-4.28614200	3.09101900	-3.46598000	H	2.34181700	-0.73193100	2.55515100
H	-4.80504000	5.48955300	-3.19135000	H	5.78163000	-2.91040700	1.29246000
H	-3.26472900	6.97381400	-1.91883000	H	4.22620000	-4.25990600	0.59079600
H	-1.20450900	6.01297500	-0.89318900	H	1.72384400	-2.09648600	-2.12125600
H	-0.70059100	3.61518300	-1.13977700	H	2.60817600	0.81369200	-2.50905700
Se	-2.09882500	1.28082700	-2.65338500	H	5.81377200	3.26677000	-1.11105300
H	-0.36008400	1.80298800	-0.32259000	H	3.74392700	4.57796800	-1.15006600
H	-0.05890600	1.52515200	-4.58219700	H	1.52184300	2.72762300	2.00475700
H	1.76217100	2.34133300	-2.28297300	N	1.24423800	7.28402100	1.66437900
H	-0.16398200	3.04215000	-3.55502800	C	2.18739700	8.22333000	2.23734800
				H	2.97051800	7.67377500	2.76814600
				H	2.67604200	8.89041500	1.50342300
				H	1.66830900	8.86284800	2.96533900
				C	0.10967300	7.87220600	0.98496200
				H	-0.55907000	7.07790200	0.64515900
				H	-0.44851600	8.51864300	1.67711800
				H	0.37883100	8.48460500	0.10368800
				N	5.58143700	2.32837800	-5.65560700
				N	2.11680100	-6.61264200	-2.79603500
				N	5.15210300	-2.51986100	5.81001200
				C	6.87649100	1.74013100	-5.94177200
				H	6.89727900	1.39235000	-6.98411200
				H	7.73613400	2.42121600	-5.80405700
				H	7.02673900	0.87369600	-5.29043000

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B3LYP-D3 SCF energy: -8699.791945 a.u.

B3LYP-D3 enthalpy: -8696.456531 a.u.

B3LYP-D3 free energy: -8696.859314 a.u.

M06 SCF energy in solution: -8698.113949 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z
C	7.20054500	0.19000000	-0.96025300
C	6.01301300	-0.08337600	-0.24997300
C	5.12332900	-1.04802900	-0.76706500
C	5.43324500	-1.69848000	-1.97215000
C	6.60797700	-1.40696700	-2.65862300

