Supporting Information

Theoretical Study of Ligand Effect in NHC-Cobalt-Catalyzed Hydrogenation of Ketones

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1. Comparison between triplet and singlet free energy profiles of pincer cobalt(I)-catalyzed hydrogenation of acetophenone with NHC ligand L1

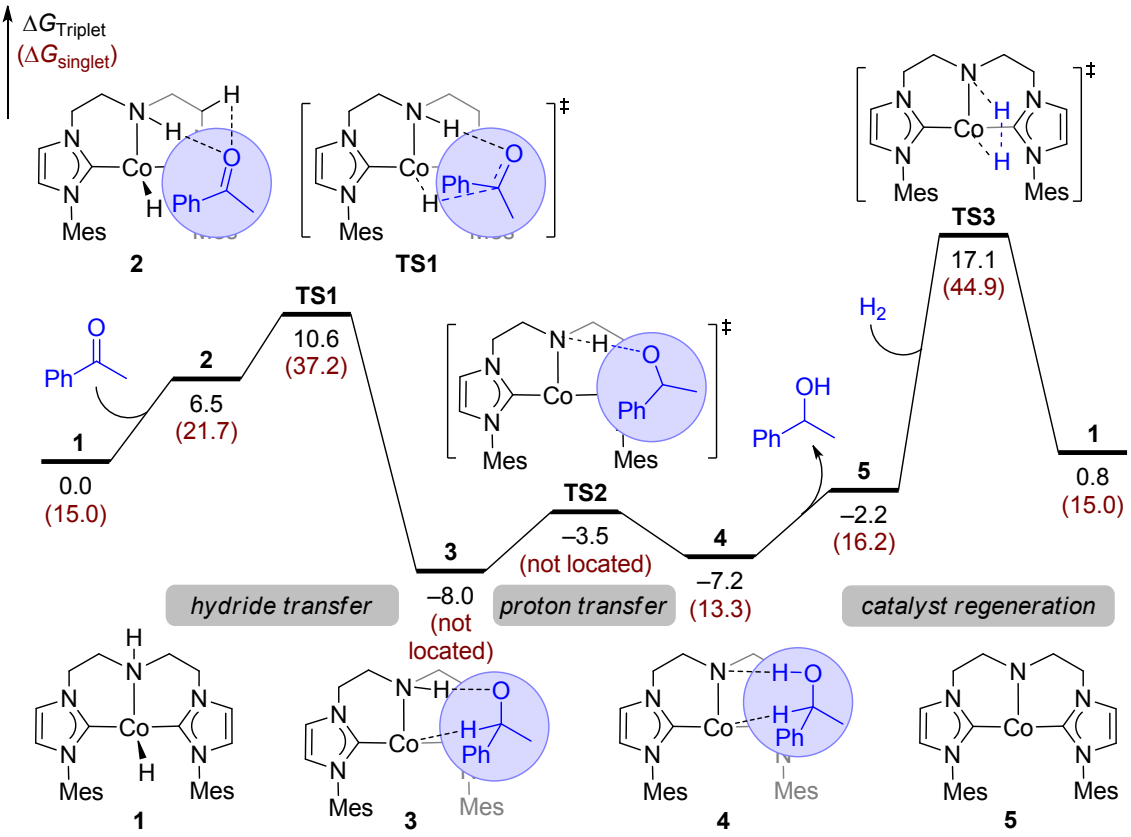


Figure S1. Comparison between triplet and singlet free energy profiles of pincer cobalt(I)-catalyzed hydrogenation of acetophenone with NHC ligand **L1**.

Both triplet and singlet free energy profiles are calculated for cobalt(I)-catalyzed hydrogenation of acetophenone. As shown in Figure S1, the relative free energies of singlet intermediate and transition state with respect to triplet cobalt(I) hydride **1** are in red. The higher relative free energy of singlet structures suggests that triplet cobalt(I) complex is more stable in this catalytic system. The <S**2> of each triplet intermediate and transition state in NHC ligand **L1** involved hydrogenation free energy profile are shown in Table S1. These results show that the <S**2> of calculated triplet complexes is very close to 2.0.

Table S1. The <S**2> of triplet cobalt complexes in NHC ligand **L1** involved hydrogenation free energy profile

Complexes	<S**2> before annihilation	<S**2> after annihilation
1	2.0629	2.0009
2	2.0662	2.0010
TS1	2.0600	2.0008
3	2.0254	2.0003
TS2	2.0166	2.0001
4	2.0387	2.0006
5	2.0432	2.0008
TS3	2.0330	2.0005

2. Free energy profiles of pincer cobalt(I)-catalyzed hydrogenation of acetophenone with NHC ligand L3

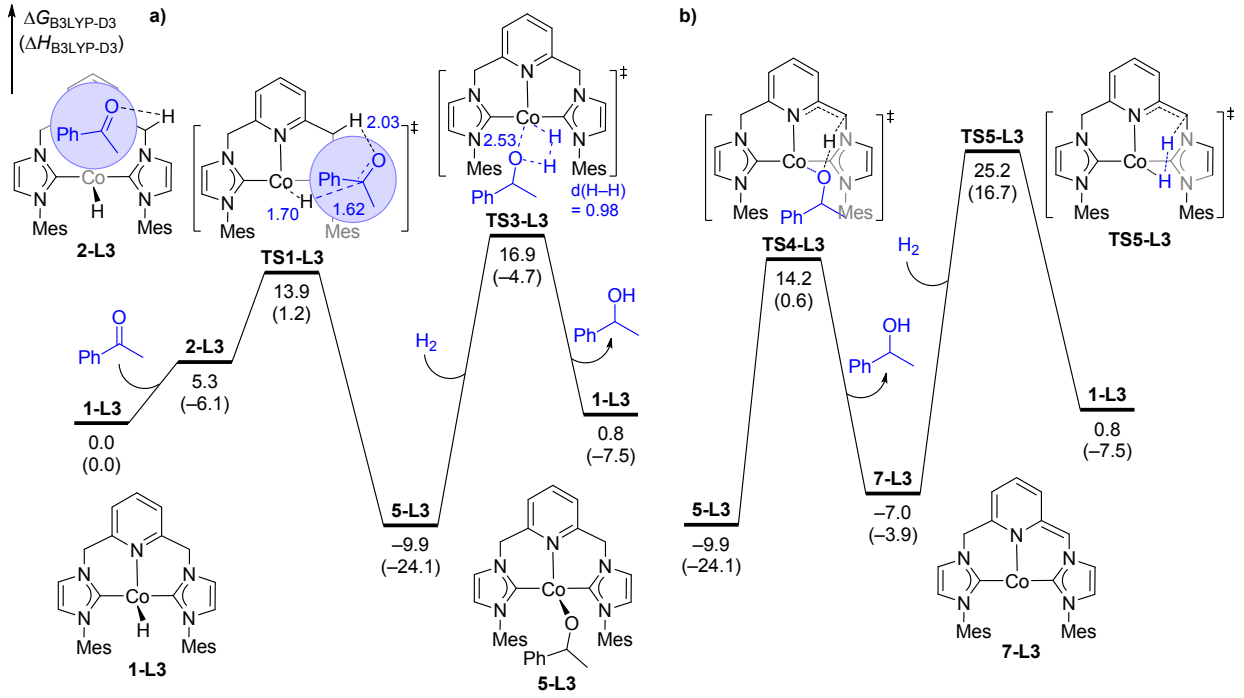


Figure S2. a) Free energy profile of pincer cobalt(I)-catalyzed hydrogenation of acetophenone with NHC ligand **L3**. b) Competing pathway for catalyst regeneration with the participation of reactive C–H bond on ligand backbone.

The complete free energy profile for cobalt(I)-catalyzed hydrogenation of acetophenone with NHC ligand **L3** are shown in Figure S2a. Besides the H_2 splitting transitions state **TS3-L3**, another possible pathway for the **L3** involved catalyst regeneration process are also proposed. The computational results are shown in Figure S2b. In this pathway, an intramolecular proton

transfer (**TS4-L3**) could occur from intermediate **5-L3** to generate the product 1-phenylethanol. The reactive C–H bond on ligand **L3** is used as the hydrogen donor. This step bears an activation free energy of 24.1 kcal/mol. However, subsequent H_2 splitting transition state (**TS5-L3**) for catalyst regeneration has an activation free energy of 35.1 kcal/mol, which is 8.3 kcal/mol higher than that of **TS3-L3** in Figure 6. Therefore, this possibility could be ruled out.

3. Non-covalent interactions between ligand and substrate in TS1 and TS1-L3

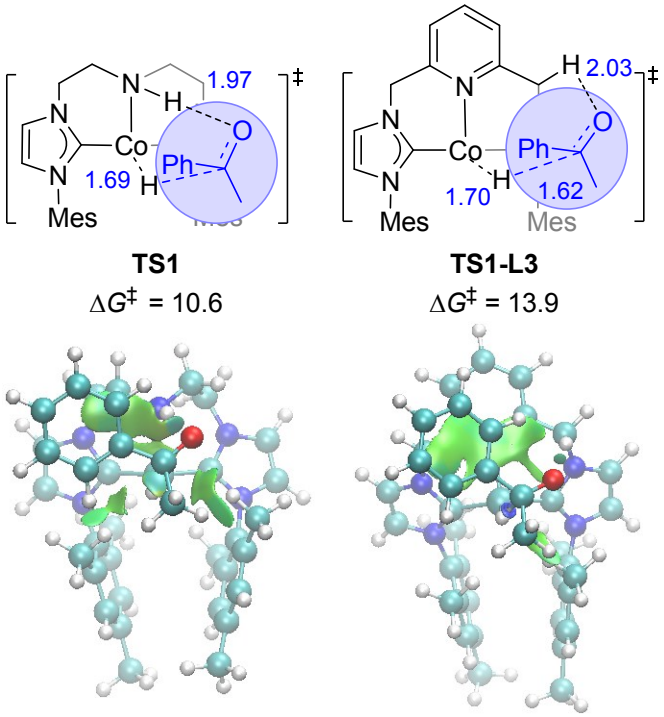
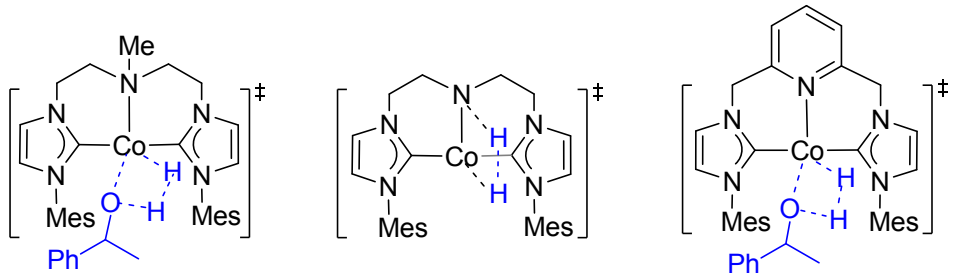


Figure S3. Non-covalent interactions between ligand and substrate in **TS1** and **TS1-L3**.

The non-covalent interactions (NCI) between pincer ligand and the substrate ketone in transition states **TS1** and **TS1-L3** are visualized with the aid of NCI plot. As shown in Figure S3, the non-covalent ligand-substrate interactions in **TS1** included the non-covalent interaction between the carbonyl group of the substrate and alkyl C–H bonds on the ligand, as well as the interaction between phenyl group of the substrate and the NHC part of ligand. It is similar to the ligand-substrate interaction in transition state **TS1-L2**. While in **TS1-L3**, the non-covalent interaction between the carbonyl group of the substrate and alkyl C–H bonds on the ligand is shown to be negligible. Therefore, the ligand-substrate interaction in **TS1-L3** is diminished

compared with that in **TS1** and **TS1-L2**, which accounts for the higher activation free energy of transition state **TS1-L3**.

4. Distortion-interaction analysis of transition states TS3-L2, TS3, and TS3-L3



TS3-L2
$\Delta G^{‡}$ = 27.3
$E^{‡}$(TS3-L2) = 17.4
$E^{‡}(\text{TS3-L2})_{int}$ = –11.0
$E^{‡}(\text{TS3-L2})_{dist}$ = **28.4**
$E^{‡}(\text{TS3-L2})_{dist\text{-}1}$ = 11.6
$E^{‡}(\text{TS3-L2})_{dist\text{-}2}$ = **16.8**

TS3
$\Delta G^{‡}$ = 25.1
$E^{‡}$(TS3) = 10.0
$E^{‡}(\text{TS3})_{int}$ = –10.9
$E^{‡}(\text{TS3})_{dist}$ = **20.9**
$E^{‡}(\text{TS3})_{dist\text{-}1}$ = 17.8
$E^{‡}(\text{TS3})_{dist\text{-}2}$ = **3.1**

TS3-L3
$\Delta G^{‡}$ = 26.8
$E^{‡}$(TS3-L3) = 18.8
$E^{‡}(\text{TS3-L3})_{int}$ = –15.2
$E^{‡}(\text{TS3-L3})_{dist}$ = **34.0**
$E^{‡}(\text{TS3-L3})_{dist\text{-}1}$ = 19.5
$E^{‡}(\text{TS3-L3})_{dist\text{-}2}$ = **14.5**

Figure S4. Distortion-interaction analysis of transition states **TS3-L2**, **TS3**, and **TS3-L3**.

Distortion-interaction analysis on **TS3-L2** and **TS3** reveals that the interaction energies between the H–H part (fragment 1) and the Co/L part (fragment 2) are nearly the same for these two transition states (Figure S4). Whereas the distortion energy of **TS3-L2** is higher than that of **TS3** by 7.5 kcal/mol and most of the increased distortion in **TS3-L2** originates from the Co/L part (fragment 2). Distortion-interaction analysis of **TS3-L3** shows that the $E^{‡}_{dist\text{-}2}$ of **TS3-L3** is 14.5 kcal/mol, which is higher than that in **TS3** by 11.4 kcal/mol. Meanwhile the variation of interaction in interaction energy is 4.3 kcal/mol. Therefore, the higher energy barrier of **TS3-L3** with respect to **TS3** is also attributed to the increased distortion of phenylethoxyl-Co/L fragment like **TS3-L2**. A conclusion could be drawn that ligand **L2** and **L3** have the same critical deficiency that the lack of N–H group on backbone suppresses the regeneration of active cobalt catalyst, thereby leading to the low reactivity of **L2** and **L3**.

5. Free energy profiles of pincer cobalt(I)-catalyzed hydrogenation of acetophenone with phosphine ligand L5

As a comparison, phosphine ligands **L4** and **L5** involved hydrogenation of acetophenone are also considered in calculation although no reactivity was observed for them in the experiment. The complete free energy profile with **L5** are shown in Figure S5. Computational studies confirm ligands **L4** and **L5** involved hydrogenation of acetophenone follow exactly the same reaction pathway as **L1** and the catalyst regeneration transition states have the same structure as **TS3**. The catalyst regeneration is still the rate-determining step. For both ligands **L4** and **L5**, the relative weak coordination ability results in the higher energy barrier for catalyst regeneration, thereby restricts their reactivity in this cobalt(I)-catalyzed ketone hydrogenation reaction.

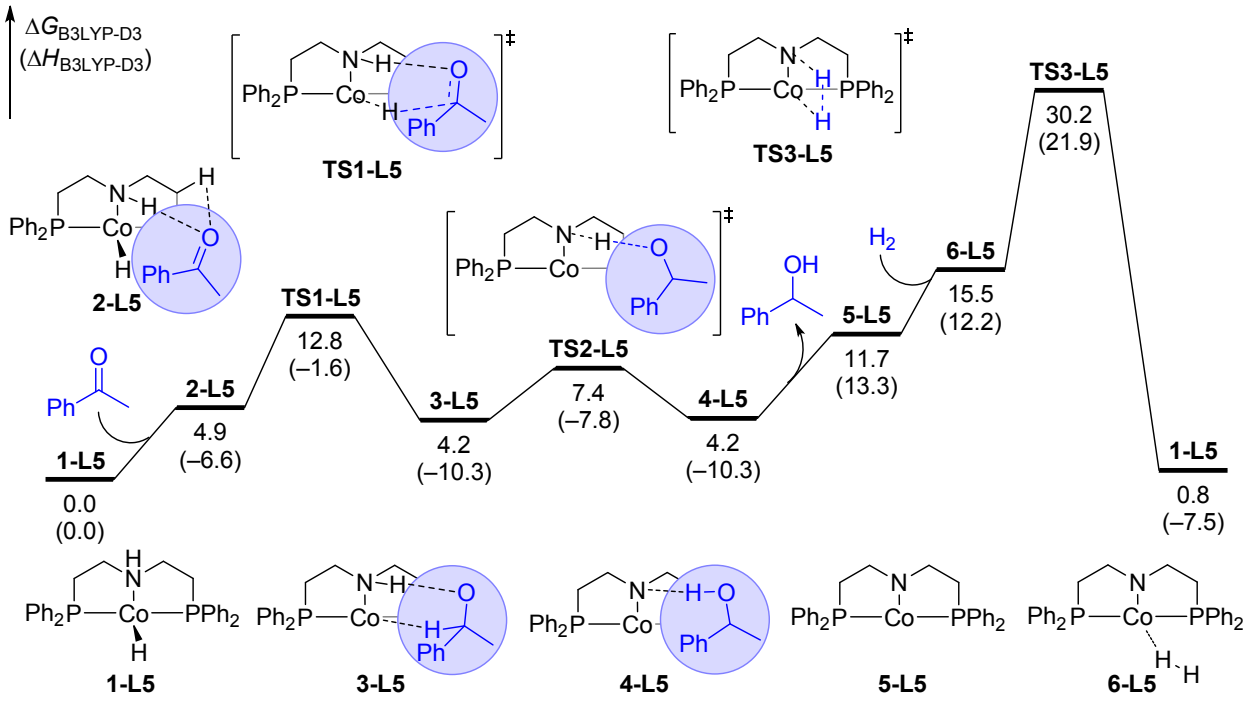


Figure S5. Free energy profile of pincer cobalt(I)-catalyzed hydrogenation of acetophenone with phosphine ligand **L5**.

6. Free energy profiles of L4 and L5 involved catalyst regeneration with ammonia borane as the hydrogen donor

To provide further advice on improving the efficiency of phosphine ligands, another widely used hydrogen donor, ammonia borane (H_3N-BH_3), was employed to replace H_2 for the calculation of **L4** and **L5** involved catalyst regeneration. As shown in Figure S6a, the interaction of cobalt complex **5** with ammonia borane leads to the formation of protonation intermediate **7-L4** directly. The corresponding protonation transition state is not obtained. This protonation step is most likely a barrier-free process because this step is highly exergonic by 17.1 kcal/mol. Subsequent hydride transfer occurs through transition state **TS4-L4**, regenerating the active cobalt hydride **1-L4**. The activation free energy of this step is only 5.6 kcal/mol, which is much lower than that with H_2 (**TS3-L4**, 29.2 kcal/mol). Ligand **L5** involved catalyst regeneration with ammonia borane follows the same pathway as **L4**. The corresponding activation free energy for catalyst regeneration is only 6.3 kcal/mol (Figure S6b), which is also much lower than that of **TS3-L5** (Figure S5, 30.2 kcal/mol). Therefore, DFT calculation indicates that using ammonia borane (H_3N–BH_3) instead of H_2 as the hydrogen donor could greatly promote the catalyst regeneration in phosphine ligands (**L4** and **L5**) involved ketone hydrogenation reactions.

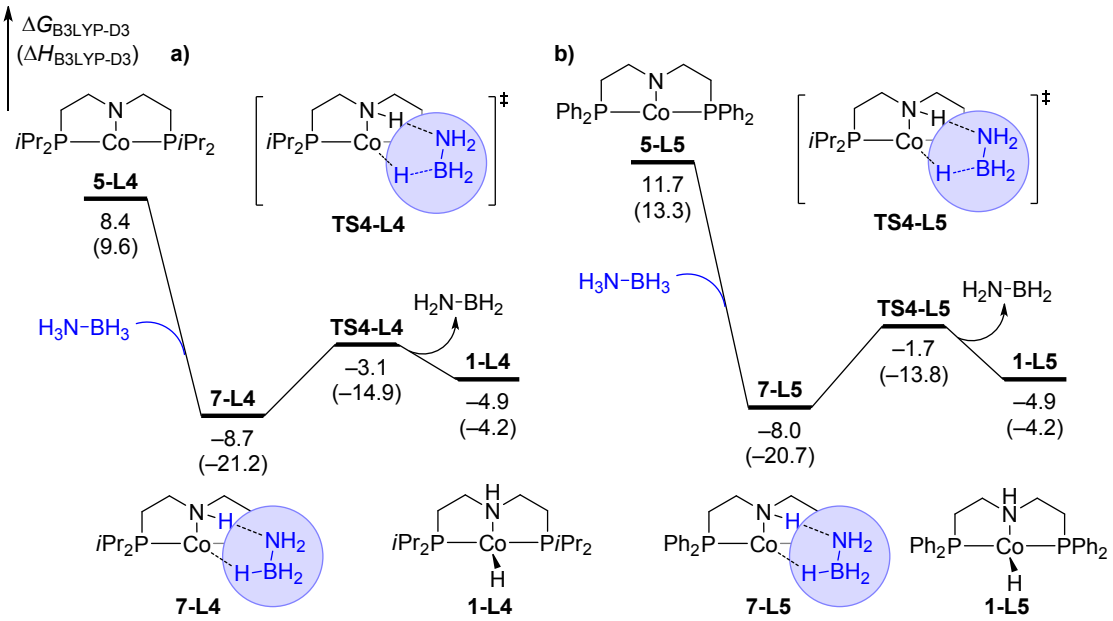


Figure S6. Free energy profile of **L4** and **L5** involved catalyst regeneration with ammonia borane as the hydrogen donor. All energies are in kcal/mol.

7. Intermediates formed through the interaction of H_2 with T-shaped tridentate cobalt(I) complex 5, 5-L4, and 5-L5.

To study the interaction of H_2 with T-shaped tridentate cobalt(I) complex **5**, **5-L4**, and **5-L5**, three different intermediates are obtained in calculation. As shown in Figure S7, not only the end-on bonding structure **6** and side-on bonding structure **6b** are located, the other structure **6c** which contains the N–H interaction is also considered in calculation. Besides cobalt(I) complex **5**, analogous complexes **5-L4** and **5-L5** are also studied to locate the H_2 bonding intermediate. In our calculation, the side-on bonding structure **6b** (**6b-L4** and **6b-L5**) is shown to be a distorted trigonal pyramidal geometry. This result is consistent with Arnold's study that the 16*e* triplet PNP-CoCl complex possesses a distorted trigonal pyramidal structure (ref. 28: S. S. Rozenel, R. Padilla and J. Arnold, *Inorg. Chem.*, 2013, **52**, 11544-11550.). The computational results show that the formation of these three H_2 bonding intermediates are endergonic and the end-on intermediate **6** (**6-L4** and **6-L5**) has the lowest relative free energy.

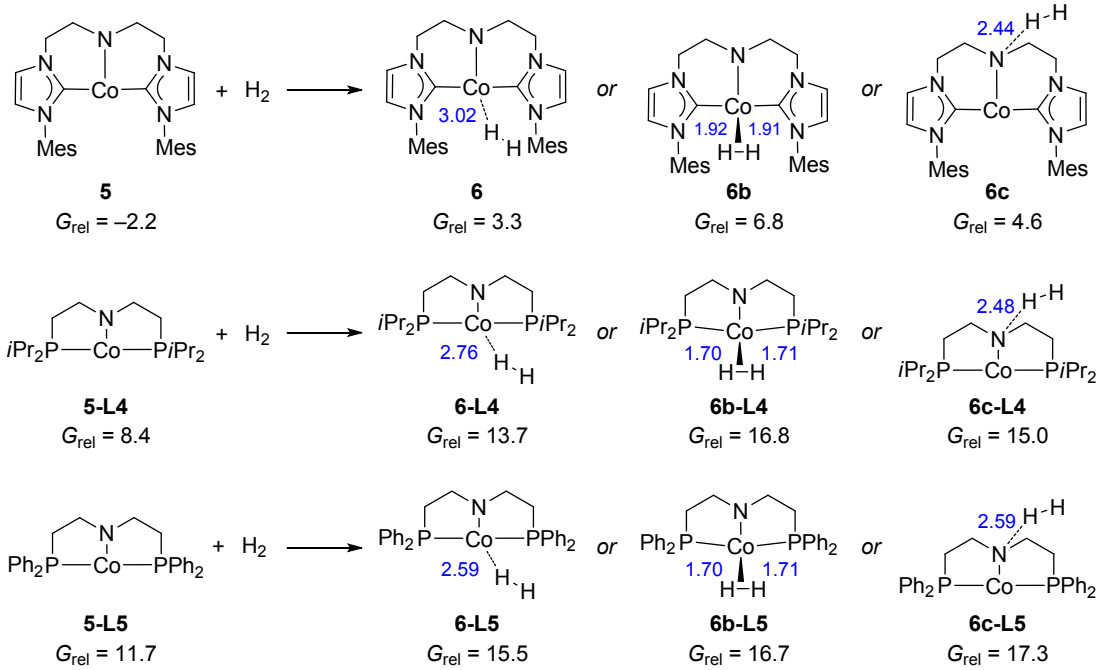


Figure S7. Possible intermediates formed through the interaction of H_2 with T-shaped tridentate cobalt(I) complex **5**, **5-L4**, and **5-L5**. All energies are with respect to triplet cobalt(I) hydride complex **1** (**1-L4** or **1-L5**) and are in kcal/mol. The bond lengths are in blue and the unit is Å.

8. Cartesian coordinates and energies of optimized structures

1

(U)B3LYP-D3(BJ) SCF energy: -1508.38726663 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1507.760613 a.u.

(U)B3LYP-D3(BJ) free energy: -1507.862682 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1508.80217646 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1508.175523 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1508.277592 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.830076	-0.187381	-0.897388
N	-4.000260	-0.095751	-0.160426
C	-3.799460	-2.438130	0.589065
C	-4.329548	-1.041850	0.899291
C	-4.500356	1.251036	0.104959
C	-3.858543	2.270469	-0.835256
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H	-3.871933	-0.681086	1.827319
H	-2.130804	-0.394297	-2.519089
N	-2.503016	2.612079	-0.439967
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C	-2.061140	3.915887	-0.253289

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H	-4.055227	-2.704624	-0.447430
N	-2.368231	-2.588097	0.785649
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C	-1.415090	-1.738526	0.246954
C	-0.469769	-3.635415	1.161620
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H	0.339461	-4.293590	1.435027
N	-0.243636	-2.424450	0.505004
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C	1.766732	1.805999	-0.949719
C	1.481127	2.123270	1.464336
C	3.140141	1.659804	-0.736495
C	2.858950	1.965997	1.628556
C	3.707239	1.764725	0.535703
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H	5.742144	1.826684	-0.195363
H	5.558220	2.354377	1.486763
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2

(U)B3LYP-D3(BJ) SCF energy: -1893.33236423 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1892.555885 a.u.

(U)B3LYP-D3(BJ) free energy: -1892.681273 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1893.85726312 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1893.080784 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1893.206172 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.836467	0.256757	-0.090857
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C	-1.068764	-3.812861	-0.922628
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C	3.400622	1.528006	-0.517791
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C	4.508348	1.241189	0.280754
C	3.292219	1.861192	2.256573
C	4.472978	1.401039	1.668345
H	5.415349	0.878683	-0.194320
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C	0.926855	2.750465	2.141005
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H	5.639377	0.016702	2.851680
H	6.607889	1.196427	1.966459
H	5.714354	1.687949	3.417113
H	-4.149129	-0.976372	-2.277856
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C	-4.778660	0.240983	1.358591
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3

(U)B3LYP-D3(BJ) SCF energy: -1893.36307345 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1892.583170 a.u.

(U)B3LYP-D3(BJ) free energy: -1892.705376 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1893.88688292 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1893.106979 a.u.

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Cartesian coordinates

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C	-3.337591	-1.022642	-1.818321
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N	-2.115952	-1.788366	-1.551412
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C	-2.009896	-3.158351	-1.736113
C	-0.724786	-3.493077	-1.462985
H	-2.850655	-3.763932	-2.036146
H	-0.208001	-4.438510	-1.495944

N	-0.081294	-2.309535	-1.105838
H	-2.373643	4.639699	-1.486261
H	-2.852638	3.394663	-0.288580
N	-0.793983	3.614744	-0.625450
C	-0.105772	4.752621	-0.230171
C	-0.084075	2.476721	-0.364212
C	1.079863	4.336850	0.284197
H	-0.515491	5.743437	-0.351499
H	1.913604	4.881949	0.697182
N	1.078014	2.948630	0.188894
C	1.335919	-2.221430	-0.912763
C	1.908645	-2.777094	0.237307
C	2.122675	-1.650954	-1.929948
C	3.304808	-2.788985	0.338182
C	3.508690	-1.678876	-1.779610
C	4.119599	-2.262560	-0.663792
H	3.760890	-3.232474	1.220188
H	4.128910	-1.250848	-2.564043
C	2.112584	2.103785	0.711623
C	3.183642	1.738734	-0.111522
C	2.021393	1.684776	2.047602
C	4.202001	0.961139	0.446385
C	3.055796	0.898491	2.556983
C	4.156662	0.534273	1.775231
H	5.047235	0.681486	-0.175908
H	3.002872	0.568783	3.592104
H	-4.051913	0.633211	-2.956421
H	-2.430101	0.096609	-3.441335
C	-2.923976	0.816827	1.397627
O	-3.786854	1.408361	0.534167
C	-3.256836	-0.653363	1.694671

C	-2.283061	-1.558102	2.132694
C	-4.562229	-1.115673	1.505435
C	-2.599815	-2.897008	2.365127
H	-1.263413	-1.204912	2.276670
C	-4.887286	-2.453761	1.737375
H	-5.296182	-0.399506	1.148465
C	-3.906037	-3.351677	2.163666
H	-1.829877	-3.589064	2.698478
H	-5.907347	-2.798821	1.582781
H	-4.155053	-4.395298	2.338990
C	-2.813196	1.600120	2.725761
H	-2.144113	1.121303	3.452432
H	-2.450014	2.613956	2.520328
H	-3.811476	1.677663	3.171203
C	1.050418	-3.366693	1.327405
H	0.752258	-4.397416	1.095389
H	1.593257	-3.386547	2.277131
H	0.130927	-2.792706	1.458536
C	1.494593	-1.047841	-3.160848
H	0.770991	-1.732398	-3.617592
H	0.944673	-0.131092	-2.916048
H	2.258846	-0.803565	-3.904339
C	5.623689	-2.339342	-0.571099
H	5.947256	-2.705809	0.407146
H	6.030464	-3.016342	-1.332787
H	6.087368	-1.359431	-0.733030
C	0.834123	2.063235	2.892483
H	0.704564	3.150290	2.948468
H	-0.088541	1.658939	2.466066
H	0.940035	1.678070	3.910496
C	3.222153	2.156321	-1.558917

H	3.169682	3.245347	-1.671090
H	4.138827	1.804663	-2.040715
H	2.367207	1.739446	-2.103159
C	5.254425	-0.319719	2.359009
H	4.945678	-1.371309	2.406060
H	6.165547	-0.271000	1.755407
H	5.503576	-0.007518	3.379131

4

(U)B3LYP-D3(BJ) SCF energy: -1893.36621610 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1892.585246 a.u.

(U)B3LYP-D3(BJ) free energy: -1892.708727 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1893.88536309 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1893.104393 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1893.227874 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.659354	0.510638	-0.893117
N	-2.441443	0.907060	-1.779430
C	-2.261475	3.368310	-1.640586
C	-2.499664	2.146045	-2.525019
C	-3.073821	-0.166991	-2.510151
C	-3.213146	-1.427456	-1.658974
H	-3.505927	2.303229	-2.965281
H	-3.837976	-2.160980	-2.177348
H	-3.689901	-1.179587	-0.708470
H	-3.347183	1.211083	-0.355075
H	-1.792056	2.177453	-3.379382

H	-1.948062	1.048387	1.303790
N	-1.931737	-2.085908	-1.388638
C	-0.787817	-1.418228	-1.055578
C	-1.735410	-3.455891	-1.448338
C	-0.426106	-3.678992	-1.174121
H	-2.537025	-4.140742	-1.676714
H	0.155624	-4.586224	-1.141723
N	0.140619	-2.426803	-0.937864
H	-2.414702	4.281744	-2.224407
H	-2.975325	3.350141	-0.810508
N	-0.908748	3.451340	-1.072494
C	-0.292641	4.650929	-0.747200
C	-0.184763	2.375065	-0.641211
C	0.860808	4.341472	-0.102520
H	-0.723118	5.605856	-1.006647
H	1.643005	4.960609	0.307118
N	0.912380	2.951628	-0.048971
C	1.550022	-2.228777	-0.774940
C	2.159353	-2.586190	0.435793
C	2.294974	-1.744268	-1.862314
C	3.550024	-2.488562	0.527622
C	3.680911	-1.647393	-1.716530
C	4.327548	-2.031376	-0.538719
H	4.034851	-2.776294	1.457238
H	4.269898	-1.275534	-2.551780
C	1.933656	2.211641	0.631210
C	3.046978	1.759829	-0.087713
C	1.793946	1.985811	2.008832
C	4.052705	1.091928	0.615105
C	2.817216	1.299357	2.665961
C	3.955103	0.851689	1.987572

H	4.929909	0.749431	0.074929
H	2.726301	1.118538	3.734695
H	-4.104358	0.105603	-2.818777
H	-2.541207	-0.433868	-3.447576
C	-3.018808	0.952879	1.558912
O	-3.803865	1.483908	0.514303
C	-3.290325	-0.530073	1.774120
C	-2.241757	-1.424401	2.007079
C	-4.598171	-1.025981	1.710540
C	-2.485925	-2.789752	2.163274
H	-1.223944	-1.044099	2.034018
C	-4.848954	-2.388459	1.870806
H	-5.406061	-0.332875	1.496592
C	-3.792078	-3.276367	2.092655
H	-1.657061	-3.473506	2.323960
H	-5.868455	-2.761738	1.813396
H	-3.986253	-4.339635	2.206983
C	-3.291776	1.761114	2.828049
H	-2.702353	1.384359	3.671734
H	-3.041179	2.813955	2.658695
H	-4.353155	1.697621	3.092730
C	1.337311	-3.045133	1.613176
H	0.769277	-3.955148	1.390423
H	1.976529	-3.245529	2.477672
H	0.607964	-2.279049	1.894844
C	1.623646	-1.350778	-3.153304
H	0.983468	-2.156381	-3.530879
H	0.973225	-0.479261	-3.009357
H	2.367012	-1.110625	-3.918971
C	5.831792	-1.974221	-0.431328
H	6.154471	-1.840838	0.605786

H	6.290396	-2.900924	-0.800575
H	6.244768	-1.151444	-1.025033
C	0.573020	2.467031	2.750395
H	0.451532	3.553425	2.669567
H	-0.336811	2.018647	2.338838
H	0.634410	2.207992	3.811165
C	3.142575	1.978421	-1.575299
H	3.065146	3.040466	-1.834967
H	4.089439	1.594230	-1.964342
H	2.324657	1.464262	-2.092256
C	5.039641	0.103674	2.722636
H	4.786025	-0.959897	2.816481
H	5.997063	0.167137	2.195808
H	5.181567	0.494883	3.735786

5

(U)B3LYP-D3(BJ) SCF energy: -1507.20858049 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1506.601523 a.u.

(U)B3LYP-D3(BJ) free energy: -1506.703029 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1507.60740884 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1507.000351 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1507.101857 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.624866	-0.025745	-0.316823
N	-3.568526	0.072541	0.044850
C	-3.901110	-2.350117	0.372744
C	-4.194864	-0.932549	0.859301

C	-4.263550	1.326181	0.119488
C	-3.779320	2.307350	-0.949013
H	-5.301725	-0.851261	0.828494
H	-4.414021	3.198654	-0.971745
H	-3.818768	1.815313	-1.926849
H	-3.927890	-0.874888	1.938934
N	-2.409406	2.761127	-0.707595
C	-1.378777	1.885935	-0.504429
C	-2.016401	4.079673	-0.535833
C	-0.698387	4.057431	-0.214541
H	-2.700049	4.905503	-0.658983
H	-0.000424	4.848647	0.008179
N	-0.322657	2.713922	-0.202681
H	-4.458337	-3.076317	0.974409
H	-4.224559	-2.435761	-0.671821
N	-2.488075	-2.736012	0.445247
C	-2.045969	-4.020575	0.727702
C	-1.460735	-1.913670	0.073329
C	-0.700812	-4.024156	0.547740
H	-2.719568	-4.806199	1.033889
H	0.036795	-4.802110	0.664510
N	-0.360019	-2.732506	0.152312
C	0.970307	2.266207	0.220277
C	2.033502	2.291500	-0.692152
C	1.144211	1.860720	1.551824
C	3.305790	1.949302	-0.228630
C	2.433234	1.516794	1.967450
C	3.526632	1.573728	1.099360
H	4.142489	1.977645	-0.922637
H	2.585599	1.204104	2.997824
C	0.963060	-2.325279	-0.214821

C	1.883153	-2.004396	0.790901
C	1.302877	-2.281865	-1.575447
C	3.184891	-1.672626	0.407771
C	2.610441	-1.925252	-1.911416
C	3.565607	-1.626487	-0.935148
H	3.913521	-1.435095	1.177478
H	2.891352	-1.890051	-2.961680
C	1.795890	2.659293	-2.134473
H	1.044350	1.997651	-2.580122
H	1.417900	3.682977	-2.238209
H	2.719513	2.575771	-2.714493
C	4.918180	1.258275	1.590926
H	5.439879	2.169260	1.912721
H	4.894356	0.578286	2.449015
H	5.525649	0.795699	0.806795
C	-0.026649	1.793209	2.498430
H	-0.562235	2.748577	2.541854
H	-0.754515	1.042756	2.163284
H	0.304275	1.535516	3.508793
C	0.282754	-2.601643	-2.637627
H	-0.202662	-3.566354	-2.450879
H	-0.511571	-1.845675	-2.650028
H	0.748697	-2.634190	-3.626839
C	1.466080	-1.989518	2.239103
H	0.628551	-1.298932	2.388910
H	1.130887	-2.975380	2.581537
H	2.294259	-1.668628	2.877053
C	4.967030	-1.232429	-1.331113
H	5.017309	-0.163862	-1.576739
H	5.679777	-1.417204	-0.520919
H	5.305295	-1.784830	-2.214407

H	-5.353522	1.202872	-0.054983
H	-4.180845	1.838908	1.106735

TS1

(U)B3LYP-D3(BJ) SCF energy: -1893.33047859 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1892.555023 a.u.

(U)B3LYP-D3(BJ) free energy: -1892.676411 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1893.85366099 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1893.078205 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1893.199593 a.u.