C	5.21281700	3.47857200	-6.45881000	H	7.30385500	0.95988700	4.09954000
H	4.16355200	3.72966400	-6.27224300	O	7.68223900	-0.49469000	1.85575800
H	5.81715300	4.38460000	-6.26253300	O	8.02063900	1.15053500	-0.42615600
H	5.32063500	3.23238000	-7.52363400	C	8.72544900	-0.61947200	2.80709000
C	1.13526200	-7.52850300	-2.25353500	H	8.35910100	-1.02745200	3.75882200
H	0.70600300	-8.13406700	-3.06365600	H	9.44335400	-1.31993000	2.37662600
H	1.53257300	-8.22535800	-1.49151000	H	9.22099200	0.34362100	2.98904600
H	0.32649000	-6.95764500	-1.79078400	C	9.42104800	0.95019100	-0.54996500
C	3.18458700	-7.21587800	-3.56991900	H	9.78477800	1.18252700	-1.55909800
H	3.83601300	-7.90538500	-3.00196500	H	9.88864900	1.63999400	0.15703400
H	2.75151500	-7.78601600	-4.40349300	H	9.69044000	-0.08151600	-0.29203000
H	3.81543500	-6.42731100	-3.99153500	C	6.95603100	3.87995000	-3.48848100
C	5.91919300	-1.44377000	6.41335800	H	7.07404400	4.00644700	-4.56638800
H	5.30634200	-0.58917700	6.75603000	C	6.73657700	5.28473400	-2.89808700
H	6.47347200	-1.82824700	7.27984900	H	6.67635200	5.25474200	-1.80456400
H	6.64115300	-1.06031300	5.68470400	H	7.56937800	5.94714700	-3.16369000
C	4.27037400	-3.22927500	6.72316800	H	5.80974300	5.73284200	-3.27242100
H	3.70688000	-3.98463600	6.16797900	C	8.25472000	3.26094600	-2.94322600
H	4.87426100	-3.74408800	7.48357100	H	8.18417800	3.10982900	-1.86244800
H	3.54372500	-2.59107300	7.25483300	H	8.44382100	2.28385200	-3.40089000
C	3.04813300	7.13046700	-0.73757300	H	9.11309500	3.91184100	-3.15148700
H	2.43222300	7.98412400	-0.44396300	C	3.27193500	0.72031400	-5.15899400
C	2.85514700	6.93971100	-2.25411300	H	3.52401600	1.19953500	-6.10952800
H	3.48572600	6.13482500	-2.64718900	C	3.85465100	-0.70643500	-5.19673400
H	1.81754600	6.69223100	-2.49779500	H	3.64808500	-1.23155900	-4.25773800
H	3.12315400	7.85994600	-2.78727700	H	3.41207700	-1.28710800	-6.01521700
C	4.51562100	7.47806700	-0.41925000	H	4.94108600	-0.68163600	-5.33466200
H	4.83559900	8.37039600	-0.97152200	C	1.74050000	0.67986100	-5.03423300
H	4.65712000	7.66649000	0.65012800	H	1.40983500	0.14801900	-4.13503700
H	5.17574100	6.65132000	-0.70314100	H	1.31434200	1.68644400	-4.99337000
C	0.33311500	4.91731700	3.02827200	H	1.30643200	0.15770000	-5.89468300
H	0.13583000	5.97538700	3.22398300	C	6.68152900	-3.74398500	3.73833600
C	-0.99625700	4.23969800	2.63941500	H	7.25993200	-3.26524000	4.53852300
H	-0.85733000	3.17711100	2.41954100	C	7.61953300	-3.97861600	2.54229800
H	-1.72949800	4.32525300	3.45119600	H	7.14824400	-4.62188100	1.78806500
H	-1.42761500	4.69296800	1.74030600	H	7.90340700	-3.04632000	2.04817600
C	0.91825900	4.30423800	4.31349200	H	8.52946200	-4.48922400	2.87806100
H	1.12265200	3.23410300	4.19693200	C	6.20491300	-5.10991300	4.27478900
H	1.85681400	4.79712500	4.59434800	H	5.59306100	-5.62194900	3.52218200
H	0.21290800	4.41341300	5.14595500	H	7.06363500	-5.75326600	4.50462400
C	0.76851100	-4.18068800	-3.54860500	H	5.61065700	-4.99710600	5.18283400
H	0.67816200	-5.19922600	-3.93712000	C	2.69338500	-0.83259900	5.22003500
C	1.18080100	-3.26890300	-4.71642600	H	3.20422500	-0.89299700	6.18334800
H	1.25441600	-2.22197300	-4.40474500	C	2.46822300	0.66391600	4.92961700
H	2.15336800	-3.56353300	-5.12755200	H	1.89393600	0.81620100	4.00904300
H	0.43961100	-3.32011700	-5.52333400	H	1.90518600	1.12738200	5.74836700
C	-0.59510200	-3.75840900	-2.96399800	H	3.41909400	1.19149300	4.81409500
H	-1.37908900	-3.80739600	-3.72995000	C	1.34426100	-1.56373500	5.34951100
H	-0.89134700	-4.40685200	-2.13327200	H	0.78884700	-1.51862300	4.40647700
H	-0.56772100	-2.73684900	-2.57075900	H	1.48276000	-2.62019600	5.60094100
C	3.95652900	-6.71513300	-0.40145800	H	0.72326300	-1.10206500	6.12679100
H	3.51497300	-7.57359900	-0.91280100	Rh	1.86705700	0.14399400	0.04051300
C	5.46392900	-6.70039100	-0.72484300	Cl	-0.11519700	1.61274600	0.13291200
H	5.95956600	-5.86311000	-0.21796900	C	-7.20041800	-0.18972400	-0.95992000
H	5.94459400	-7.62871000	-0.39239800	C	-6.01280000	0.08349600	-0.24971400
H	5.63874000	-6.58809600	-1.80030500	C	-5.12317500	1.04826800	-0.76668300
C	3.73322200	-6.92501500	1.10828200	C	-5.43319900	1.69894400	-1.97161200
H	4.19752400	-6.12930400	1.70105500	C	-6.60799500	1.40757200	-2.65803500
H	2.66842600	-6.94058600	1.35808300	C	-7.50187100	0.46581400	-2.15438000
H	4.17529100	-7.87629800	1.42842400	C	-5.79560800	-0.66530000	1.02732300
H	8.41587600	-0.23234200	-2.69015000	C	-4.77581200	-1.62398100	1.20242600