Imaginary frequency: -72.1858 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.641426	0.376636	-0.376151
N	-2.662669	1.077689	-1.061140
C	-1.505215	2.257727	-2.969815
C	-2.701242	2.198187	-2.008791
C	-3.510345	-0.067429	-1.404438
C	-2.925817	-0.999971	-2.467647
H	-3.622567	2.170125	-2.614398
H	-4.498944	0.266092	-1.766905
H	-3.671507	-0.645257	-0.494006
H	-2.592548	-0.429344	-3.343885
H	-3.720267	-1.673850	-2.803799
H	-2.940494	1.438122	-0.144173
H	-1.032504	0.306114	1.269374
N	-1.832967	-1.833498	-1.989201
C	-0.747596	-1.347420	-1.291494

C	-1.706096	-3.188050	-2.284674
C	-0.522171	-3.590788	-1.765267
H	-2.465889	-3.735819	-2.821059
H	-0.040302	-4.555569	-1.748657
N	0.047403	-2.469357	-1.162939
N	-0.263659	2.613805	-2.305176
C	0.520350	3.726685	-2.594260
C	0.277281	1.843337	-1.305159
C	1.590303	3.672178	-1.761943
H	0.251372	4.443776	-3.354698
H	2.437187	4.329470	-1.643796
N	1.427326	2.526465	-0.987774
C	1.350775	-2.467872	-0.570280
C	1.483824	-2.562089	0.822940
C	2.465984	-2.390743	-1.416255
C	2.775482	-2.585719	1.356070
C	3.737555	-2.433906	-0.839478
C	3.911053	-2.534173	0.543291
H	2.894024	-2.650570	2.435378
H	4.610800	-2.376473	-1.485398
C	2.297342	2.102638	0.066942
C	3.413370	1.318574	-0.247168
C	1.978225	2.459827	1.383935
C	4.219220	0.875875	0.803935
C	2.806991	1.986390	2.403880
C	3.921206	1.185416	2.133750
H	5.088265	0.264409	0.578527
H	2.572475	2.246157	3.433745
C	0.270990	-2.610150	1.711353
H	-0.235032	-1.635269	1.693787
H	-0.452824	-3.355661	1.362876

H	0.551899	-2.849165	2.741941
C	5.293045	-2.609036	1.145459
H	6.045350	-2.181242	0.474327
H	5.343589	-2.071886	2.097845
H	5.584957	-3.649212	1.341827
C	2.286904	-2.239605	-2.905894
H	1.840747	-3.134346	-3.356377
H	1.613956	-1.404036	-3.129332
H	3.247173	-2.055799	-3.396419
C	0.775211	3.318000	1.674854
H	0.786163	4.237741	1.078197
H	-0.152176	2.787516	1.432061
H	0.745989	3.598959	2.731826
C	3.716908	0.961814	-1.679109
H	2.853202	0.478573	-2.145559
H	3.950449	1.851496	-2.276810
H	4.566742	0.277311	-1.737087
C	4.764323	0.637828	3.259451
H	4.355262	-0.313861	3.624631
H	5.793399	0.448872	2.936107
H	4.795028	1.325154	4.111626
H	-2.717135	3.127939	-1.430459
H	-1.699988	3.012496	-3.738841
H	-1.366103	1.290614	-3.464009
C	-2.616835	1.234237	2.267445
O	-2.838866	2.280219	1.635908
C	-3.561250	0.071874	2.093343
C	-3.219362	-1.257849	2.373439
C	-4.859549	0.356914	1.648552
C	-4.143900	-2.280655	2.181768
H	-2.211872	-1.492096	2.694931

C	-5.792776	-0.665418	1.468974
H	-5.115335	1.390892	1.441178
C	-5.435342	-1.988792	1.726712
H	-3.857542	-3.309873	2.381105
H	-6.796155	-0.428307	1.124820
H	-6.155290	-2.789344	1.579278
C	-1.755958	1.249212	3.516978
H	-1.342703	0.268738	3.756561
H	-0.944796	1.966710	3.401388
H	-2.391988	1.570761	4.356350

TS2

(U)B3LYP-D3(BJ) SCF energy: -1893.34610099 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1892.569772 a.u.

(U)B3LYP-D3(BJ) free energy: -1892.693948 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1893.87420931 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1893.097880 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1893.222056 a.u.

Imaginary frequency: -1141.4500 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.395464	0.226198	-1.070744
N	-2.316557	0.264947	-1.941279
C	-2.360900	2.707631	-2.399535
C	-2.359165	1.289797	-2.969524
C	-2.757234	-1.008697	-2.468046
C	-2.617736	-2.155832	-1.463823
H	-3.289975	1.227469	-3.568207

H	-3.153820	-3.032881	-1.837824
H	-3.050328	-1.875414	-0.500490
H	-2.873935	0.705726	-0.856169
H	-1.525587	1.179644	-3.688034
H	-4.591625	1.465482	1.608917
N	-1.227219	-2.581971	-1.240699
C	-0.180575	-1.725300	-1.082983
C	-0.822718	-3.903369	-1.136848
C	0.521406	-3.887340	-0.928873
H	-1.514854	-4.726665	-1.221210
H	1.237421	-4.684859	-0.809706
N	0.892057	-2.548667	-0.897833
H	-2.459253	3.427386	-3.219337
H	-3.208466	2.807080	-1.715681
N	-1.162589	3.081323	-1.629189
C	-0.937474	4.382068	-1.202656
C	-0.322736	2.207953	-1.015657
C	0.072789	4.331685	-0.295151
H	-1.512048	5.216148	-1.574922
H	0.558552	5.103634	0.280200
N	0.437930	2.995561	-0.201729
C	2.236599	-2.070375	-0.740845
C	2.765579	-1.925082	0.546669
C	2.973920	-1.756170	-1.892211
C	4.088434	-1.489382	0.662408
C	4.283534	-1.302286	-1.725285
C	4.857920	-1.166767	-0.456927
H	4.517589	-1.380307	1.654695
H	4.868467	-1.050365	-2.606876
C	1.313424	2.439296	0.791167
C	2.645248	2.169231	0.463252

C	0.770571	2.148033	2.054687
C	3.462198	1.623054	1.457625
C	1.622268	1.581994	3.005813
C	2.968967	1.318771	2.727318
H	4.502228	1.414152	1.224526
H	1.222057	1.340482	3.987973
C	1.920283	-2.157693	1.771294
H	1.231307	-1.315843	1.912232
H	1.315013	-3.065853	1.691883
H	2.544311	-2.234874	2.666284
C	6.262552	-0.638022	-0.300662
H	6.703331	-0.946383	0.652808
H	6.916512	-0.985472	-1.107555
H	6.273289	0.460217	-0.326586
C	2.353525	-1.872108	-3.260378
H	1.922612	-2.865879	-3.427631
H	1.537145	-1.147318	-3.368757
H	3.094812	-1.681768	-4.041734
C	-0.677873	2.430919	2.366525
H	-0.863006	3.511299	2.426966
H	-1.357890	2.035193	1.601714
H	-0.953589	1.990153	3.328825
C	3.163213	2.398048	-0.932619
H	2.718520	1.668655	-1.620714
H	2.906079	3.394586	-1.307392
H	4.250367	2.281541	-0.968659
C	3.859229	0.696255	3.775319
H	3.537801	-0.326463	4.010379
H	4.899712	0.649865	3.438585
H	3.833510	1.262995	4.713460
H	-3.825051	-0.986036	-2.768353

H	-2.192258	-1.283016	-3.378794
C	-4.203498	0.729441	0.878014
O	-3.176626	1.314710	0.155147
C	-3.741357	-0.484532	1.701285
C	-2.394166	-0.862693	1.699893
C	-4.637065	-1.239785	2.472721
C	-1.957326	-1.978987	2.416196
H	-1.694429	-0.274929	1.113275
C	-4.205591	-2.351290	3.196916
H	-5.686243	-0.956350	2.510334
C	-2.861281	-2.731615	3.166211
H	-0.907877	-2.257742	2.385689
H	-4.919708	-2.923331	3.784550
H	-2.524498	-3.600429	3.726159
C	-5.390374	0.348764	-0.036078
H	-5.697479	1.233247	-0.604477
H	-5.093557	-0.428044	-0.750390
H	-6.257508	-0.021810	0.522786

TS3

(U)B3LYP-D3(BJ) SCF energy: -1508.36489454 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1507.744005 a.u.

(U)B3LYP-D3(BJ) free energy: -1507.845927 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1508.77063349 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1508.149744 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1508.251666 a.u.

Imaginary frequency: -1231.8340 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.551232	-0.056731	-0.403564
N	-3.716026	0.007873	-0.028037
C	-3.842408	-2.411855	0.407655
C	-4.225868	-0.997887	0.850867
C	-4.329837	1.289535	0.131409
C	-3.805086	2.294525	-0.902923
H	-5.336296	-0.992060	0.884699
H	-4.436692	3.187257	-0.910648
H	-3.830641	1.840368	-1.898444
H	-3.891020	-0.859905	1.902076
N	-2.441317	2.740327	-0.624670
C	-1.389475	1.879660	-0.457133
C	-2.069733	4.062309	-0.422950
C	-0.747957	4.056268	-0.118643
H	-2.769284	4.878401	-0.518245
H	-0.060989	4.854701	0.112592
N	-0.349485	2.720714	-0.144232
H	-4.388521	-3.142310	1.012533
H	-4.136441	-2.544092	-0.640726
N	-2.421292	-2.741926	0.532258
C	-1.959105	-4.010262	0.864759
C	-1.401360	-1.915805	0.141813
C	-0.613858	-3.997165	0.695305
H	-2.622330	-4.796711	1.190724
H	0.134713	-4.759655	0.841023
N	-0.290250	-2.713697	0.260396
C	0.963818	2.287243	0.229091
C	1.980624	2.282051	-0.734451
C	1.201395	1.924513	1.562401
C	3.274760	1.958782	-0.320049

C	2.509713	1.600060	1.929292
C	3.560515	1.632377	1.008581
H	4.077159	1.963566	-1.053852
H	2.711808	1.320927	2.960758
C	1.020946	-2.307713	-0.148805
C	1.964188	-1.957382	0.824764
C	1.323734	-2.295649	-1.519430
C	3.253778	-1.627929	0.400684
C	2.620227	-1.938133	-1.896219
C	3.598667	-1.611441	-0.952588
H	4.000742	-1.368819	1.145481
H	2.873950	-1.927527	-2.953901
C	1.670088	2.598780	-2.174842
H	0.907069	1.913732	-2.561596
H	1.273664	3.614187	-2.291708
H	2.566152	2.507637	-2.795421
C	4.975692	1.342854	1.445332
H	5.553047	0.867462	0.646551
H	5.500464	2.266879	1.721849
H	4.997322	0.683976	2.319821
C	0.072523	1.875247	2.559837
H	-0.461552	2.830983	2.611627
H	-0.666666	1.118078	2.270394
H	0.445753	1.633351	3.559232
C	0.282119	-2.656441	-2.547244
H	-0.181119	-3.624321	-2.322232
H	-0.525708	-1.914743	-2.561639
H	0.726804	-2.711026	-3.545355
C	1.584258	-1.909205	2.282563
H	0.744792	-1.221875	2.436650
H	1.267365	-2.888590	2.659392

H	2.425475	-1.564666	2.890469
C	4.987618	-1.221978	-1.394908
H	5.024688	-0.163205	-1.682266
H	5.720107	-1.371451	-0.595104
H	5.310118	-1.804763	-2.264527
H	-5.433017	1.245165	0.003665
H	-4.160818	1.726468	1.140214
H	-2.512513	-0.417439	-1.994772
H	-3.195575	-0.293442	-1.258093

L1

(U)B3LYP-D3(BJ) SCF energy: -1361.84340084 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1361.225988 a.u.

(U)B3LYP-D3(BJ) free energy: -1361.336944 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1362.27977556 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1361.662363 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1361.773319 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.000055	-2.563426	-0.456454
C	2.447994	-2.567998	-0.606931
C	1.217707	-1.962659	0.071913
C	-1.217544	-1.962606	0.071974
C	-2.447894	-2.567906	-0.606794
H	1.317010	-2.059037	1.170742
H	-2.479505	-3.654225	-0.452927
H	-2.408217	-2.373260	-1.679229
H	0.000038	-3.560240	-0.239989

H	1.203913	-0.889747	-0.150467
N	-3.678626	-1.986279	-0.095387
C	-4.241946	-0.870410	-0.656396
C	-4.329260	-2.415288	1.060313
C	-5.362504	-1.558058	1.248215
H	-4.012906	-3.277599	1.628106
H	-6.129851	-1.517122	2.005917
N	-5.290039	-0.637442	0.200696
H	2.479581	-3.654317	-0.453063
H	2.408247	-2.373357	-1.679365
N	3.678774	-1.986410	-0.095596
C	4.329512	-2.415512	1.060015
C	4.241974	-0.870429	-0.656493
C	5.362724	-1.558250	1.247940
H	4.013263	-3.277926	1.627711
H	6.130145	-1.517386	2.005569
N	5.290131	-0.637507	0.200535
C	-6.210427	0.447851	0.035088
C	-7.477738	0.192019	-0.503720
C	-5.816714	1.736471	0.422630
C	-8.367194	1.262956	-0.632718
C	-6.735558	2.777348	0.271647
C	-8.014690	2.560253	-0.251364
H	-9.354744	1.078806	-1.049775
H	-6.444395	3.782354	0.569056
C	6.210406	0.447895	0.035029
C	5.816368	1.736530	0.422174
C	7.477949	0.192159	-0.503304
C	6.735100	2.777526	0.271260
C	8.367273	1.263205	-0.632234
C	8.014430	2.560536	-0.251286

H	6.443678	3.782544	0.568372
H	9.354993	1.079118	-1.048917
C	-7.855077	-1.197157	-0.953483
H	-7.087437	-1.609022	-1.617645
H	-7.946633	-1.890117	-0.108400
H	-8.810250	-1.187615	-1.486370
C	-8.977497	3.709080	-0.432348
H	-10.015930	3.362495	-0.447310
H	-8.876296	4.446502	0.371301
H	-8.793617	4.233817	-1.379165
C	-4.434471	1.980050	0.972081
H	-4.263401	1.405373	1.890658
H	-3.675645	1.656642	0.251900
H	-4.283947	3.039767	1.197461
C	7.855687	-1.197037	-0.952683
H	7.947205	-1.889815	-0.107448
H	7.088299	-1.609211	-1.616946
H	8.810983	-1.187393	-1.485348
C	4.433932	1.980038	0.971170
H	3.675356	1.656744	0.250675
H	4.262534	1.405208	1.889590
H	4.283346	3.039721	1.196665
C	8.977121	3.709462	-0.432255
H	8.794653	4.232797	-1.380123
H	8.874305	4.447960	0.370191
H	10.015708	3.363236	-0.445007
H	-1.316788	-2.058965	1.170810
H	-1.203723	-0.889697	-0.150421

1-singlet

(U)B3LYP-D3(BJ) SCF energy: -1508.37195529 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1507.742869 a.u.

(U)B3LYP-D3(BJ) free energy: -1507.843431 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1508.78215068 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1508.153064 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1508.253626 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.585360	-0.090127	-0.268176
N	-3.665154	-0.164003	-0.092865
C	-3.756287	-2.572187	0.516721
C	-4.143046	-1.148452	0.893060
C	-4.365961	1.120472	0.070224
C	-3.922342	2.152537	-0.962077
H	-5.243740	-1.115789	0.976529
H	-4.602692	3.009048	-0.923610
H	-3.986993	1.721238	-1.970814
H	-3.876510	-0.521045	-1.029305
H	-3.719034	-0.885973	1.866532
H	-0.108383	-0.053300	-0.495510
N	-2.579257	2.631480	-0.709717
C	-1.537680	1.767443	-0.425638
C	-2.185315	3.964581	-0.717585
C	-0.863357	3.969915	-0.419536
H	-2.867308	4.772949	-0.933723
H	-0.161776	4.781325	-0.307776
N	-0.481579	2.641571	-0.246121
H	-4.244207	-3.260884	1.214370
H	-4.147269	-2.799205	-0.488012

N	-2.330527	-2.822256	0.561146
C	-1.778628	-4.060770	0.870159
C	-1.383163	-1.907542	0.121686
C	-0.447758	-3.950155	0.647656
H	-2.372048	-4.889236	1.226504
H	0.356115	-4.658292	0.772050
N	-0.217331	-2.653324	0.198454
C	0.844800	2.283784	0.164353
C	1.845937	2.152966	-0.804920
C	1.113011	2.133912	1.530607
C	3.153943	1.927634	-0.371654
C	2.433305	1.897135	1.919182
C	3.469070	1.811900	0.984446
H	3.941831	1.824762	-1.113926
H	2.656194	1.775483	2.977155
C	1.099012	-2.212286	-0.161321
C	1.975553	-1.806432	0.850089
C	1.492210	-2.270821	-1.504678
C	3.291809	-1.500999	0.496099
C	2.811245	-1.938944	-1.816479
C	3.728067	-1.564472	-0.828691
H	3.985683	-1.190610	1.272616
H	3.131045	-1.977100	-2.855910
C	1.491464	2.174464	-2.266896
H	0.802760	1.346769	-2.477572
H	0.983980	3.101767	-2.557075
H	2.384426	2.059334	-2.888694
C	4.895717	1.609715	1.433812
H	5.495780	1.128417	0.655583
H	5.377897	2.566753	1.674790
H	4.946602	0.987515	2.334339

C	-0.007989	2.174380	2.534909
H	-0.570904	3.114014	2.479247
H	-0.717770	1.363015	2.324879
H	0.373593	2.060328	3.554258
C	0.493820	-2.624887	-2.572880
H	0.008303	-3.587791	-2.373895
H	-0.297516	-1.864515	-2.595467
H	0.971023	-2.674517	-3.556584
C	1.480509	-1.639283	2.261944
H	0.646304	-0.927809	2.271260
H	1.110095	-2.579669	2.687686
H	2.273505	-1.255336	2.910226
C	5.145872	-1.201929	-1.197935
H	5.202711	-0.178220	-1.591253
H	5.811988	-1.256707	-0.330699
H	5.542956	-1.867058	-1.973185
H	-5.457743	0.982220	-0.013329
H	-4.150133	1.497220	1.074858

2-singlet

(U)B3LYP-D3(BJ) SCF energy: -1893.32973410 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1892.549883 a.u.

(U)B3LYP-D3(BJ) free energy: -1892.666864 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1893.84480966 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1893.064959 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1893.181940 a.u.

Cartesian coordinates

ATOM X Y Z

Co	-0.908064	0.524238	-0.522189
N	-2.636730	0.955778	-1.632731
C	-2.329539	3.400039	-1.548920
C	-2.575990	2.184226	-2.434066
C	-3.190070	-0.162249	-2.400524
C	-3.512535	-1.348521	-1.501790
H	-3.526840	2.344316	-2.970480
H	-4.084513	-2.085603	-2.073400
H	-4.130523	-1.023803	-0.660083
H	-3.253197	1.151360	-0.828386
H	-1.779639	2.086720	-3.181497
H	0.260956	0.205047	0.369965
N	-2.316463	-2.013533	-1.010396
C	-1.161149	-1.347441	-0.677014
C	-2.175140	-3.392857	-0.943255
C	-0.888542	-3.628465	-0.598289
H	-2.998230	-4.066283	-1.125021
H	-0.343392	-4.547569	-0.454769
N	-0.274693	-2.383904	-0.447598
H	-2.487437	4.310597	-2.134028
H	-3.028347	3.382804	-0.706141
N	-0.968715	3.441559	-1.033338
C	-0.209021	4.600229	-0.960542
C	-0.311028	2.342175	-0.536460
C	0.978767	4.243675	-0.417569
H	-0.577967	5.555737	-1.300173
H	1.866777	4.815952	-0.203362
N	0.908643	2.876728	-0.162322
C	1.162559	-2.305351	-0.483188
C	1.919277	-2.396479	0.690104
C	1.773181	-2.310858	-1.749388

C	3.304964	-2.543736	0.571887
C	3.161287	-2.440809	-1.818642
C	3.943755	-2.578523	-0.667878
H	3.896041	-2.639619	1.479540
H	3.639143	-2.457423	-2.795889
C	2.055486	2.157274	0.311607
C	2.769342	1.355949	-0.594232
C	2.497683	2.357821	1.624474
C	3.938621	0.744098	-0.149334
C	3.666846	1.704090	2.032067
C	4.399647	0.896444	1.162870
H	4.499037	0.128379	-0.845075
H	4.014844	1.843745	3.053328
C	1.279037	-2.302212	2.045320
H	1.061005	-1.249442	2.259640
H	0.331725	-2.844398	2.086661
H	1.944466	-2.685716	2.824799
C	5.442034	-2.728492	-0.766913
H	5.853734	-3.219714	0.120717
H	5.728555	-3.316022	-1.645861
H	5.936112	-1.751699	-0.854058
C	0.944002	-2.195498	-3.002975
H	0.219713	-3.015198	-3.082133
H	0.369683	-1.262092	-3.001314
H	1.580034	-2.211851	-3.892792
C	1.774671	3.276099	2.578833
H	2.086519	4.320592	2.444490
H	0.694403	3.241256	2.433383
H	1.993681	3.002665	3.615671
C	2.276980	1.161795	-2.001381
H	1.305999	0.649830	-1.979694

H	2.124923	2.120978	-2.511468
H	2.981627	0.560945	-2.582306
C	5.650838	0.191866	1.625735
H	5.454189	-0.868587	1.827241
H	6.438879	0.232611	0.865053
H	6.044379	0.636059	2.545672
H	-4.121496	0.137510	-2.910575
H	-2.466267	-0.457734	-3.169484
C	-2.621503	1.127676	1.454398
O	-3.478927	1.820012	0.832293
C	-2.964340	-0.277676	1.809986
C	-2.046925	-1.172857	2.386159
C	-4.294396	-0.704154	1.642444
C	-2.431566	-2.464107	2.727539
H	-1.021316	-0.858520	2.519563
C	-4.680106	-1.999680	1.984834
H	-5.011862	0.011545	1.254092
C	-3.748709	-2.891256	2.518840
H	-1.704238	-3.145961	3.160284
H	-5.713561	-2.309500	1.847720
H	-4.045519	-3.901640	2.786874
C	-1.576709	1.828394	2.302184
H	-0.626186	1.295101	2.320459
H	-1.417676	2.831081	1.903089
H	-1.953642	1.918851	3.333686

4-singlet

(U)B3LYP-D3(BJ) SCF energy: -1893.33797754 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1892.556204 a.u.

(U)B3LYP-D3(BJ) free energy: -1892.676549 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1893.85675169 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1893.074978 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1893.195323 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.624361	0.551499	-1.048442
N	-2.344728	0.839855	-1.826273
C	-2.418191	3.312117	-1.693128
C	-2.438540	2.078482	-2.589003
C	-2.887097	-0.260822	-2.607763
C	-3.091935	-1.512119	-1.764293
H	-3.402528	2.117093	-3.125270
H	-3.633429	-2.269086	-2.340738
H	-3.674963	-1.269704	-0.872357
H	-3.308248	1.042955	-0.422275
H	-1.651165	2.174575	-3.359970
H	-1.948236	0.892442	1.232918
N	-1.816978	-2.099570	-1.364457
C	-0.703756	-1.346122	-1.127789
C	-1.579464	-3.454079	-1.201146
C	-0.270091	-3.584404	-0.876831
H	-2.357733	-4.191502	-1.319091
H	0.340406	-4.452967	-0.688683
N	0.256788	-2.291057	-0.836896
H	-2.572683	4.214732	-2.294460
H	-3.218094	3.233136	-0.948821
N	-1.145538	3.457636	-0.989531
C	-0.674507	4.643756	-0.444184
C	-0.352372	2.394076	-0.669337

C	0.463024	4.340296	0.229269
H	-1.178446	5.585977	-0.594957
H	1.158946	4.956112	0.776409
N	0.650276	2.967600	0.080703
C	1.665057	-2.044442	-0.734450
C	2.315590	-2.231879	0.492952
C	2.379153	-1.732638	-1.906812
C	3.712536	-2.170147	0.514379
C	3.769538	-1.640925	-1.824871
C	4.455775	-1.881233	-0.629846
H	4.227969	-2.343615	1.455078
H	4.332034	-1.409201	-2.726638
C	1.707006	2.228352	0.701256
C	2.818599	1.846187	-0.062804
C	1.608960	1.932586	2.070997
C	3.868015	1.195928	0.591489
C	2.675425	1.264462	2.675898
C	3.819908	0.905559	1.956126
H	4.740796	0.906253	0.015213
H	2.614537	1.029593	3.736425
H	-3.882397	0.013860	-2.999083
H	-2.266822	-0.521062	-3.488165
C	-3.011941	0.747700	1.487625
O	-3.814516	1.239415	0.434524
C	-3.211796	-0.745278	1.709390
C	-2.131074	-1.568139	2.040977
C	-4.481443	-1.319493	1.578341
C	-2.310975	-2.937461	2.241464
H	-1.139312	-1.131394	2.117220
C	-4.665954	-2.688473	1.774252
H	-5.311172	-0.680400	1.291912

C	-3.580106	-3.503137	2.106142
H	-1.460758	-3.565186	2.494485
H	-5.657009	-3.122299	1.665454
H	-3.722199	-4.570259	2.256030
C	-3.340375	1.541193	2.753698
H	-2.749808	1.189573	3.607347
H	-3.133679	2.604604	2.590069
H	-4.402297	1.430264	3.000425
C	1.548571	-2.445995	1.772917
H	0.650617	-3.049714	1.626441
H	2.176637	-2.927962	2.528540
H	1.227802	-1.477290	2.177060
C	1.667256	-1.525632	-3.218371
H	1.023096	-2.379338	-3.459677
H	1.014720	-0.644872	-3.167608
H	2.385804	-1.392182	-4.032397
C	5.962056	-1.802609	-0.580135
H	6.357045	-2.273552	0.325516
H	6.417814	-2.295814	-1.445915
H	6.308570	-0.760312	-0.586830
C	0.388055	2.327956	2.861760
H	0.323049	3.414997	2.991903
H	-0.527550	2.016039	2.352512
H	0.404626	1.870988	3.855402
C	2.874975	2.123836	-1.542791
H	2.738913	3.190292	-1.756871
H	3.833104	1.802424	-1.960442
H	2.071144	1.590409	-2.064664
C	4.979207	0.235488	2.651893
H	4.641553	-0.603698	3.270943
H	5.710363	-0.146296	1.934073

H 5.499584 0.936662 3.316835

5-singlet

(U)B3LYP-D3(BJ) SCF energy: -1507.17892406 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1506.571432 a.u.

(U)B3LYP-D3(BJ) free energy: -1506.672376 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1507.57902973 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1506.971538 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1507.072482 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.602424	0.080337	-0.069106
N	-3.487305	0.235270	-0.013127
C	-4.048290	-2.099421	0.601214
C	-4.120725	-0.622497	0.970382
C	-4.056819	1.563585	0.080107
C	-3.563816	2.487130	-1.027179
H	-5.199809	-0.393374	1.033446
H	-4.140994	3.417146	-1.037562
H	-3.675265	1.985171	-1.995862
H	-3.725544	-0.494262	1.999886
N	-2.162706	2.839774	-0.823128
C	-1.257322	1.911009	-0.398223
C	-1.589822	4.090289	-0.998918
C	-0.279274	3.967784	-0.669402
H	-2.159285	4.945305	-1.329537
H	0.522230	4.688483	-0.638158
N	-0.088960	2.634749	-0.302179

H	-4.598400	-2.700724	1.334177
H	-4.504945	-2.241990	-0.386744
N	-2.675934	-2.595886	0.555608
C	-2.307360	-3.932640	0.633393
C	-1.620143	-1.790743	0.238205
C	-0.975907	-3.987347	0.379122
H	-3.014349	-4.711974	0.873437
H	-0.283956	-4.814164	0.351187
N	-0.568741	-2.674446	0.145622
C	1.139495	2.129245	0.232175
C	2.212724	1.889469	-0.636104
C	1.251199	1.938672	1.620260
C	3.436087	1.506794	-0.079844
C	2.484769	1.522712	2.125138
C	3.591985	1.322363	1.294634
H	4.279838	1.329697	-0.740872
H	2.585684	1.367615	3.197126
C	0.748005	-2.299547	-0.273475
C	1.744912	-2.106948	0.691925
C	1.005039	-2.158841	-1.647206
C	3.040222	-1.827394	0.250048
C	2.310010	-1.852789	-2.039464
C	3.342077	-1.704498	-1.107628
H	3.826762	-1.686841	0.985857
H	2.526356	-1.739836	-3.099546
C	2.038921	2.003603	-2.129377
H	1.232970	1.343824	-2.470554
H	1.772432	3.020083	-2.440455
H	2.958788	1.717799	-2.647757
C	4.921812	0.911245	1.878205
H	5.373808	1.726596	2.457290

H	4.812837	0.057978	2.558292
H	5.632014	0.629511	1.094492
C	0.073376	2.166976	2.530703
H	-0.362216	3.161320	2.378222
H	-0.718756	1.437919	2.313361
H	0.368907	2.073928	3.580020
C	-0.100600	-2.318418	-2.658541
H	-0.614765	-3.279449	-2.542290
H	-0.857575	-1.535507	-2.522362
H	0.292458	-2.256866	-3.677646
C	1.413129	-2.167233	2.160711
H	0.651814	-1.418372	2.408258
H	1.007469	-3.143515	2.450031
H	2.301487	-1.969397	2.767309
C	4.751764	-1.423650	-1.567185
H	4.774344	-0.631090	-2.324095
H	5.389160	-1.114155	-0.733381
H	5.207462	-2.313762	-2.019822
H	-5.156163	1.510097	-0.022785
H	-3.866520	2.074038	1.051289

TS1-singlet

(U)B3LYP-D3(BJ) SCF energy: -1893.29760971 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1892.521294 a.u.

(U)B3LYP-D3(BJ) free energy: -1892.638316 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1893.81650311 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1893.040187 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1893.157209 a.u.

Imaginary frequency: -594.9319 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.095861	0.560482	-0.708073
N	-2.898768	0.885018	-1.594211
C	-3.055501	3.271748	-0.986214
C	-3.219130	2.231030	-2.084019
C	-3.427507	-0.147046	-2.498822
C	-3.476296	-1.502632	-1.808663
H	-4.267652	2.275913	-2.423854
H	-4.023767	-2.209121	-2.439548
H	-3.999381	-1.395429	-0.852726
H	-3.364169	0.746036	-0.671506
H	-2.575912	2.470628	-2.937649
H	-1.104047	0.191757	0.859430
N	-2.146814	-2.047570	-1.586270
C	-1.072108	-1.284845	-1.193654
C	-1.813983	-3.382772	-1.775326
C	-0.490408	-3.485757	-1.517987
H	-2.544093	-4.124551	-2.060065
H	0.183593	-4.326714	-1.547877
N	-0.047930	-2.209627	-1.168808
H	-3.439368	4.233674	-1.338684
H	-3.648046	2.969395	-0.112746
N	-1.668985	3.457850	-0.600965
C	-1.088810	4.689572	-0.318015
C	-0.799369	2.406883	-0.411834
C	0.185255	4.434189	0.057445
H	-1.627443	5.619126	-0.419745
H	0.992770	5.091159	0.337343
N	0.350442	3.050104	0.006766

C	1.357700	-1.952200	-1.035286
C	1.960516	-2.002172	0.227008
C	2.109169	-1.809042	-2.213400
C	3.358818	-1.980781	0.280429
C	3.500323	-1.780458	-2.109044
C	4.143028	-1.895114	-0.871127
H	3.841569	-2.046266	1.252278
H	4.095106	-1.687101	-3.015423
C	1.575808	2.417943	0.387720
C	2.384514	1.825997	-0.594967
C	1.968583	2.474616	1.732747
C	3.630073	1.331846	-0.205404
C	3.217538	1.950485	2.076712
C	4.066957	1.390076	1.121481
H	4.270296	0.886858	-0.960114
H	3.534650	1.990682	3.116564
C	1.124433	-2.073561	1.472379
H	0.482130	-1.188064	1.540199
H	0.453379	-2.938135	1.471541
H	1.753153	-2.124629	2.365757
C	5.650435	-1.898732	-0.794912
H	6.000331	-2.216332	0.191996
H	6.084611	-2.572664	-1.542274
H	6.064250	-0.899681	-0.983235
C	1.422727	-1.705265	-3.552132
H	0.895944	-2.632156	-3.809590
H	0.672783	-0.906614	-3.541162
H	2.146563	-1.493234	-4.344520
C	1.084193	3.093343	2.786543
H	1.177012	4.186834	2.809207
H	0.032117	2.864159	2.604036

H	1.354687	2.720988	3.779371
C	1.927223	1.744562	-2.027580
H	0.996701	1.163106	-2.101290
H	1.708379	2.739670	-2.434473
H	2.689017	1.268494	-2.650432
C	5.411949	0.837427	1.522668
H	6.148543	0.952933	0.720753
H	5.799293	1.338952	2.415631
H	5.347056	-0.233913	1.749453
H	-4.457639	0.105084	-2.801432
H	-2.809054	-0.192273	-3.401665
C	-2.679290	0.063412	1.742949
O	-3.655122	0.065189	0.933209
C	-2.252707	-1.242915	2.347011
C	-1.486090	-1.333005	3.520616
C	-2.673900	-2.438427	1.742974
C	-1.133048	-2.571764	4.053199
H	-1.150353	-0.431396	4.021194
C	-2.305811	-3.675736	2.261055
H	-3.290540	-2.375366	0.857157
C	-1.531100	-3.752485	3.422374
H	-0.539783	-2.614480	4.963183
H	-2.630308	-4.585809	1.762361
H	-1.247775	-4.717680	3.833229
C	-2.429405	1.336430	2.540981
H	-1.444004	1.364978	3.006785
H	-2.519837	2.196187	1.875365
H	-3.195831	1.420951	3.326463

TS3-singlet

(U)B3LYP-D3(BJ) SCF energy: -1508.31554431 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1507.694868 a.u.

(U)B3LYP-D3(BJ) free energy: -1507.795803 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1508.72713133 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1508.106455 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1508.207390 a.u.

Imaginary frequency: -1457.7790 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.609904	0.109904	-0.301348
N	-3.554459	0.428237	-0.033351
C	-4.142112	-1.918357	0.546924
C	-4.241627	-0.438583	0.902808
C	-4.021326	1.794675	0.088962
C	-3.390595	2.720620	-0.948812
H	-5.317738	-0.195057	0.922014
H	-3.914219	3.680943	-0.954186
H	-3.470886	2.265392	-1.944049
H	-3.854264	-0.285284	1.925396
N	-1.994314	2.974259	-0.648846
C	-1.129517	1.951263	-0.353365
C	-1.364928	4.211322	-0.672234
C	-0.060073	3.985583	-0.387971
H	-1.896578	5.126474	-0.883092
H	0.776721	4.657397	-0.282065
N	0.074005	2.608235	-0.194655
H	-4.788516	-2.495951	1.215889
H	-4.492833	-2.064357	-0.484518
N	-2.790687	-2.433598	0.667364

C	-2.462510	-3.768063	0.889787
C	-1.702875	-1.694227	0.280175
C	-1.133675	-3.887619	0.654726
H	-3.194134	-4.496231	1.205032
H	-0.467395	-4.732953	0.723840
N	-0.681742	-2.620036	0.285795
C	1.303118	2.023203	0.249166
C	2.342839	1.849709	-0.674422
C	1.469209	1.737450	1.614608
C	3.588831	1.438323	-0.193748
C	2.725330	1.304296	2.043528
C	3.801440	1.172919	1.160103
H	4.406950	1.310501	-0.897561
H	2.869041	1.080093	3.098233
C	0.634536	-2.331433	-0.193426
C	1.659185	-2.087457	0.729981
C	0.860419	-2.317794	-1.581115
C	2.947486	-1.867876	0.237534
C	2.159646	-2.059722	-2.025272
C	3.214931	-1.847594	-1.132604
H	3.755036	-1.690953	0.941046
H	2.353104	-2.043129	-3.095694
C	2.113366	2.086166	-2.146089
H	1.262117	1.496815	-2.504463
H	1.886098	3.136328	-2.364118
H	2.997116	1.802606	-2.725138
C	5.160740	0.753338	1.664692
H	5.084913	-0.071610	2.382638
H	5.809224	0.429711	0.844410
H	5.667860	1.580155	2.178810
C	0.323857	1.897373	2.578262

H	-0.077345	2.917779	2.552903
H	-0.499702	1.227001	2.298723
H	0.640924	1.675001	3.601667
C	-0.259933	-2.587553	-2.553294
H	-0.767501	-3.530406	-2.317310
H	-1.022811	-1.799181	-2.513843
H	0.124930	-2.650351	-3.575597
C	1.363985	-2.044978	2.207217
H	0.575022	-1.314480	2.417095
H	1.012017	-3.013715	2.581709
H	2.256406	-1.761977	2.772114
C	4.612371	-1.605077	-1.648199
H	4.995882	-2.479650	-2.188482
H	4.636737	-0.759874	-2.346328
H	5.306469	-1.386340	-0.831249
H	-5.116459	1.833124	-0.045769
H	-3.804334	2.196592	1.095370
H	-2.577448	-0.183464	-2.026020
H	-3.289346	0.052532	-1.202687

1-L2

(U)B3LYP-D3(BJ) SCF energy: -1547.69931453 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1547.043073 a.u.