C	-6.70969900	-0.44143100	2.08562800	H	-5.32123500	-3.22987500	-7.52423000
C	-4.70729200	-2.34364300	2.40856800	C	-1.13597500	7.52904200	-2.25371600
C	-6.61222300	-1.14529000	3.28662700	H	-0.70753700	8.13468400	-3.06420900
C	-5.61315600	-2.10490200	3.43305300	H	-1.53261700	8.22582300	-1.49126200
P	-3.50030200	1.40847200	0.06501000	H	-0.32671900	6.95822200	-1.79176100
P	-3.37646900	-1.82014600	-0.01616000	C	-3.18648500	7.21656200	-3.56814700
C	-4.00157200	1.82158200	1.78550100	H	-3.83683500	7.90665800	-2.99969400
C	-3.21673000	1.31820400	2.81946300	H	-2.75415700	7.78610100	-4.40252300
C	-5.14373000	2.56656900	2.09856400	H	-3.81821600	6.42809600	-3.98860500
C	-3.56804500	1.49823600	4.16156400	C	-5.91845700	1.44215000	6.41397300
C	-5.48918100	2.84020900	3.42216800	H	-5.30563100	0.58744000	6.75639300
C	-4.70280800	2.28019200	4.46449900	H	-6.47265100	1.82645500	7.28059400
C	-3.04433500	3.02411600	-0.70792900	H	-6.64048500	1.05891800	5.68526800
C	-3.57374500	4.23940500	-0.27096100	C	-4.26952200	3.22751200	6.72409300
C	-2.16979000	3.03151800	-1.79831500	H	-3.70601800	3.98296500	6.16903900
C	-3.28532900	5.44570200	-0.91710200	H	-4.87333700	3.74219900	7.48464100
C	-1.82244000	4.21913700	-2.44959000	H	-3.54287900	2.58915600	7.25558300
C	-2.41995400	5.43308700	-2.03449400	C	-3.04844500	-7.13047100	-0.73883700
C	-4.14123200	-2.03740500	-1.67590200	H	-2.43251000	-7.98418900	-0.44541100
C	-3.48279300	-1.41467300	-2.73953800	C	-2.85531900	-6.93922700	-2.25530300
C	-5.28211200	-2.80066800	-1.93714500	H	-3.48592500	-6.13427000	-2.64819400
C	-3.95065400	-1.51408800	-4.04975300	H	-1.81771200	-6.69160800	-2.49881000
C	-5.75523800	-2.96922900	-3.24533600	H	-3.12321800	-7.85932700	-2.78875300
C	-5.10444800	-2.29074600	-4.30212200	C	-4.51598200	-7.47816900	-0.42081900
C	-2.72197100	-3.49902400	0.40045300	H	-4.83584000	-8.37038400	-0.97333900
C	-3.08062300	-4.65334000	-0.29842400	H	-4.65765900	-7.66682700	0.64849000
C	-1.83287700	-3.62144300	1.47446000	H	-5.17607200	-6.65138100	-0.70464400
C	-2.59550800	-5.91541200	0.06644500	C	-0.33324500	-4.91828600	3.02737500
C	-1.32691100	-4.86015300	1.87472100	H	-0.13613200	-5.97640100	3.22299900
C	-1.73422800	-6.02449600	1.18126200	C	0.99622700	-4.24082000	2.63844800