(U)B3LYP-D3(BJ) free energy: -1547.147577 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1548.12179925 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1547.465558 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1547.570062 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.686956	-0.118383	-0.792884
N	-3.921452	0.008379	-0.116318
C	-3.711472	-2.244253	1.009436
C	-4.127702	-0.782445	1.104322
C	-4.300250	1.404576	0.158908
C	-3.621334	2.403107	-0.776089
H	-5.195808	-0.765041	1.394802
H	-4.184957	3.340973	-0.774922
H	-3.595350	2.014287	-1.801520
H	-3.550839	-0.311846	1.905312
H	-1.833085	-0.201632	-2.444607
N	-2.265368	2.707336	-0.357960
C	-1.289944	1.737438	-0.212627
C	-1.766479	3.996610	-0.223525
C	-0.444073	3.871550	0.027605
H	-2.391612	4.871630	-0.315560
H	0.325830	4.607304	0.197224
N	-0.166344	2.501688	0.036914
H	-4.124083	-2.759658	1.883131
H	-4.151372	-2.719144	0.123951
N	-2.275181	-2.464463	1.021668
C	-1.720685	-3.628469	1.546772
C	-1.338443	-1.672353	0.381260
C	-0.401071	-3.591008	1.258800
H	-2.311114	-4.362499	2.073656
H	0.399644	-4.278887	1.479001
N	-0.180447	-2.407585	0.555530
C	1.182981	2.053067	0.203557
C	1.955088	1.774339	-0.934036
C	1.738924	2.071668	1.489886

C	3.328189	1.587567	-0.757763
C	3.116047	1.872590	1.617421
C	3.929832	1.658077	0.501539
H	3.944255	1.401030	-1.633723
H	3.563546	1.905980	2.608639
C	1.114678	-2.091345	0.034527
C	2.106486	-1.670624	0.932152
C	1.392686	-2.336551	-1.319127
C	3.411043	-1.537102	0.456948
C	2.707942	-2.148681	-1.755751
C	3.730526	-1.768690	-0.883410
H	4.191433	-1.236946	1.150215
H	2.941671	-2.337596	-2.801103
C	1.325475	1.725211	-2.301231
H	0.531777	0.970372	-2.349529
H	0.856000	2.683501	-2.555817
H	2.075583	1.495272	-3.063675
C	5.420317	1.482036	0.658545
H	5.955017	1.786776	-0.247150
H	5.805810	2.073120	1.496151
H	5.683230	0.434112	0.850833
C	0.868122	2.326291	2.694801
H	0.517682	3.365212	2.731592
H	-0.024825	1.692572	2.668041
H	1.415557	2.121554	3.619702
C	0.325065	-2.821678	-2.263467
H	-0.209413	-3.683146	-1.845437
H	-0.423563	-2.039561	-2.446118
H	0.763941	-3.118583	-3.221065
C	1.769509	-1.386100	2.374141
H	0.873879	-0.761274	2.444038

H	1.565226	-2.304998	2.938092
H	2.594136	-0.861889	2.864311
C	5.142231	-1.588989	-1.384729
H	5.321696	-0.552896	-1.699483
H	5.877415	-1.821886	-0.606794
H	5.344829	-2.231552	-2.247909
H	-5.396814	1.521862	0.094787
H	-4.002300	1.649320	1.182381
C	-4.714541	-0.510126	-1.238770
H	-5.786442	-0.589976	-0.974733
H	-4.597874	0.151230	-2.096990
H	-4.334229	-1.482511	-1.551244

2-L2

(U)B3LYP-D3(BJ) SCF energy: -1932.64149627 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1931.835497 a.u.

(U)B3LYP-D3(BJ) free energy: -1931.962068 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1933.17797628 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1932.371977 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1932.498548 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.721656	0.838060	-0.148795
N	-2.454192	1.687601	-1.469609
C	-1.265106	3.915369	-1.463241
C	-1.961728	2.822971	-2.263531
C	-2.959220	0.666269	-2.403628
C	-3.099900	-0.714669	-1.775151

H	-2.800547	3.289898	-2.813445
H	-3.769800	-1.320833	-2.390759
H	-3.541412	-0.652848	-0.778271
H	-1.250576	2.434334	-2.997843
H	-1.279244	0.843882	1.414999
N	-1.831559	-1.420678	-1.695260
C	-0.685074	-0.886840	-1.138151
C	-1.680425	-2.748728	-2.067924
C	-0.411009	-3.093882	-1.758365
H	-2.486772	-3.320110	-2.500401
H	0.129764	-4.019494	-1.874436
N	0.184419	-1.960472	-1.197135
H	-1.207988	4.808317	-2.093815
H	-1.849049	4.185196	-0.575336
N	0.093524	3.581824	-1.070061
C	1.089317	4.548320	-0.967918
C	0.487145	2.357240	-0.562861
C	2.155815	3.943410	-0.400030
H	0.948172	5.561145	-1.313227
H	3.136984	4.310995	-0.144900
N	1.781966	2.620898	-0.159352
C	1.555887	-2.015693	-0.788339
C	1.871393	-2.219438	0.562257
C	2.540084	-2.037971	-1.788504
C	3.194946	-2.535852	0.881334
C	3.849256	-2.354594	-1.421065
C	4.188111	-2.639198	-0.095016
H	3.448087	-2.724210	1.921453
H	4.616592	-2.397111	-2.191349
C	2.653601	1.740944	0.559544
C	3.724307	1.152280	-0.126071

C	2.502216	1.618796	1.949769
C	4.682403	0.462226	0.617900
C	3.467084	0.884840	2.645783
C	4.571035	0.318646	2.003110
H	5.530852	0.024285	0.099946
H	3.369234	0.785583	3.724626
C	0.809786	-2.148343	1.628153
H	0.272060	-1.193347	1.594480
H	0.062504	-2.940185	1.492856
H	1.252837	-2.265380	2.621488
C	5.601175	-3.024337	0.267663
H	5.642660	-3.516180	1.244505
H	6.030129	-3.706601	-0.474589
H	6.256932	-2.146096	0.317553
C	2.180319	-1.747658	-3.224496
H	1.607946	-2.566768	-3.676872
H	1.556393	-0.850165	-3.293451
H	3.081598	-1.594038	-3.825276
C	1.365072	2.291419	2.671862
H	1.325811	3.361702	2.434802
H	0.401200	1.861319	2.369915
H	1.478691	2.183417	3.755058
C	3.840250	1.285150	-1.623227
H	2.890894	1.033116	-2.105701
H	4.091240	2.310189	-1.923987
H	4.613374	0.616340	-2.011084
C	5.604694	-0.447864	2.790849
H	5.313571	-1.499447	2.909574
H	6.579598	-0.436274	2.292437
H	5.730923	-0.030647	3.795567
H	-3.936837	0.978189	-2.813147

H	-2.258040	0.589715	-3.239293
C	-4.803945	0.378320	2.356633
O	-5.846815	0.983842	2.137722
C	-4.550057	-0.944460	1.696682
C	-3.287412	-1.557750	1.705140
C	-5.611069	-1.558415	1.013068
C	-3.098278	-2.770852	1.042142
H	-2.442245	-1.063293	2.168958
C	-5.421411	-2.773259	0.361673
H	-6.573133	-1.056665	1.007743
C	-4.161557	-3.382051	0.377431
H	-2.113451	-3.225495	1.021646
H	-6.249624	-3.247211	-0.158331
H	-4.007010	-4.327787	-0.135453
C	-3.731451	0.942759	3.254284
H	-2.814413	1.124216	2.667548
H	-4.087963	1.875367	3.696173
H	-3.466488	0.232569	4.046801
C	-3.532930	2.107610	-0.561351
H	-4.334059	2.641497	-1.104660
H	-3.964563	1.235406	-0.074594
H	-3.134659	2.742654	0.229253

5-L2

(U)B3LYP-D3(BJ) SCF energy: -1932.68779079 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1931.876319 a.u.

(U)B3LYP-D3(BJ) free energy: -1931.998716 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1933.20982197 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1932.398350 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1932.520747 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	1.425012	0.193227	-0.056959
N	3.444758	0.928216	0.792412
C	3.370458	3.073325	-0.575500
C	3.443856	2.397688	0.789233
C	3.622126	0.448072	2.176789
C	2.870112	-0.855211	2.452222
H	4.361908	2.787168	1.269756
H	3.276034	-1.335614	3.347601
H	2.961203	-1.529131	1.593536
H	2.586393	2.717755	1.388654
H	1.063457	-2.351777	-2.061261
N	1.451650	-0.603950	2.693179
C	0.648798	0.034225	1.773679
C	0.758037	-0.983131	3.832959
C	-0.522053	-0.574412	3.657785
H	1.227979	-1.511009	4.648673
H	-1.393794	-0.658825	4.286949
N	-0.572239	0.044775	2.407171
H	3.476013	4.150644	-0.400331
H	4.223165	2.771872	-1.197168
N	2.134924	2.863067	-1.315512
C	1.787107	3.662884	-2.404631
C	1.282491	1.784361	-1.167869
C	0.689631	3.103732	-2.966632
H	2.341428	4.551076	-2.667668
H	0.093357	3.400166	-3.815297
N	0.393578	1.973968	-2.210753

C	-1.734542	0.771247	1.986160
C	-2.766752	0.106031	1.313481
C	-1.841904	2.118421	2.365473
C	-3.947183	0.815739	1.068308
C	-3.036098	2.788806	2.091867
C	-4.104425	2.148354	1.455854
H	-4.763395	0.308317	0.559269
H	-3.134781	3.831541	2.385390
C	-0.609465	1.000980	-2.511765
C	-1.924295	1.224064	-2.088008
C	-0.229065	-0.167760	-3.188233
C	-2.860829	0.208575	-2.296060
C	-1.198447	-1.156750	-3.371588
C	-2.507746	-0.999022	-2.905223
H	-3.880804	0.356632	-1.951135
H	-0.919946	-2.075547	-3.881886
C	-2.605449	-1.320597	0.869420
H	-1.768848	-1.424010	0.172393
H	-2.389961	-1.989907	1.706723
H	-3.509683	-1.677264	0.368875
C	-5.376765	2.897839	1.144422
H	-6.237041	2.222494	1.092157
H	-5.587834	3.662030	1.899940
H	-5.305251	3.410897	0.175555
C	-0.687921	2.813331	3.041644
H	-0.404433	2.309748	3.973522
H	0.194207	2.798467	2.390739
H	-0.938345	3.852694	3.273419
C	1.182843	-0.343180	-3.687892
H	1.516624	0.538278	-4.247307
H	1.874276	-0.480910	-2.848151

H	1.256052	-1.216657	-4.342125
C	-2.292816	2.515889	-1.408718
H	-1.788754	2.600925	-0.441048
H	-1.995277	3.384591	-2.006662
H	-3.369041	2.569934	-1.234922
C	-3.502363	-2.127491	-3.015677
H	-3.396755	-2.810052	-2.161923
H	-4.533429	-1.758609	-3.019327
H	-3.346284	-2.716976	-3.925696
H	4.694303	0.311479	2.397137
H	3.244149	1.211522	2.863426
C	1.537975	-2.648045	-1.107731
O	2.160539	-1.576674	-0.488242
C	0.428191	-3.305859	-0.285947
C	-0.688209	-3.868312	-0.917191
C	0.526129	-3.418747	1.104571
C	-1.675058	-4.531340	-0.185206
H	-0.782074	-3.783333	-1.997050
C	-0.456632	-4.075459	1.844567
H	1.383092	-2.982487	1.600675
C	-1.562285	-4.638683	1.202461
H	-2.531704	-4.963461	-0.697443
H	-0.362134	-4.142640	2.925686
H	-2.330396	-5.149626	1.777239
C	2.594134	-3.716932	-1.458545
H	2.156151	-4.578964	-1.977647
H	3.363237	-3.269025	-2.098219
H	3.075404	-4.073159	-0.539715
C	4.463330	0.341707	-0.085148
H	5.484821	0.653131	0.202165
H	4.368425	-0.743850	-0.049251

H 4.270462 0.629184 -1.119866

TS1-L2

(U)B3LYP-D3(BJ) SCF energy: -1932.63895943 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1931.834283 a.u.

(U)B3LYP-D3(BJ) free energy: -1931.959600 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1933.17090977 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1932.366233 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1932.491550 a.u.

Imaginary frequency: -92.1647 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	1.202775	-0.791665	0.008418
N	2.931292	-1.949752	-0.879541
C	1.988192	-4.133693	0.002285
C	2.467735	-3.310568	-1.188182
C	3.378546	-1.309274	-2.132267
C	3.351091	0.219165	-2.085623
H	3.280386	-3.893302	-1.662494
H	3.980600	0.606444	-2.892975
H	3.742571	0.600621	-1.137852
H	1.648193	-3.222904	-1.907407
H	2.058560	0.119031	1.136157
N	2.003309	0.741425	-2.308662
C	0.900396	0.283238	-1.629640
C	1.686920	1.733626	-3.224259
C	0.347292	1.919727	-3.144788
H	2.434899	2.215917	-3.834585

H	-0.318423	2.582063	-3.674796
N	-0.117183	1.029306	-2.174589
H	1.838699	-5.158481	-0.355886
H	2.762275	-4.179364	0.777327
N	0.731989	-3.694689	0.595565
C	-0.050382	-4.549122	1.367919
C	0.243097	-2.403158	0.582254
C	-1.073042	-3.807631	1.851945
H	0.189537	-5.593710	1.496049
H	-1.906632	-4.067884	2.484730
N	-0.888450	-2.513421	1.370848
C	-1.520253	0.842507	-1.951591
C	-2.207314	1.737822	-1.124730
C	-2.181470	-0.170956	-2.662439
C	-3.600949	1.641358	-1.073461
C	-3.571906	-0.239975	-2.566465
C	-4.299293	0.670345	-1.791965
H	-4.150467	2.335102	-0.442699
H	-4.098746	-1.018754	-3.113806
C	-1.790417	-1.440159	1.661802
C	-3.040294	-1.429927	1.027291
C	-1.430752	-0.466749	2.608394
C	-3.937452	-0.411663	1.355499
C	-2.346262	0.555767	2.870755
C	-3.600670	0.600330	2.256113
H	-4.911990	-0.396321	0.876699
H	-2.075694	1.326117	3.589574
C	-1.457052	2.747832	-0.300915
H	-0.748762	2.252963	0.370686
H	-0.865213	3.430824	-0.918065
H	-2.143263	3.344303	0.307402

C	-5.804421	0.582986	-1.719355
H	-6.210240	1.299157	-0.997975
H	-6.266678	0.790871	-2.692498
H	-6.132606	-0.419656	-1.417684
C	-1.400310	-1.155104	-3.494171
H	-0.791813	-0.646243	-4.251406
H	-0.709014	-1.721456	-2.858750
H	-2.069862	-1.854878	-4.003260
C	-0.114296	-0.528569	3.334950
H	0.067094	-1.529991	3.742779
H	0.716857	-0.306781	2.651850
H	-0.096762	0.189501	4.160994
C	-3.400570	-2.485020	0.011939
H	-2.623370	-2.563925	-0.754625
H	-3.506193	-3.476448	0.468830
H	-4.342757	-2.236900	-0.482882
C	-4.555681	1.733142	2.541157
H	-4.231482	2.654627	2.039638
H	-5.565973	1.503617	2.187337
H	-4.612563	1.954006	3.613104
H	4.400853	-1.644012	-2.379573
H	2.718792	-1.640300	-2.939990
C	3.479571	1.383459	1.529868
O	4.407347	1.195603	0.720436
C	2.533046	2.533355	1.307936
C	1.580460	2.940264	2.254016
C	2.673036	3.286738	0.133475
C	0.793716	4.068972	2.031367
H	1.445698	2.371794	3.167591
C	1.878818	4.406811	-0.096724
H	3.429426	2.981235	-0.580128

C	0.940118	4.809981	0.856057
H	0.063216	4.371388	2.777418
H	1.999577	4.974642	-1.015862
H	0.326089	5.689901	0.684061
C	3.612936	0.808978	2.933974
H	2.660822	0.666868	3.445470
H	4.128874	-0.150733	2.869921
H	4.233697	1.493578	3.531771
C	4.026016	-1.947423	0.104424
H	4.858183	-2.599373	-0.220947
H	4.390301	-0.928817	0.248281
H	3.653718	-2.288763	1.071309

TS3-L2

(U)B3LYP-D3(BJ) SCF energy: -1933.82543896 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1932.998374 a.u.

(U)B3LYP-D3(BJ) free energy: -1933.121887 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1934.36133401 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1933.534269 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1933.657782 a.u.

Imaginary frequency: -222.0634 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	0.572934	1.424466	-0.110604
N	1.745643	3.227293	0.732545
C	-0.163676	4.701320	-0.053616
C	3.148460	1.467654	1.844831
H	3.942676	1.395478	2.593205

H	3.603686	1.319718	0.860371
H	2.817368	-1.000129	-3.306969
N	2.210426	0.385430	2.101960
C	1.012954	0.257858	1.440291
C	2.448332	-0.662036	2.982291
C	1.374554	-1.482419	2.891527
H	3.351155	-0.733243	3.568521
H	1.133512	-2.406319	3.392120
N	0.514388	-0.909804	1.955506
H	-0.641184	5.634730	0.262346
H	0.423569	4.929635	-0.950455
N	-1.230949	3.773995	-0.401357
C	-2.414688	4.208018	-0.992985
C	-1.108279	2.401247	-0.418151
C	-3.081932	3.096342	-1.374664
H	-2.669698	5.253334	-1.078178
H	-4.036555	2.965702	-1.858573
N	-2.286676	2.007682	-1.015368
C	-0.775860	-1.485897	1.701919
C	-0.904985	-2.490220	0.733205
C	-1.836029	-1.106371	2.536568
C	-2.125770	-3.169890	0.674824
C	-3.036373	-1.811181	2.434881
C	-3.187382	-2.865190	1.529560
H	-2.243028	-3.962607	-0.059443
H	-3.866198	-1.536064	3.081993
C	-2.720706	0.663730	-1.274848
C	-3.779899	0.163960	-0.498771
C	-2.188136	-0.061804	-2.352113
C	-4.337944	-1.064415	-0.850971
C	-2.762015	-1.305365	-2.641851

C	-3.842788	-1.813107	-1.921504
H	-5.170417	-1.449417	-0.268619
H	-2.362352	-1.875978	-3.477379
C	0.229431	-2.832196	-0.195697
H	0.603523	-1.950613	-0.732080
H	1.086748	-3.244667	0.349104
H	-0.091813	-3.578081	-0.929090
C	-4.467475	-3.663400	1.488703
H	-4.426382	-4.511100	2.185531
H	-5.330098	-3.051660	1.774428
H	-4.655101	-4.070597	0.490952
C	-1.672729	0.034597	3.508482
H	-0.880116	-0.165837	4.239744
H	-1.391107	0.951224	2.976543
H	-2.602885	0.217265	4.054600
C	-1.052964	0.445893	-3.200068
H	-0.990001	1.536080	-3.190046
H	-0.091454	0.065741	-2.829911
H	-1.175249	0.108960	-4.235512
C	-4.302157	0.935601	0.687400
H	-3.478450	1.252851	1.334919
H	-4.842696	1.842028	0.388690
H	-4.981936	0.315273	1.277722
C	-4.441134	-3.151572	-2.278206
H	-3.826216	-3.974850	-1.891640
H	-5.446087	-3.266326	-1.859286
H	-4.507963	-3.284004	-3.363719
C	3.023379	-0.611705	-2.287102
O	1.848854	-0.225974	-1.656676
C	3.746529	-1.728373	-1.534551
C	4.638127	-2.587142	-2.187551

C	3.560330	-1.882927	-0.158324
C	5.331805	-3.572229	-1.482930
H	4.785627	-2.485762	-3.261404
C	4.250237	-2.865219	0.552972
H	2.844273	-1.236150	0.328023
C	5.141438	-3.714657	-0.106216
H	6.016107	-4.233970	-2.008628
H	4.081005	-2.971784	1.622062
H	5.676049	-4.485303	0.443364
C	4.006245	0.570075	-2.462021
H	4.921106	0.265074	-2.984320
H	3.531102	1.380041	-3.026120
H	4.292465	0.957886	-1.475686
H	1.511678	1.100072	-1.839117
H	1.173232	1.986682	-1.820357
C	2.476716	2.837105	1.952399
H	1.767222	2.796707	2.783332
H	3.235966	3.599557	2.200407
C	0.741539	4.244679	1.086949
H	1.243395	5.145910	1.487188
H	0.114149	3.827094	1.879395
C	2.700953	3.736723	-0.262011
H	3.193775	4.661229	0.089936
H	3.461205	2.979450	-0.456867
H	2.197861	3.916849	-1.210279

1-L3

(U)B3LYP-D3(BJ) SCF energy: -1621.52558802 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1620.904208 a.u.