H	-4.75657700	2.44263500	-2.37354200	H	0.85741500	-3.17817100	2.41884100
H	-6.82878300	1.91826200	-3.59152100	H	1.72956500	-4.32667200	3.45011300
H	-3.93980800	-3.09211400	2.55330000	H	1.42738700	-4.69394300	1.73917600
H	-5.54117300	-2.66797100	4.35996000	C	-0.91811000	-4.30522300	4.31270100
H	-2.34139500	0.73117800	2.55523000	H	-1.12246300	-3.23507600	4.19619200
H	-5.78127100	2.91006900	1.29345600	H	-1.85664000	-4.79805800	4.59373800
H	-4.22596800	4.25979000	0.59198200	H	-0.21260500	-4.41445300	5.14503200
H	-1.72366500	2.09712800	-2.12070300	C	-0.76876800	4.18172200	-3.54780100
H	-2.60814700	-0.81318100	-2.50905600	H	-0.67844100	5.20038600	-3.93600000
H	-5.81381300	-3.26647300	-1.11158900	C	-1.18113500	3.27036100	-4.71594200
H	-3.74396200	-4.57782800	-1.15092200	H	-1.25479100	2.22334300	-4.40459000
H	-1.52157000	-2.72827200	2.00413900	H	-2.15367800	3.56515300	-5.12701000
N	-1.24542900	-7.28473500	1.66370600	H	-0.43993700	3.32177400	-5.52282000
C	-2.18911600	-8.22406900	2.23574900	C	0.59480700	3.75907400	-2.96341700
H	-2.97294100	-7.67453000	2.76551500	H	1.37885200	3.80833800	-3.72931800
H	-2.67678900	-8.89135600	1.50136800	H	0.89110300	4.40701600	-2.13234500
H	-1.67078800	-8.86337500	2.96447200	H	0.56731200	2.73730200	-2.57069900
C	-0.11029300	-7.87299300	0.98528500	C	-3.95667900	6.71524700	-0.39989600
H	0.55889700	-7.07877000	0.64622100	H	-3.51496200	7.57385700	-0.91087900
H	0.44711500	-8.51962300	1.67787300	C	-5.46406900	6.70070700	-0.72337000
H	-0.37875600	-8.48520000	0.10366100	H	-5.95975700	5.86332500	-0.21671200
N	-5.58184900	-2.32661600	-5.65581800	H	-5.94467500	7.62898400	-0.39073000
N	-2.11800500	6.61318400	-2.79528900	H	-5.63883100	6.58867300	-1.79886200
N	-5.15134200	2.51834600	5.81083200	C	-3.73350700	6.92461300	1.10994500
C	-6.87692300	-1.73822800	-5.94158900	H	-4.19798800	6.12877600	1.70240800
H	-6.89783200	-1.39001800	-6.98378600	H	-2.66873800	6.93999900	1.35989100
H	-7.73655800	-2.41936300	-5.80405800	H	-4.17554400	7.87583500	1.43033400
H	-7.02709400	-0.87206600	-5.28986900	H	-8.41591800	0.23299600	-2.68962000
C	-5.21339400	-3.47651100	-6.45951000	H	-7.30329700	-0.96046000	4.09972300
H	-4.16414900	-3.72780300	-6.27309700	O	-7.68181600	0.49449800	1.85622500
H	-5.81782600	-4.38255200	-6.26357400	O	-8.02048800	-1.15032500	-0.42592000