(U)B3LYP-D3(BJ) free energy: -1621.006851 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1621.96236891 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1621.340989 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1621.443632 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.545488	-0.263981	-1.184243
N	-3.450159	-0.154427	-0.357640
C	-3.406607	-2.534646	0.113454
C	-4.014728	-1.182879	0.341344
C	-4.094329	1.050013	-0.302870
C	-3.497317	2.119168	-1.165422
H	-4.132305	3.007890	-1.184470
H	-3.377124	1.735381	-2.189865
H	-1.356981	-0.481156	-2.786337
N	-2.175247	2.525097	-0.687681
C	-1.141683	1.634445	-0.563413
C	-1.808896	3.822498	-0.366634
C	-0.499867	3.772274	-0.026916
H	-2.499559	4.649915	-0.418686
H	0.192866	4.542206	0.272532
N	-0.106913	2.436638	-0.145628
H	-3.962782	-3.296851	0.663966
H	-3.460075	-2.769490	-0.960881
N	-2.004394	-2.635613	0.515813
C	-1.476854	-3.702638	1.230248
C	-1.033738	-1.801781	0.026147
C	-0.132010	-3.550352	1.206389
H	-2.098244	-4.460732	1.681581
H	0.663949	-4.145713	1.623887

N	0.123758	-2.391320	0.471183
C	1.252002	2.068100	0.120630
C	2.116871	1.799078	-0.950355
C	1.712510	2.154138	1.443344
C	3.482703	1.698710	-0.670893
C	3.086137	2.047430	1.670742
C	3.988798	1.850953	0.622066
H	4.169157	1.517923	-1.494048
H	3.458669	2.134814	2.689328
C	1.461498	-2.019509	0.116932
C	2.311624	-1.534703	1.119831
C	1.917936	-2.281284	-1.185425
C	3.660013	-1.352988	0.807155
C	3.268495	-2.046894	-1.457189
C	4.156527	-1.603623	-0.473763
H	4.332729	-0.998942	1.583227
H	3.640638	-2.249605	-2.458871
C	1.597392	1.668764	-2.357806
H	0.895686	0.832227	-2.452512
H	1.047358	2.567258	-2.662706
H	2.422001	1.513973	-3.059673
C	5.471624	1.783176	0.892399
H	6.051835	1.948237	-0.020808
H	5.776141	2.535224	1.628636
H	5.762794	0.803200	1.290511
C	0.751862	2.373660	2.586608
H	0.411879	3.414756	2.646462
H	-0.143691	1.754622	2.470188
H	1.226681	2.123275	3.539839
C	1.002993	-2.836883	-2.244887
H	0.464610	-3.718979	-1.877676

H	0.242553	-2.104108	-2.542268
H	1.575477	-3.128041	-3.130778
C	1.787861	-1.231944	2.501362
H	0.837534	-0.692494	2.447338
H	1.606787	-2.144253	3.083558
H	2.502316	-0.615899	3.053759
C	5.611569	-1.379484	-0.803390
H	5.772087	-0.379219	-1.225615
H	6.242951	-1.461009	0.087402
H	5.969408	-2.104688	-1.541964
C	-5.216055	1.273377	0.481085
H	-5.675442	2.257958	0.483847
C	-5.128985	-1.022312	1.149436
H	-5.522770	-1.879325	1.688545
C	-5.751452	0.229735	1.242756
H	-6.633633	0.374923	1.856998

2-L3

(U)B3LYP-D3(BJ) SCF energy: -2006.46856619 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2005.697595 a.u.

(U)B3LYP-D3(BJ) free energy: -2005.823405 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2007.01916457 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2006.248193 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2006.374003 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.715805	-0.268864	0.338721
N	2.317175	-0.249978	-0.999659

C	2.086380	-2.642633	-1.385877
C	2.645222	-1.310353	-1.791415
C	2.946796	0.931037	-1.262295
C	2.627783	2.041162	-0.309253
H	3.269359	2.906354	-0.485619
H	2.779566	1.690239	0.718963
H	0.960602	-0.393078	1.954140
N	1.236250	2.475078	-0.433238
C	0.189290	1.615510	-0.230266
C	0.825337	3.771997	-0.694106
C	-0.527586	3.755083	-0.656310
H	1.522651	4.576398	-0.870440
H	-1.258417	4.537413	-0.783715
N	-0.902561	2.437852	-0.377642
H	2.429803	-3.415002	-2.077283
H	2.465836	-2.892263	-0.388032
N	0.624646	-2.698766	-1.353470
C	-0.114690	-3.760607	-1.855480
C	-0.139508	-1.827867	-0.623029
C	-1.389803	-3.568863	-1.443564
H	0.330027	-4.544960	-2.448360
H	-2.286731	-4.147575	-1.594662
N	-1.390887	-2.390523	-0.694618
C	-2.288472	2.108941	-0.225534
C	-2.812896	1.911688	1.060511
C	-3.109905	2.161799	-1.361796
C	-4.202877	1.847169	1.191283
C	-4.492679	2.093172	-1.178857
C	-5.057744	1.966204	0.093002
H	-4.625811	1.721836	2.184743
H	-5.141817	2.155007	-2.049930

C	-2.557996	-1.968052	0.020011
C	-3.653978	-1.487017	-0.709188
C	-2.620496	-2.175802	1.407797
C	-4.847204	-1.250999	-0.024182
C	-3.826398	-1.887876	2.052590
C	-4.952617	-1.444310	1.354777
H	-5.709305	-0.898965	-0.583626
H	-3.893942	-2.048176	3.126280
C	-1.911753	1.820157	2.263704
H	-1.231253	0.963817	2.193608
H	-1.277126	2.710337	2.352122
H	-2.501869	1.724207	3.179876
C	-6.556464	1.935765	0.264579
H	-6.844526	2.155085	1.297450
H	-7.046309	2.667622	-0.387192
H	-6.969417	0.950734	0.013656
C	-2.515755	2.307199	-2.741560
H	-2.187796	3.334260	-2.943302
H	-1.636454	1.665541	-2.859004
H	-3.249770	2.035869	-3.506045
C	-1.449461	-2.730116	2.175898
H	-1.051348	-3.630522	1.692891
H	-0.626649	-2.005973	2.223709
H	-1.749256	-2.990419	3.195705
C	-3.552362	-1.245331	-2.194452
H	-2.611162	-0.746609	-2.444071
H	-3.582502	-2.180303	-2.767991
H	-4.377361	-0.614248	-2.535227
C	-6.241431	-1.158676	2.085055
H	-6.251540	-0.136332	2.484233
H	-7.108651	-1.257334	1.423927

H	-6.379601	-1.839318	2.931863
C	3.826612	1.101802	-2.321698
H	4.292683	2.071259	-2.472741
C	3.513447	-1.204203	-2.866887
H	3.733281	-2.086495	-3.460346
C	4.121473	0.023008	-3.157371
H	4.817063	0.123356	-3.983971
C	4.329746	-1.666204	1.403149
O	4.673656	-2.298596	0.410550
C	4.748711	-0.238969	1.568960
C	4.346978	0.541165	2.663110
C	5.569698	0.330690	0.585358
C	4.771851	1.864216	2.777409
H	3.683273	0.125351	3.412139
C	5.992875	1.651988	0.698679
H	5.852330	-0.282630	-0.262814
C	5.597124	2.420960	1.796970
H	4.452115	2.462617	3.625594
H	6.627999	2.084993	-0.069389
H	5.928629	3.452035	1.887630
C	3.476797	-2.301315	2.477698
H	2.497293	-1.803928	2.496269
H	3.348464	-3.360953	2.246789
H	3.935019	-2.195925	3.468220

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(U)B3LYP-D3(BJ) SCF energy: -2006.51244965 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2005.736275 a.u.

(U)B3LYP-D3(BJ) free energy: -2005.857705 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2007.05302486 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2006.276850 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2006.398280 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.017938	-0.352991	-0.165501
N	-2.585863	-0.788842	1.089385
C	-2.254710	-3.169330	0.692309
C	-2.867867	-2.068481	1.502625
C	-3.286544	0.213440	1.718238
C	-3.081722	1.590900	1.167549
H	-3.733019	2.306058	1.673796
H	-3.315035	1.606816	0.099734
H	-1.168112	1.658053	-2.848248
N	-1.700455	2.061868	1.333466
C	-0.622204	1.367913	0.862047
C	-1.343992	3.262660	1.923743
C	0.004144	3.347294	1.829349
H	-2.072165	3.940818	2.340844
H	0.697867	4.112491	2.137752
N	0.431830	2.184872	1.185128
H	-2.584261	-4.141250	1.065999
H	-2.575697	-3.074470	-0.355668
N	-0.789095	-3.171997	0.696219
C	-0.008637	-4.303335	0.886110
C	-0.054080	-2.094380	0.291895
C	1.263962	-3.939825	0.596579
H	-0.424095	-5.247019	1.204245
H	2.187631	-4.495918	0.600246
N	1.219092	-2.592970	0.235748

C	1.826045	1.984047	0.917861
C	2.308942	2.100183	-0.394264
C	2.688195	1.836712	2.016736
C	3.695542	2.156506	-0.569479
C	4.063375	1.899751	1.787976
C	4.584084	2.093563	0.505504
H	4.086216	2.274474	-1.576875
H	4.741607	1.809260	2.634043
C	2.367330	-1.935239	-0.319326
C	3.404761	-1.552391	0.539522
C	2.469658	-1.828869	-1.716165
C	4.591269	-1.087968	-0.031985
C	3.665974	-1.326980	-2.235704
C	4.739894	-0.970983	-1.415718
H	5.412418	-0.807827	0.621727
H	3.770205	-1.245088	-3.315293
C	1.376626	2.197576	-1.572540
H	0.858802	1.247953	-1.755210
H	0.598583	2.950781	-1.403517
H	1.929297	2.469768	-2.476719
C	6.073778	2.214333	0.299622
H	6.517808	2.910961	1.019869
H	6.577103	1.248748	0.431757
H	6.310754	2.571989	-0.706783
C	2.148346	1.628941	3.411432
H	1.811308	2.566235	3.870576
H	1.288390	0.951656	3.404271
H	2.920144	1.202409	4.058907
C	1.353310	-2.265967	-2.626759
H	0.976453	-3.256150	-2.343544
H	0.506041	-1.566983	-2.579843

H	1.707387	-2.320085	-3.661259
C	3.248758	-1.659800	2.035580
H	2.283716	-1.255597	2.356142
H	3.290777	-2.701080	2.379334
H	4.040703	-1.103711	2.544208
C	6.020828	-0.455453	-2.023771
H	5.939870	0.610300	-2.272583
H	6.866012	-0.566767	-1.337178
H	6.262997	-0.986406	-2.950788
C	-4.150792	-0.014608	2.774337
H	-4.661860	0.830001	3.228337
C	-3.721076	-2.355568	2.553784
H	-3.887823	-3.393138	2.830371
C	-4.380790	-1.319945	3.231157
H	-5.065852	-1.522917	4.046835
C	-1.689488	0.679216	-2.863601
O	-1.021060	-0.248185	-2.072559
C	-3.117244	0.948554	-2.395871
C	-3.656727	2.239027	-2.424172
C	-3.911629	-0.097394	-1.908690
C	-4.952044	2.487309	-1.961755
H	-3.046955	3.059942	-2.796418
C	-5.202750	0.143477	-1.441435
H	-3.487549	-1.095002	-1.870720
C	-5.727327	1.439331	-1.462080
H	-5.350185	3.498838	-1.981307
H	-5.797287	-0.676982	-1.047950
H	-6.730310	1.629562	-1.089387
C	-1.695655	0.194385	-4.324493
H	-2.175917	0.919139	-4.993488
H	-0.664788	0.031780	-4.657957

H -2.234189 -0.757547 -4.395731

TS1-L3

(U)B3LYP-D3(BJ) SCF energy: -2006.45710848 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2005.687058 a.u.

(U)B3LYP-D3(BJ) free energy: -2005.810787 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2007.00663580 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2006.236585 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2006.360314 a.u.

Imaginary frequency: -391.4414 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	0.878614	0.197151	-0.137023
N	2.509039	-0.088059	1.174088
C	2.299309	2.223939	1.905403
C	2.856512	0.838888	2.096560
C	3.139648	-1.283987	1.209212
C	2.799547	-2.226208	0.088680
H	3.417368	-3.125102	0.140225
H	2.992834	-1.727213	-0.865968
H	1.399288	0.745858	-1.660158
N	1.398466	-2.636445	0.122571
C	0.370814	-1.730287	0.025557
C	0.954534	-3.947807	0.196482
C	-0.396226	-3.894653	0.138032
H	1.630775	-4.785580	0.268630
H	-1.144195	-4.671018	0.140575
N	-0.739480	-2.543127	0.037929

H	2.661824	2.882000	2.698287
H	2.644655	2.592564	0.928930
N	0.835431	2.297674	1.910782
C	0.123157	3.284595	2.576811
C	0.047636	1.573470	1.057913
C	-1.157598	3.190602	2.148117
H	0.588226	3.958166	3.279809
H	-2.038958	3.761278	2.391996
N	-1.188714	2.144303	1.224175
C	-2.113620	-2.156765	-0.072441
C	-2.615499	-1.724355	-1.308613
C	-2.951915	-2.372524	1.032529
C	-4.001224	-1.595588	-1.438485
C	-4.329271	-2.234004	0.851651
C	-4.873861	-1.877431	-0.385118
H	-4.407074	-1.286517	-2.398309
H	-4.991395	-2.421110	1.694585
C	-2.357048	1.881345	0.438153
C	-3.486914	1.344380	1.068514
C	-2.378569	2.291820	-0.905389
C	-4.674127	1.268414	0.336947
C	-3.581376	2.162022	-1.603768
C	-4.741896	1.673863	-0.997089
H	-5.562352	0.874431	0.823197
H	-3.617426	2.482500	-2.642584
C	-1.697181	-1.447137	-2.470163
H	-1.023175	-0.610522	-2.253941
H	-1.057913	-2.310924	-2.687811
H	-2.273099	-1.206621	-3.368483
C	-6.369144	-1.783560	-0.562744
H	-6.644252	-1.748540	-1.621245

H	-6.877267	-2.641844	-0.108875
H	-6.773854	-0.880633	-0.089411
C	-2.381014	-2.754792	2.376507
H	-2.088443	-3.811076	2.417597
H	-1.483944	-2.168266	2.600506
H	-3.116549	-2.582496	3.167764
C	-1.162824	2.883538	-1.567689
H	-0.710772	3.671315	-0.955627
H	-0.382052	2.129204	-1.714009
H	-1.424139	3.307439	-2.541943
C	-3.427374	0.869230	2.498718
H	-2.509048	0.303556	2.682443
H	-3.440527	1.702106	3.212908
H	-4.280552	0.222588	2.721141
C	-6.025777	1.565509	-1.781851
H	-6.042642	0.650955	-2.388438
H	-6.898900	1.534778	-1.122273
H	-6.146587	2.411074	-2.467593
C	4.072310	-1.614923	2.187512
H	4.548771	-2.590153	2.166186
C	3.776968	0.573459	3.106194
H	4.017591	1.348262	3.827463
C	4.397394	-0.676096	3.163623
H	5.127035	-0.901278	3.935230
C	2.615011	1.767465	-1.963277
O	2.678962	2.682335	-1.097188
C	3.704045	0.697136	-1.962780
C	3.773489	-0.336161	-2.909880
C	4.701875	0.770453	-0.984903
C	4.797142	-1.281227	-2.862943
H	3.006489	-0.419479	-3.673201

C	5.719177	-0.182518	-0.923746
H	4.651204	1.587232	-0.274217
C	5.771919	-1.215349	-1.861415
H	4.831874	-2.075647	-3.604568
H	6.473239	-0.116484	-0.143246
H	6.566808	-1.955554	-1.820834
C	2.077766	2.151050	-3.348382
H	1.763551	1.295835	-3.951933
H	1.230825	2.827618	-3.220874
H	2.870509	2.690289	-3.886221

TS3-L3

(U)B3LYP-D3(BJ) SCF energy: -2007.65240767 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2006.861879 a.u.

(U)B3LYP-D3(BJ) free energy: -2006.986250 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2008.20227923 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2007.411751 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2007.536122 a.u.

Imaginary frequency: -756.4685 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.329124	-0.505863	-0.668133
N	-2.888650	-1.716876	0.078559
C	-2.176950	-3.438746	-1.478062
C	-2.916011	-3.029113	-0.228982
C	-3.680210	-1.260070	1.071714
C	-3.626769	0.230433	1.302626
H	-4.381587	0.536492	2.030856

H	-3.777995	0.750368	0.347077
H	-1.741335	2.009731	-2.888126
N	-2.314031	0.622658	1.819654
C	-1.158630	0.358720	1.132220
C	-2.077578	1.175061	3.069479
C	-0.731734	1.270436	3.193023
H	-2.875478	1.461379	3.737200
H	-0.108077	1.639923	3.991238
N	-0.188089	0.763117	2.011024
H	-2.354970	-4.498312	-1.677563
H	-2.583808	-2.845767	-2.310405
N	-0.729368	-3.235494	-1.459741
C	0.145910	-4.083640	-2.130448
C	-0.144187	-2.035977	-1.127163
C	1.331584	-3.439379	-2.193329
H	-0.152121	-5.054812	-2.494684
H	2.275049	-3.730943	-2.623674
N	1.155809	-2.203992	-1.560739
C	1.213159	0.464162	1.930967
C	2.112062	1.456256	1.525400
C	1.642249	-0.789855	2.390879
C	3.477222	1.191819	1.661290
C	3.016035	-1.006831	2.511073
C	3.946061	-0.019698	2.173022
H	4.189443	1.955260	1.358727
H	3.365969	-1.968353	2.879104
C	2.244971	-1.278084	-1.437521
C	3.432056	-1.732591	-0.835804
C	2.163027	0.011949	-1.993837
C	4.556020	-0.904304	-0.869240
C	3.306538	0.814741	-1.964763

C	4.516526	0.371756	-1.428470
H	5.478510	-1.260814	-0.418307
H	3.247371	1.811729	-2.395291
C	1.614965	2.759393	0.962609
H	0.945125	2.597792	0.112852
H	1.036532	3.329412	1.696224
H	2.448762	3.383044	0.627908
C	5.424090	-0.255285	2.364115
H	5.744971	0.035940	3.373102
H	5.681378	-1.312251	2.235396
H	6.016663	0.327288	1.651700
C	0.643004	-1.866248	2.729780
H	-0.075965	-1.527936	3.485396
H	0.065302	-2.138154	1.838104
H	1.147477	-2.759234	3.111087
C	0.905174	0.548756	-2.619147
H	0.375802	-0.201641	-3.209305
H	0.197475	0.895921	-1.853348
H	1.130002	1.408700	-3.257757
C	3.518598	-3.066286	-0.131623
H	2.580340	-3.307230	0.375915
H	3.743037	-3.894622	-0.814467
H	4.314399	-3.038512	0.618109
C	5.728167	1.269453	-1.403921
H	5.698549	1.946174	-0.539196
H	6.655172	0.690797	-1.334498
H	5.783411	1.895543	-2.300934
C	-4.482798	-2.113389	1.826378
H	-5.104971	-1.708759	2.618826
C	-3.681356	-3.940794	0.495038
H	-3.668937	-4.992493	0.225829

C	-4.475081	-3.479043	1.545988
H	-5.087333	-4.167098	2.120918
C	-2.486339	2.341293	-2.134989
O	-2.991076	1.237727	-1.447579
C	-1.782270	3.342852	-1.225270
C	-0.757686	4.161492	-1.715491
C	-2.192288	3.515542	0.101258
C	-0.170571	5.140375	-0.911258
H	-0.422480	4.032847	-2.742980
C	-1.607404	4.487460	0.912099
H	-2.976710	2.875955	0.485880
C	-0.597746	5.310484	0.406960
H	0.622474	5.767052	-1.312015
H	-1.937515	4.600396	1.941921
H	-0.141079	6.069406	1.036932
C	-3.616922	3.054793	-2.901946
H	-3.246809	3.914024	-3.475744
H	-4.093789	2.346598	-3.587975
H	-4.373502	3.411523	-2.193489
H	-2.517546	0.192273	-2.074214
H	-2.005250	-0.555404	-2.445335

L4

(U)B3LYP-D3(BJ) SCF energy: -1369.53317016 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1368.990659 a.u.

(U)B3LYP-D3(BJ) free energy: -1369.078403 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1369.82032375 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1369.277813 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1369.365557 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	4.060587	-0.315695	-0.544509
N	0.014825	-0.020191	0.354164
C	-1.205922	0.010729	-0.447169
C	1.223037	-0.191125	-0.448239
C	2.461752	-0.275018	0.445588
C	5.109826	-1.351636	0.642700
C	5.390805	-0.717393	2.009504
C	6.398978	-1.848295	-0.028048
C	4.648543	1.453206	-0.250282
C	6.063515	1.667071	-0.802333
C	3.664543	2.433863	-0.905196
H	-1.311062	-0.877171	-1.099464
H	1.299291	0.673236	-1.119525
H	1.185610	-1.081625	-1.104573
H	2.413141	-1.197113	1.040560
H	2.453420	0.560835	1.155617
H	6.056475	0.147940	1.917695
H	5.884171	-1.438206	2.674368
H	4.471907	-0.382972	2.502976
H	6.187994	-2.328607	-0.989074
H	6.908219	-2.577553	0.614871
H	7.102589	-1.030158	-0.213365
H	6.809977	1.076352	-0.263464
H	6.351781	2.722400	-0.715413
H	6.118969	1.391845	-1.862332
H	3.565958	2.236834	-1.979630
H	4.022237	3.464411	-0.786420
H	2.667231	2.377850	-0.458059

H	-0.048674	-0.789598	1.021305
H	-1.144854	0.873619	-1.122377
C	-2.438017	0.157495	0.446772
H	-2.495454	-0.683254	1.152692
H	-2.319349	1.065708	1.048666
P	-4.034329	0.294720	-0.539686
C	-4.747067	-1.424485	-0.228103
C	-5.002181	1.413730	0.640882
C	-3.850321	-2.475496	-0.898415
H	-4.270356	-3.479301	-0.756676
H	-3.769842	-2.295429	-1.977098
H	-2.837365	-2.479511	-0.483461
C	-6.183527	-1.537412	-0.754121
H	-6.543744	-2.570045	-0.662899
H	-6.876515	-0.896927	-0.201128
H	-6.238805	-1.256847	-1.812727
C	-6.256138	1.993873	-0.029517
H	-6.709099	2.763469	0.608436
H	-6.015862	2.449299	-0.995759
H	-7.017060	1.226350	-0.204446
C	-5.319478	0.815111	2.015779
H	-6.042428	-0.004413	1.937295
H	-4.422589	0.426267	2.509834
H	-5.759766	1.575303	2.673943
H	-4.301328	2.248175	0.788169
H	-4.749130	-1.613301	0.853660
H	4.471119	-2.232742	0.802196
H	4.655444	1.645520	0.830579

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(U)B3LYP-D3(BJ) SCF energy: -1516.03743661 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1515.485253 a.u.

(U)B3LYP-D3(BJ) free energy: -1515.572084 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1516.32865761 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1515.776474 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1515.863305 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.021042	-0.880780	-0.818379
P	-1.900072	0.095003	0.015785
N	-0.097271	-2.099386	1.068296
C	0.839885	-1.599853	2.084107
C	-1.484487	-2.240191	1.541207
C	-2.207581	-0.885123	1.588719
C	-2.102066	1.850543	0.672428
C	-3.519518	2.233631	1.111952
C	-1.504834	2.881591	-0.293909
C	-3.477823	-0.221685	-0.959127
C	-3.454907	0.568970	-2.273918
C	-3.621016	-1.723100	-1.246152
H	0.962152	-2.321039	2.910378
H	-1.526576	-2.720198	2.533217
H	-1.991733	-2.900911	0.834215
H	-1.829787	-0.284914	2.424575
H	-3.276282	-1.045008	1.773676
H	-4.196844	2.306576	0.254269
H	-3.514424	3.212777	1.607430
H	-3.942765	1.507050	1.814370
H	-0.506093	2.577634	-0.620841

H	-1.427991	3.862982	0.190659
H	-2.124457	3.003982	-1.187904
H	-3.467649	1.650183	-2.107854
H	-4.330730	0.316591	-2.884496
H	-2.557316	0.324440	-2.854210
H	-2.726176	-2.112251	-1.746335
H	-4.482822	-1.899465	-1.901671
H	-3.782475	-2.302445	-0.331045
H	0.232526	-2.992119	0.709201
H	0.403316	-0.691892	2.510413
H	0.317308	-1.982652	-1.986521
C	2.192182	-1.270434	1.449975
H	2.878493	-0.874106	2.207311
H	2.644276	-2.188425	1.054432
P	1.966939	-0.080183	0.010461
C	2.581220	1.525205	0.795925
C	3.394780	-0.612223	-1.095569
C	1.671996	1.927462	1.963082
H	2.010840	2.874843	2.400686
H	0.640197	2.065256	1.625167
H	1.668380	1.178922	2.762225
C	2.661220	2.654860	-0.238161
H	2.910276	3.605087	0.251038
H	3.424026	2.462391	-0.997106
H	1.703465	2.786819	-0.754284
C	3.236434	-0.061117	-2.518961
H	3.988490	-0.508349	-3.181191
H	2.244702	-0.307080	-2.910590
H	3.369522	1.025282	-2.558261
C	4.797510	-0.368029	-0.529264
H	5.036512	0.700716	-0.490453

H	4.912341	-0.774365	0.482292
H	5.552481	-0.845580	-1.166357
H	3.222837	-1.694837	-1.159617
H	3.587352	1.339291	1.193486
H	-1.462746	1.832338	1.565773
H	-4.334544	0.103916	-0.355584

2-L4

(U)B3LYP-D3(BJ) SCF energy: -1900.98499670 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1900.282995 a.u.

(U)B3LYP-D3(BJ) free energy: -1900.391899 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1901.38623330 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1900.684232 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1900.793136 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.265473	-0.022970	-0.665787
P	-0.549166	-2.198805	-0.023876
N	0.652226	0.186044	1.384296
C	-0.332019	0.645902	2.377730
C	1.324593	-1.071426	1.749561
C	0.388138	-2.279571	1.601126
C	-2.125416	-3.116461	0.456506
C	-1.948485	-4.594075	0.823150
C	-3.232777	-2.922074	-0.588117
C	0.405499	-3.433174	-1.077199
C	-0.219659	-3.532935	-2.474793
C	1.871991	-2.994140	-1.190020

H	0.152361	0.862142	3.345194
H	1.717993	-1.031150	2.779346
H	2.178522	-1.175023	1.077775
H	-0.352426	-2.288519	2.409083
H	0.965432	-3.206357	1.695629
H	-1.681671	-5.191698	-0.055294
H	-2.883880	-5.004611	1.224709
H	-1.168821	-4.739998	1.578866
H	-3.314068	-1.873205	-0.888846
H	-4.201930	-3.242571	-0.185547
H	-3.041704	-3.512011	-1.490020
H	-1.231695	-3.947596	-2.449380
H	0.388330	-4.181720	-3.117961
H	-0.266884	-2.541307	-2.939757
H	1.934488	-1.973558	-1.581686
H	2.411310	-3.662920	-1.873324
H	2.389930	-3.021091	-0.226019
H	1.352376	0.918237	1.284186
H	-1.046943	-0.165176	2.544204
H	0.692606	0.274331	-1.983434
C	-1.061632	1.880961	1.850806
H	-1.826866	2.210206	2.562474
H	-0.343595	2.698386	1.729967
P	-1.783633	1.499160	0.160881
C	-3.621566	1.387164	0.551207
C	-1.577306	3.176230	-0.671156
C	-3.881895	0.263168	1.561516
H	-4.955940	0.182000	1.770549
H	-3.542547	-0.700186	1.170461
H	-3.372131	0.438338	2.514617
C	-4.436914	1.165962	-0.728827

H	-5.494933	1.002834	-0.487545
H	-4.377889	2.023659	-1.404506
H	-4.076958	0.286683	-1.275587
C	-1.729381	3.083649	-2.195268
H	-1.407080	4.022338	-2.664226
H	-1.119905	2.267711	-2.596563
H	-2.769617	2.911121	-2.492760
C	-2.421078	4.308163	-0.075755
H	-3.487418	4.170236	-0.288823
H	-2.300667	4.383389	1.010838
H	-2.125165	5.271796	-0.509309
H	-0.521108	3.388775	-0.461102
H	-3.927075	2.337106	1.008061
H	-2.430888	-2.574341	1.362683
H	0.366655	-4.414615	-0.587558
C	2.455492	2.496775	-0.389118
O	1.840634	3.003154	0.547739
C	3.413612	1.380600	-0.122663
C	3.727337	0.425646	-1.099100
C	3.962123	1.261557	1.163514
C	4.574015	-0.637789	-0.786955
H	3.266678	0.484807	-2.077707
C	4.820682	0.208625	1.468096
H	3.704298	2.007526	1.908623
C	5.123865	-0.745696	0.492306
H	4.794866	-1.388461	-1.539698
H	5.250924	0.127856	2.462236
H	5.786478	-1.573362	0.729874
C	2.236440	2.945934	-1.809147
H	1.604570	2.183864	-2.289505
H	1.711526	3.903176	-1.812062

H 3.175601 3.022313 -2.366356

3-L4

(U)B3LYP-D3(BJ) SCF energy: -1900.98781369 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1900.283339 a.u.

(U)B3LYP-D3(BJ) free energy: -1900.390172 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1901.39284305 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1900.688368 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1900.795201 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.171191	-0.040226	-0.202340
P	-0.652279	2.060319	0.050210
N	-0.018770	-0.254290	1.905388
C	1.278982	-0.181353	2.588485
C	-1.028748	0.658971	2.446447
C	-0.836968	2.092917	1.913009
C	0.386146	3.593487	-0.253815
C	-0.268378	4.914543	0.167132
C	0.908514	3.650717	-1.694403
C	-2.361334	2.475009	-0.603201
C	-2.430923	2.157392	-2.104520
C	-3.440937	1.692898	0.156293
H	1.186784	-0.511069	3.636398
H	-1.012320	0.675037	3.548574
H	-2.006390	0.274346	2.143496
H	0.091866	2.517110	2.312893
H	-1.652124	2.746245	2.242784

H	-1.103320	5.174712	-0.492264
H	0.459767	5.732860	0.107572
H	-0.646626	4.878285	1.194175
H	1.347883	2.693894	-1.994237
H	1.674830	4.429278	-1.791877
H	0.106518	3.891189	-2.400577
H	-1.676358	2.697895	-2.683795
H	-3.417333	2.427122	-2.501319
H	-2.284109	1.085139	-2.272139
H	-3.254241	0.617200	0.125552
H	-4.418986	1.862980	-0.308452
H	-3.514374	2.001286	1.203414
H	-0.338107	-1.274038	1.901714
H	1.620432	0.860282	2.608171
H	-0.148982	-1.831674	-0.462278
C	2.295994	-1.065415	1.859774
H	3.277727	-1.023843	2.345728
H	1.922753	-2.095254	1.895360
P	2.368537	-0.614372	0.048154
C	3.916486	0.437801	-0.081367
C	2.828695	-2.264259	-0.715785
C	3.797678	1.675434	0.815191
H	4.687854	2.307578	0.709230
H	2.925788	2.275417	0.534606
H	3.700820	1.410833	1.872409
C	4.178948	0.845132	-1.536272
H	5.043150	1.518417	-1.595147
H	4.386392	-0.018432	-2.174292
H	3.313325	1.371376	-1.955475
C	2.496121	-2.319459	-2.212643
H	2.622840	-3.341513	-2.589788

H	1.458887	-2.020256	-2.393888
H	3.147144	-1.665798	-2.803120
C	4.257324	-2.735635	-0.424001
H	5.000946	-2.118699	-0.941270
H	4.484276	-2.713676	0.647504
H	4.392024	-3.767606	-0.770315
H	2.133732	-2.939179	-0.203008
H	4.758059	-0.167899	0.277635
H	1.246641	3.416192	0.404436
H	-2.534283	3.547526	-0.452915
C	-0.808846	-2.652610	0.111512
O	-0.479221	-2.795699	1.388476
C	-2.251137	-2.166560	-0.142635
C	-2.693413	-1.752010	-1.406595
C	-3.164734	-2.192020	0.914032
C	-4.026212	-1.396788	-1.616818
H	-1.987088	-1.717599	-2.234536
C	-4.499371	-1.831567	0.710363
H	-2.793353	-2.516729	1.881013
C	-4.936819	-1.441072	-0.556942
H	-4.354860	-1.082101	-2.604270
H	-5.201230	-1.861174	1.540444
H	-5.975219	-1.163581	-0.717379
C	-0.538946	-3.916133	-0.741589
H	-0.720786	-3.758401	-1.811390
H	0.496508	-4.239740	-0.599609
H	-1.196451	-4.717940	-0.387475

4-L4

(U)B3LYP-D3(BJ) SCF energy: -1900.98957237 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1900.284304 a.u.

(U)B3LYP-D3(BJ) free energy: -1900.390597 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1901.39039858 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1900.685130 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1900.791423 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.016230	-0.254801	-0.019788
P	-2.008347	0.803021	0.229592
N	0.202300	-0.344481	2.025492
C	1.157342	0.587341	2.603972
C	-1.101806	-0.222927	2.655308
C	-1.934832	0.958405	2.089724
C	-2.208259	2.589085	-0.319265
C	-3.416175	3.324621	0.271777
C	-2.147264	2.746160	-1.845221
C	-3.715729	0.049545	-0.025849
C	-3.995432	-0.231130	-1.508170
C	-3.878039	-1.232485	0.803835
H	1.463347	0.273453	3.620161
H	-1.019923	-0.097363	3.750245
H	-1.654284	-1.157309	2.495926
H	-1.422146	1.901696	2.314510
H	-2.933787	1.018245	2.540757
H	-4.357351	2.935309	-0.131966
H	-3.371984	4.392005	0.020485
H	-3.454812	3.238756	1.362431
H	-1.358344	2.125440	-2.282116
H	-1.951362	3.791771	-2.113262

H	-3.094816	2.465404	-2.314715
H	-4.038603	0.683957	-2.103627
H	-4.959516	-0.743701	-1.619566
H	-3.219548	-0.873322	-1.933707
H	-3.096535	-1.960069	0.568727
H	-4.847683	-1.696307	0.582883
H	-3.843066	-1.034683	1.878370
H	0.671372	-1.886843	2.143111
H	0.735364	1.601510	2.723816
H	2.303781	-2.228439	0.604590
C	2.413658	0.687869	1.730732
H	3.128600	1.416544	2.129907
H	2.911849	-0.289509	1.715788
P	1.927526	1.053196	-0.035621
C	2.120037	2.923417	-0.176481
C	3.436233	0.389897	-0.952860
C	1.486700	3.658252	1.012184
H	1.551991	4.742321	0.856734
H	0.428054	3.402391	1.123825
H	1.985285	3.424850	1.956351
C	1.525245	3.432729	-1.495670
H	1.675129	4.515986	-1.586566
H	1.977531	2.958214	-2.370158
H	0.451188	3.235996	-1.534608
C	3.292132	0.501707	-2.477365
H	4.029450	-0.136273	-2.980020
H	2.294009	0.206063	-2.817973
H	3.469264	1.527981	-2.815819
C	4.790019	0.938111	-0.485816
H	4.902697	1.998946	-0.735778
H	4.927609	0.827459	0.593839

H	5.607377	0.400770	-0.983158
H	3.405065	-0.676501	-0.689192
H	3.195658	3.138373	-0.166613
H	-1.298600	3.043631	0.091822
H	-4.446816	0.781330	0.340931
C	1.511546	-2.984425	0.770491
O	0.969528	-2.875354	2.053062
C	0.463470	-2.779543	-0.325456
C	0.776425	-2.110207	-1.525058
C	-0.810626	-3.357229	-0.193469
C	-0.158865	-2.037936	-2.570629
H	1.778958	-1.724781	-1.674233
C	-1.719053	-3.325542	-1.250847
H	-1.055366	-3.843731	0.745238
C	-1.397170	-2.666502	-2.442245
H	0.101434	-1.518711	-3.488823
H	-2.688120	-3.805069	-1.144033
H	-2.110069	-2.638325	-3.261126
C	2.158025	-4.365614	0.625322
H	2.617583	-4.490513	-0.362031
H	2.924214	-4.491261	1.396830
H	1.402205	-5.146699	0.759903

5-L4

(U)B3LYP-D3(BJ) SCF energy: -1514.83873649 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1514.306650 a.u.

(U)B3LYP-D3(BJ) free energy: -1514.393907 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1515.11551058 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1514.583424 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1514.670681 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.000002	0.120329	-0.000008
P	-2.214261	0.010346	0.129440
N	-0.000001	-1.794466	0.000065
C	1.185776	-2.607514	-0.154644
C	-1.185781	-2.607501	0.154824
C	-2.384272	-1.772630	0.648861
C	-3.237462	0.887132	1.439615
C	-4.747239	0.636430	1.347706
C	-2.906865	2.383828	1.519934
C	-3.213037	0.115970	-1.452649
C	-3.262932	1.552957	-1.986647
C	-2.609027	-0.829902	-2.500630
H	1.021932	-3.426325	-0.882855
H	-1.021942	-3.426263	0.883090
H	-1.457248	-3.116455	-0.792423
H	-2.380889	-1.750787	1.744928
H	-3.340670	-2.206401	0.331053
H	-5.176838	1.111035	0.458523
H	-5.259126	1.057564	2.221977
H	-4.982348	-0.432591	1.305959
H	-1.827278	2.543621	1.611086
H	-3.396883	2.836089	2.391277
H	-3.249697	2.925307	0.632261
H	-3.793380	2.229436	-1.310188
H	-3.777653	1.580586	-2.955144
H	-2.250373	1.948338	-2.132750
H	-1.556938	-0.586892	-2.685036

H	-3.157365	-0.740741	-3.446904
H	-2.653652	-1.874828	-2.181693
H	1.457244	-3.116406	0.792637
C	2.384268	-1.772679	-0.648740
H	3.340666	-2.206429	-0.330901
H	2.380884	-1.750913	-1.744808
P	2.214258	0.010333	-0.129444
C	3.213031	0.116073	1.452639
C	3.237465	0.887029	-1.439674
C	4.747237	0.636298	-1.347767
H	5.259125	1.057380	-2.222063
H	5.176854	1.110935	-0.458610
H	4.982323	-0.432726	-1.305973
C	2.906902	2.383729	-1.520057
H	3.396926	2.835941	-2.391423
H	1.827318	2.543543	-1.611210
H	3.249752	2.925238	-0.632409
C	2.609013	-0.829712	2.500694
H	3.157348	-0.740478	3.446963
H	1.556924	-0.586684	2.685078
H	2.653634	-1.874664	2.181842
C	3.262934	1.553102	1.986521
H	2.250376	1.948498	2.132598
H	3.777659	1.580808	2.955013
H	3.793379	2.229526	1.310005
H	4.234240	-0.217870	1.227454
H	2.867999	0.423973	-2.365417
H	-2.868016	0.424112	2.365384
H	-4.234248	-0.217949	-1.227436

TS1-L4

(U)B3LYP-D3(BJ) SCF energy: -1900.97997625 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1900.279077 a.u.