C	-8.72501500	0.61908400	2.80759900
H	-8.35864400	1.02682300	3.75942800
H	-9.44289700	1.31967300	2.37730600
H	-9.22059300	-0.34403200	2.98932900
C	-9.42089900	-0.94985200	-0.54944200
H	-9.78481600	-1.18180800	-1.55859400
H	-9.88843000	-1.63987000	0.15739300
H	-9.69018400	0.08178300	-0.29110200
C	-6.95622700	-3.87890700	-3.48913700
H	-7.07431700	-4.00503200	-4.56707900
C	-6.73673200	-5.28390200	-2.89925400
H	-6.67643900	-5.25429700	-1.80572800
H	-7.56954600	-5.94622600	-3.16503800
H	-5.80991300	-5.73186900	-3.27380000
C	-8.25487400	-3.26010600	-2.94356900
H	-8.18422700	-3.10932900	-1.86274900
H	-8.44402000	-2.28287100	-3.40091400
H	-9.11326400	-3.91093900	-3.15195100
C	-3.27210600	-0.71902200	-5.15897800
H	-3.52399900	-1.19827000	-6.10955800
C	-3.85510700	0.70761600	-5.19670400
H	-3.64862100	1.23276500	-4.25770300
H	-3.41264700	1.28837900	-6.01518300
H	-4.94153400	0.68261600	-5.33464100
C	-1.74067800	-0.67827000	-5.03413300
H	-1.41016300	-0.14629000	-4.13497000
H	-1.31434100	-1.68476900	-4.99320700
H	-1.30670800	-0.15605500	-5.89460200
C	-6.68090800	3.74302700	3.73965200
H	-7.25933900	3.26399000	4.53965000
C	-7.61889300	3.97818300	2.54369300
H	-7.14754200	4.62167900	1.78969600
H	-7.90286000	3.04609600	2.04922900
H	-8.52878000	4.48875000	2.87963600
C	-6.20423500	5.10871400	4.27664300
H	-5.59235900	5.62101600	3.52423300
H	-7.06294000	5.75200400	4.50671600
H	-5.60998700	4.99553000	5.18464400
C	-2.69270000	0.83116300	5.22017200
H	-3.20346600	0.89126700	6.18354100
C	-2.46751500	-0.66526200	4.92931000
H	-1.89326000	-0.81724400	4.00866400
H	-1.90441700	-1.12895600	5.74788800
H	-3.41836900	-1.19285000	4.81367600
C	-1.34357900	1.56229800	5.34974300
H	-0.78827300	1.51749000	4.40663100
H	-1.48206400	2.61867800	5.60151900
H	-0.72249600	1.10038900	6.12681500
Rh	-1.86685500	-0.14407400	0.04041500
Cl	0.11531900	-1.61283400	0.13279700

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B3LYP-D3 SCF energy: -4349.836568 a.u.

B3LYP-D3 enthalpy: -4348.170907 a.u.

B3LYP-D3 free energy: -4348.396376 a.u.

M06 SCF energy in solution: -4349.018822 a.u.

#### Cartesian coordinates

ATOM	X	Y	Z
C	-0.00238800	1.25395300	3.36668700
C	0.31753700	0.49682900	2.22174700

C	1.18658800	1.05873500	1.26411600
C	1.70680700	2.34603000	1.45997400
C	1.37020600	3.07749200	2.59622600
C	0.51723500	2.53672100	3.55542800
C	-0.25608500	-0.88244400	2.11544500
C	-1.18927000	-1.26936000	1.12918300
C	0.14170200	-1.83644800	3.08273700
C	-1.72180200	-2.56949200	1.14486300
C	-0.38678400	-3.12930800	3.08027000
C	-1.32867200	-3.48146400	2.11607200
P	1.54352900	0.12804800	-0.29462100
P	-1.61099600	-0.17272800	-0.31150500
C	2.25249000	-1.44195400	0.33150300
C	1.88176300	-2.63661100	-0.27841100
C	3.14562300	-1.46717100	1.40805300
C	2.36615000	-3.86895300	0.17875100
C	3.68419300	-2.66708600	1.87062300
C	3.28198200	-3.88118900	1.25315700
C	2.95923200	1.02370200	-1.05452200
C	4.28803000	0.61537900	-0.92964000
C	2.67291300	2.15735800	-1.82630600
C	5.33053900	1.32099000	-1.53996300
C	3.68381600	2.88920300	-2.45516100
C	5.02848700	2.47113800	-2.30499500
C	-2.12619000	1.42574800	0.42981500
C	-1.72871100	2.59602800	-0.22256500
C	-2.91153500	1.51836900	1.58149800
C	-2.06557500	3.85488400	0.27354700
C	-3.33019900	2.76273800	2.07151100
C	-2.86366900	3.93744700	1.43892800
C	-3.14286400	-0.93007100	-0.99161300
C	-4.42471800	-0.58249800	-0.56220400
C	-3.00207200	-1.92158200	-1.96596200
C	-5.56224000	-1.20657200	-1.08819600
C	-4.10836200	-2.59075500	-2.49235600
C	-5.40326300	-2.23250100	-2.04757200
H	2.37792800	2.77762000	0.72647100
H	1.77280300	4.07700200	2.73466600
H	-2.44047000	-2.87092400	0.39320200
H	-1.75230400	-4.48208000	2.12102200
H	1.17525400	-2.59738300	-1.10321000
H	3.40757900	-0.53306200	1.89128800
H	4.52277000	-0.26975900	-0.34988800
H	1.63776900	2.47142300	-1.93679500
H	-1.11939100	2.49822100	-1.11491800
H	-3.20115400	0.61299200	2.10776500
H	-4.55177100	0.20211700	0.17448000
H	-2.00998900	-2.15519300	-2.33596200
N	-6.51563400	-2.93659900	-2.62041600
C	-7.28728500	-3.81084000	-1.75696000
H	-6.60962300	-4.33287800	-1.07409300
H	-8.05798200	-3.30382300	-1.14769900
H	-7.79818900	-4.56568800	-2.36998500
C	-7.25916900	-2.25755000	-3.66677500
H	-6.55979600	-1.74059400	-4.33047100
H	-7.81060600	-2.99748300	-4.26189400
H	-7.98973600	-1.51314600	-3.29799000
N	-3.14573500	5.25298300	1.93926800
N	6.03974200	3.25498600	-2.95603800
N	3.83242900	-5.09376600	1.79827600
C	-2.65695600	5.60624900	3.25950500

H	-2.48700500	6.69095900	3.30636500	H	6.65493000	-0.68476700	-2.92276700
H	-3.33544800	5.34304900	4.09094400	H	7.96932100	-0.94730500	-1.75608200
H	-1.70043800	5.10372700	3.43332300	H	0.25173700	3.10862800	4.43791400
C	-4.41234600	5.85053700	1.55684400	H	-0.07533400	-3.85962000	3.81689100
H	-4.61071700	5.64016000	0.50113800	O	1.06239000	-1.41381900	4.00088100
H	-5.27857000	5.48872700	2.14226400	O	-0.85714200	0.66836900	4.26043300
H	-4.35723300	6.93982300	1.68369900	C	1.40344200	-2.28999800	5.06187100
C	6.65852100	2.68688500	-4.14132700	H	1.93514100	-3.17836800	4.69550400
H	7.12551800	3.49006700	-4.72601500	H	2.06893900	-1.72452000	5.71628100
H	7.43536300	1.92692200	-3.93821800	H	0.51609200	-2.60222800	5.62854400
H	5.88717400	2.22038000	-4.76202800	C	-0.64073500	0.93212900	5.63927500
C	6.89633000	4.07020900	-2.11344600	H	-0.98541000	1.93255800	5.92919200
H	7.71663600	3.52078500	-1.61578400	H	-1.22930800	0.19021800	6.18400500
H	7.35067800	4.86446200	-2.72010000	H	0.42064300	0.82182300	5.89369100
H	6.29035400	4.54469400	-1.33492500	C	-4.29179700	2.80671400	3.25597600
C	2.95740400	-5.84284800	2.68368900	H	-4.63130300	3.83720800	3.37820100
H	2.17149200	-6.42089800	2.16311500	C	-5.54876600	1.95560500	2.99491400
H	3.55392400	-6.54796800	3.27716000	H	-5.30570300	0.88921500	2.92885900
H	2.45920800	-5.15198400	3.37212100	H	-6.27074200	2.07825900	3.81117900
C	4.68949400	-5.90924000	0.95138400	H	-6.03754200	2.24611600	2.05857400
H	5.27945600	-5.25902700	0.29937100	C	-3.60919100	2.37921500	4.56629400
H	5.38410300	-6.48077500	1.58225100	H	-3.23480000	1.35418300	4.49257600
H	4.15402600	-6.63081500	0.31050100	H	-2.75413100	3.02620000	4.78883200
C	-6.93101400	-0.74435800	-0.59718300	H	-4.31212500	2.43650200	5.40656700
H	-7.69744600	-1.24780000	-1.18887000	C	-1.51440900	5.11146900	-0.39112500
C	-7.13148000	0.76889100	-0.80462200	H	-2.23857000	5.91698900	-0.23453700
H	-6.42541800	1.35712300	-0.20780100	C	-0.20639900	5.53223200	0.30840600
H	-6.98703600	1.04314300	-1.85522500	H	0.54273600	4.73647100	0.22793100
H	-8.14507500	1.06348700	-0.50656100	H	0.20515300	6.44098600	-0.14791500
C	-7.15285900	-1.13708300	0.87564700	H	-0.37702900	5.72544400	1.37221800
H	-8.14892200	-0.82800700	1.21549400	C	-1.29260800	4.96057600	-1.90464800
H	-7.06387800	-2.22053000	1.01259600	H	-0.48003400	4.26248300	-2.13626200
H	-6.41290300	-0.65590400	1.52500600	H	-2.19262700	4.59615600	-2.41165000
C	-3.88560900	-3.64841000	-3.56368600	H	-1.01893200	5.92865400	-2.33966400
H	-4.84197600	-4.15754700	-3.71502200	C	4.71404700	-2.66546000	2.99736700
C	-3.47504300	-2.98144600	-4.89213500	H	4.49005200	-3.51720900	3.65018800
H	-2.55679700	-2.39431800	-4.77495400	C	4.69626400	-1.38520900	3.84950800
H	-3.31076100	-3.73910600	-5.66868200	H	5.11708800	-0.53303600	3.30126700
H	-4.25484000	-2.29652500	-5.24404100	H	3.68371200	-1.10953600	4.15665400
C	-2.84667400	-4.70019200	-3.13331700	H	5.31058900	-1.52580800	4.74615600
H	-1.84571600	-4.26514800	-3.02958800	C	6.13263100	-2.88391700	2.43205600
H	-3.11494200	-5.15742500	-2.17330800	H	6.39350400	-2.07830800	1.73391600
H	-2.78002300	-5.49653600	-3.88427600	H	6.87481000	-2.88302600	3.23998700
C	3.30969400	4.12365900	-3.26349900	H	6.20807700	-3.83522500	1.90130200
H	4.22372000	4.47112600	-3.75290600	C	1.89752700	-5.13448800	-0.53422400
C	2.81467200	5.24891600	-2.33438400	H	2.23770500	-6.00127400	0.03524100
H	1.90306100	4.95294300	-1.80311200	C	0.36292000	-5.23121200	-0.61160600
H	3.57164100	5.50538300	-1.58363500	H	-0.07167000	-4.41533800	-1.19897900
H	2.58510300	6.15323800	-2.91087000	H	0.06773100	-6.17401400	-1.08729800
C	2.26708100	3.80690300	-4.35157900	H	-0.08256800	-5.18906900	0.38623000
H	2.06923800	4.69936000	-4.95716600	C	2.52390700	-5.22245600	-1.93975200
H	2.61962000	3.01229200	-5.01833800	H	2.20287000	-4.37830300	-2.56131500
H	1.31174100	3.47805200	-3.92643800	H	3.61821900	-5.20358200	-1.88885200
C	6.75359500	0.81166300	-1.32993300	H	2.21860700	-6.14766600	-2.44311100
H	7.43843800	1.44884800	-1.89148900	Rh	-0.05035900	0.03263200	-1.85206300
C	7.15994000	0.90161800	0.15399100	Cl	-1.14636900	0.15093400	-3.94285300
H	6.52249400	0.26484900	0.77932300				
H	8.19731000	0.57342500	0.29092500				
H	7.07245100	1.92869300	0.52576800				
C	6.92723500	-0.62305100	-1.86343000				
H	6.29880100	-1.33439800	-1.31496400				