(U)B3LYP-D3(BJ) free energy: -1900.384954 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1901.37832805 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1900.677429 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1900.783306 a.u.

Imaginary frequency: -322.3192 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	0.174357	-0.036249	-0.371835
P	-0.105793	2.181907	0.010225
N	-0.249411	-0.270656	1.759310
C	0.973812	-0.447738	2.554852
C	-1.123395	0.807293	2.240782
C	-0.596456	2.190723	1.821460
C	1.246972	3.489023	-0.001002
C	0.775597	4.918316	0.288898
C	2.093381	3.412783	-1.278341
C	-1.583962	3.004376	-0.804650
C	-1.358299	3.137954	-2.316360
C	-2.846236	2.178050	-0.525490
H	0.732920	-0.759910	3.585037
H	-1.240087	0.774258	3.337124
H	-2.108858	0.634067	1.803478
H	0.299858	2.445062	2.399015
H	-1.344031	2.961694	2.041589
H	0.164823	5.310221	-0.531656
H	1.636704	5.588582	0.403879

H	0.182468	4.976333	1.208088
H	2.390323	2.381346	-1.490516
H	3.000475	4.020954	-1.173991
H	1.545054	3.787285	-2.148617
H	-0.532353	3.814135	-2.555668
H	-2.260593	3.530521	-2.801382
H	-1.134726	2.160640	-2.761070
H	-2.720999	1.137747	-0.841533
H	-3.698533	2.591640	-1.078374
H	-3.115824	2.174294	0.534598
H	-0.746084	-1.172045	1.727029
H	1.484602	0.518520	2.621182
H	-0.684790	-1.331841	-1.004239
C	1.883698	-1.480246	1.888498
H	2.814216	-1.599433	2.455368
H	1.365640	-2.444981	1.874467
P	2.195220	-1.010605	0.100825
C	3.967231	-0.379384	0.175893
C	2.330138	-2.716468	-0.672988
C	4.047297	0.856423	1.080038
H	5.073647	1.243226	1.107242
H	3.398028	1.654578	0.706958
H	3.749922	0.633655	2.109833
C	4.500972	-0.061357	-1.226036
H	5.496569	0.395849	-1.163296
H	4.585803	-0.958405	-1.845545
H	3.841840	0.642712	-1.747099
C	2.176149	-2.665134	-2.198385
H	2.086673	-3.680856	-2.604504
H	1.276532	-2.105710	-2.472728
H	3.038226	-2.193960	-2.682941

C	3.550785	-3.535393	-0.240786
H	4.481138	-3.118175	-0.642834
H	3.646415	-3.584958	0.849626
H	3.468270	-4.564245	-0.612978
H	1.430129	-3.196261	-0.269455
H	4.584537	-1.171209	0.619316
H	1.883321	3.163928	0.833531
H	-1.711631	4.003677	-0.369418
C	-1.579404	-2.636865	-0.127076
O	-1.031910	-2.875727	0.975917
C	-2.883472	-1.864132	-0.130678
C	-3.527126	-1.444899	-1.303686
C	-3.500105	-1.607169	1.099814
C	-4.746859	-0.776048	-1.245480
H	-3.053364	-1.613198	-2.265153
C	-4.716007	-0.923813	1.162426
H	-3.014679	-1.967759	2.000617
C	-5.344841	-0.505520	-0.010241
H	-5.228145	-0.452332	-2.164552
H	-5.178108	-0.730724	2.127269
H	-6.293566	0.022194	0.033834
C	-1.359181	-3.613899	-1.275936
H	-1.608902	-3.199269	-2.253532
H	-0.319037	-3.941290	-1.284394
H	-1.995860	-4.492218	-1.095463

TS2-L4

(U)B3LYP-D3(BJ) SCF energy: -1900.98859727 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1900.287624 a.u.

(U)B3LYP-D3(BJ) free energy: -1900.392909 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1901.38408063 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1900.683107 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1900.788392 a.u.

Imaginary frequency: -1075.4970 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.014887	-0.202675	-0.075248
P	-1.530949	1.488871	0.282088
N	0.092780	-0.402799	2.000284
C	1.246756	0.263102	2.587892
C	-1.160183	-0.003176	2.613813
C	-1.609119	1.404702	2.152254
C	-1.006628	3.271616	0.000867
C	-2.036483	4.330849	0.407861
C	-0.490133	3.490871	-1.426560
C	-3.355975	1.462783	-0.164861
C	-3.559458	1.566162	-1.681282
C	-4.016121	0.194771	0.393032
H	1.370826	-0.015245	3.650849
H	-1.105510	-0.016684	3.717461
H	-1.929894	-0.731189	2.327961
H	-0.918655	2.159677	2.545072
H	-2.606396	1.657914	2.531365
H	-2.903327	4.324866	-0.261857
H	-1.591932	5.332734	0.356597
H	-2.398121	4.177659	1.430404
H	0.219302	2.706838	-1.707680
H	0.013229	4.462335	-1.509465
H	-1.306023	3.480035	-2.156631

H	-3.211397	2.524209	-2.078797
H	-4.624501	1.472331	-1.928827
H	-3.021004	0.767306	-2.200423
H	-3.518106	-0.705663	0.025451
H	-5.066636	0.150383	0.078710
H	-3.997441	0.169589	1.486735
H	0.357264	-1.660417	1.756414
H	1.132391	1.360904	2.570545
H	0.143874	-4.438514	0.465463
C	2.518744	-0.114522	1.821866
H	3.393825	0.411571	2.219890
H	2.688049	-1.190398	1.928274
P	2.290399	0.210321	-0.006758
C	3.344279	1.745829	-0.271754
C	3.309369	-1.200482	-0.721925
C	2.840046	2.905975	0.594997
H	3.492952	3.778794	0.470510
H	1.829954	3.202332	0.299144
H	2.819191	2.653031	1.659071
C	3.390494	2.161993	-1.747106
H	3.934678	3.108344	-1.857832
H	3.890334	1.417613	-2.371257
H	2.380561	2.309861	-2.145470
C	3.202991	-1.320104	-2.250115
H	3.516011	-2.320416	-2.573156
H	2.183369	-1.153599	-2.611071
H	3.852686	-0.599004	-2.756052
C	4.775255	-1.225622	-0.273917
H	5.340457	-0.389855	-0.702822
H	4.873274	-1.179885	0.815034
H	5.257765	-2.151463	-0.611404

H	2.796151	-2.060740	-0.271054
H	4.360096	1.491628	0.057438
H	-0.148535	3.357533	0.679576
H	-3.823358	2.330996	0.316637
C	-0.285902	-3.486344	0.831183
O	0.764987	-2.674242	1.256349
C	-1.010679	-2.871656	-0.378588
C	-2.379265	-3.001126	-0.636050
C	-0.226209	-2.171320	-1.323392
C	-2.952011	-2.456521	-1.792309
H	-3.011984	-3.538515	0.062701
C	-0.802419	-1.603299	-2.469600
H	0.849990	-2.194036	-1.202846
C	-2.173089	-1.746589	-2.704708
H	-4.017846	-2.575508	-1.968339
H	-0.173296	-1.087879	-3.190266
H	-2.623308	-1.320983	-3.596780
C	-1.240346	-3.844777	1.980901
H	-1.965186	-4.619829	1.703538
H	-0.643952	-4.217952	2.818232
H	-1.792476	-2.961519	2.322919

TS3-L4

(U)B3LYP-D3(BJ) SCF energy: -1515.99251312 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1515.446989 a.u.

(U)B3LYP-D3(BJ) free energy: -1515.533041 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1516.27757877 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1515.732055 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1515.818107 a.u.

Imaginary frequency: -828.8597 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.014457	-0.799010	0.680197
P	1.982750	0.045580	-0.011103
N	-0.004447	-2.054956	-1.058508
C	-0.837947	-1.506841	-2.101473
C	1.362893	-2.297611	-1.439810
C	2.227842	-1.005446	-1.540089
C	2.206062	1.781955	-0.690705
C	3.626462	2.095061	-1.175844
C	1.674925	2.856283	0.267067
C	3.525249	-0.308548	0.996507
C	3.582627	0.568452	2.253572
C	3.557125	-1.795560	1.378136
H	-0.966821	-2.213243	-2.945111
H	1.438353	-2.833352	-2.404725
H	1.814983	-2.957849	-0.686963
H	1.896082	-0.405327	-2.395555
H	3.287544	-1.240501	-1.702717
H	4.331914	2.146697	-0.339302
H	3.649896	3.067551	-1.683205
H	3.991927	1.340728	-1.880558
H	0.670820	2.605797	0.621838
H	1.630724	3.828504	-0.239330
H	2.318735	2.971787	1.144463
H	3.698773	1.628928	2.013673
H	4.432909	0.275064	2.881533
H	2.669457	0.455860	2.850461
H	2.660530	-2.076705	1.944382

H	4.431281	-2.003249	2.007380
H	3.614937	-2.445512	0.500548
H	-0.400311	-0.587347	-2.544607
C	-2.223847	-1.150025	-1.545604
H	-2.853965	-0.681756	-2.310944
H	-2.724395	-2.069436	-1.219433
P	-2.043931	-0.061855	-0.029351
C	-2.558257	1.625915	-0.670850
C	-3.490755	-0.646983	1.017727
C	-1.601535	2.077793	-1.781087
H	-1.900026	3.063309	-2.159673
H	-0.578588	2.159090	-1.402042
H	-1.590603	1.382275	-2.625583
C	-2.603197	2.661754	0.459123
H	-2.794353	3.662925	0.053045
H	-3.389697	2.443405	1.186872
H	-1.648673	2.694805	0.997591
C	-3.340784	-0.228152	2.486712
H	-4.113574	-0.709055	3.099467
H	-2.361769	-0.524641	2.877257
H	-3.443592	0.854041	2.617900
C	-4.875899	-0.305594	0.458085
H	-5.074808	0.770894	0.507957
H	-4.984106	-0.620446	-0.585633
H	-5.657791	-0.808191	1.041000
H	-3.359567	-1.736862	0.981315
H	-3.562556	1.523744	-1.101861
H	1.543586	1.765139	-1.566531
H	4.398082	-0.092101	0.367438
H	-0.476962	-2.502940	0.291365
H	-0.644982	-2.464659	1.230534

1-L5

(U)B3LYP-D3(BJ) SCF energy: -1968.51139431 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1967.972655 a.u.

(U)B3LYP-D3(BJ) free energy: -1968.067991 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1968.92101171 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1968.382272 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1968.477608 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.018869	-1.757267	-0.100223
P	-1.791650	-0.352503	0.167455
N	-0.131612	-1.937808	2.131704
C	0.799214	-1.056687	2.861293
C	-1.541046	-1.788830	2.543989
C	-2.133553	-0.478958	2.008765
H	0.985648	-1.427080	3.882095
H	-1.651278	-1.830075	3.640009
H	-2.088349	-2.636323	2.120432
H	-1.669182	0.382860	2.498840
H	-3.206066	-0.439348	2.224696
H	0.153215	-2.908027	2.241092
H	0.310970	-0.085181	2.965579
H	-0.025443	-3.279427	-0.707069
C	2.119548	-0.884410	2.107547
H	2.744912	-0.126186	2.591796
H	2.680921	-1.825706	2.112325
P	1.819803	-0.490824	0.294062

C	1.934905	1.345203	0.205530
C	1.345298	2.154992	1.187795
C	2.487723	1.965720	-0.925798
C	1.326517	3.541940	1.056615
H	0.882141	1.703930	2.059291
C	2.469963	3.353929	-1.057597
H	2.946350	1.359062	-1.700725
C	1.891950	4.147642	-0.066077
H	0.857877	4.148750	1.825921
H	2.910425	3.815262	-1.937564
H	1.872722	5.228546	-0.171550
C	3.433239	-1.007585	-0.427400
C	3.444082	-2.117494	-1.281966
C	4.643906	-0.370174	-0.113879
C	4.648255	-2.582979	-1.815822
H	2.504600	-2.615224	-1.511257
C	5.844031	-0.835457	-0.647754
H	4.643580	0.499602	0.537244
C	5.847160	-1.943390	-1.500744
H	4.646771	-3.443800	-2.478807
H	6.776821	-0.335447	-0.400819
H	6.783508	-2.304170	-1.917827
C	-3.402004	-0.918416	-0.537672
C	-3.464840	-2.231995	-1.023346
C	-4.553954	-0.119283	-0.571038
C	-4.667032	-2.743581	-1.516570
H	-2.562530	-2.840637	-1.020934
C	-5.751045	-0.629963	-1.070775
H	-4.511904	0.907594	-0.220103
C	-5.810747	-1.944919	-1.540618
H	-4.705056	-3.763058	-1.890888

H	-6.637175	-0.001206	-1.098038
H	-6.744552	-2.340451	-1.931091
C	-1.816473	1.457812	-0.136230
C	-2.458331	2.387218	0.695061
C	-1.120346	1.925404	-1.260991
C	-2.409473	3.751760	0.404624
H	-3.002575	2.050634	1.572629
C	-1.080116	3.285532	-1.557052
H	-0.589635	1.215512	-1.888929
C	-1.723638	4.202352	-0.723633
H	-2.910215	4.461195	1.058206
H	-0.525507	3.632174	-2.423483
H	-1.681717	5.264675	-0.947265

2-L5

(U)B3LYP-D3(BJ) SCF energy: -2353.45807203 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2352.769610 a.u.

(U)B3LYP-D3(BJ) free energy: -2352.888008 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2353.97877855 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2353.290317 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2353.408715 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.362243	-0.506930	0.409515
P	0.552116	1.715380	-0.020561
N	0.825008	-0.691701	-1.792942
C	-0.369569	-0.881156	-2.639446
C	1.656351	0.447692	-2.222825

C	1.005179	1.782111	-1.838438
H	-0.095091	-1.336145	-3.604088
H	1.847042	0.423221	-3.308762
H	2.621706	0.351622	-1.718053
H	0.084821	1.946812	-2.408157
H	1.684398	2.611266	-2.061696
H	1.370021	-1.553835	-1.834266
H	-0.783627	0.104830	-2.862441
H	1.156868	-1.434374	1.505594
C	-1.423154	-1.736567	-1.936603
H	-2.342909	-1.790002	-2.529733
H	-1.039874	-2.754994	-1.811453
P	-1.737338	-1.103852	-0.200468
C	2.336257	-3.456508	-0.453612
O	1.703679	-3.476020	-1.508721
C	3.524211	-2.560592	-0.315185
C	4.056462	-2.215485	0.934970
C	4.102609	-2.029583	-1.477024
C	5.138181	-1.341843	1.019009
H	3.598224	-2.593718	1.840410
C	5.184845	-1.156605	-1.393010
H	3.690892	-2.316328	-2.439412
C	5.700874	-0.807006	-0.142742
H	5.533835	-1.067165	1.992499
H	5.627153	-0.750586	-2.298277
H	6.539270	-0.119730	-0.073831
C	1.929283	-4.321965	0.712054
H	1.546577	-3.659999	1.497777
H	1.134577	-4.999905	0.396229
H	2.778291	-4.887508	1.111739
C	2.027804	2.548363	0.710775

C	3.087362	1.717848	1.106099
C	2.166367	3.937635	0.831679
C	4.274267	2.270560	1.588072
H	2.969105	0.638335	1.050914
C	3.348163	4.487004	1.329667
H	1.346937	4.590275	0.545775
C	4.406892	3.655284	1.702488
H	5.089042	1.616046	1.884469
H	3.442675	5.565349	1.427632
H	5.326898	4.085985	2.088606
C	-0.793299	2.949975	0.129950
C	-0.958985	4.036224	-0.741699
C	-1.734986	2.749835	1.150433
C	-2.041265	4.904971	-0.593055
H	-0.243264	4.207129	-1.540692
C	-2.810039	3.621941	1.304625
H	-1.631733	1.888468	1.803864
C	-2.966324	4.700095	0.431601
H	-2.160815	5.741420	-1.276610
H	-3.540106	3.444205	2.088058
H	-3.812418	5.372518	0.542932
C	-3.195153	0.010035	-0.357138
C	-3.275466	0.946196	-1.399736
C	-4.169363	0.054220	0.652703
C	-4.304704	1.883873	-1.444110
H	-2.520747	0.957270	-2.178883
C	-5.199398	0.993894	0.609894
H	-4.126873	-0.658242	1.470819
C	-5.272775	1.910986	-0.439151
H	-4.342351	2.603103	-2.257271
H	-5.946974	1.006955	1.398774

H	-6.071608	2.646482	-0.469357
C	-2.480137	-2.603805	0.568238
C	-3.678836	-3.172972	0.111345
C	-1.779624	-3.226679	1.608785
C	-4.165355	-4.346783	0.683790
H	-4.236739	-2.689068	-0.685758
C	-2.267849	-4.403735	2.181363
H	-0.848252	-2.780860	1.949791
C	-3.458834	-4.964777	1.720144
H	-5.094250	-4.780950	0.323524
H	-1.717993	-4.879736	2.989007
H	-3.839378	-5.880002	2.165745

3-L5

(U)B3LYP-D3(BJ) SCF energy: -2353.47116309 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2352.779874 a.u.

(U)B3LYP-D3(BJ) free energy: -2352.893319 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2353.98755518 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2353.296266 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2353.409711 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.081367	0.924256	0.337182
P	1.747208	-0.605136	0.404468
N	0.084528	1.008581	2.364595
C	-0.999843	0.327733	3.053839
C	1.390842	0.625499	2.868737
C	1.900432	-0.714587	2.262635

H	-1.184296	0.761472	4.054177
H	1.403473	0.533891	3.969267
H	2.107527	1.420592	2.618187
H	1.247766	-1.532616	2.586294
H	2.918577	-0.964587	2.584295
H	-0.041347	2.685730	2.259142
H	-0.785653	-0.741264	3.237813
H	-1.589959	3.211988	0.630243
C	-2.303791	0.423254	2.246045
H	-3.106448	-0.168418	2.699257
H	-2.622106	1.472332	2.208660
P	-1.960989	-0.067535	0.477156
C	-0.604743	3.714669	0.690968
O	-0.089354	3.670588	1.993474
C	0.314980	3.036965	-0.335866
C	-0.200177	2.524910	-1.550109
C	1.716905	3.074639	-0.164536
C	0.668843	2.078851	-2.555291
H	-1.273913	2.524761	-1.713706
C	2.572363	2.674819	-1.193112
H	2.101362	3.460462	0.773784
C	2.052462	2.176691	-2.389628
H	0.256906	1.678111	-3.478144
H	3.646755	2.722514	-1.050621
H	2.723280	1.840257	-3.173685
C	-0.809908	5.183266	0.308432
H	-1.237369	5.274804	-0.696109
H	-1.482059	5.658790	1.029457
H	0.151207	5.707779	0.330656
C	3.468923	-0.283114	-0.155865
C	4.356883	0.470894	0.624363

C	3.865270	-0.664970	-1.446173
C	5.610125	0.832659	0.128561
H	4.067853	0.794863	1.618903
C	5.115300	-0.300729	-1.943418
H	3.189571	-1.250445	-2.062979
C	5.992496	0.452298	-1.158873
H	6.286626	1.414337	0.749021
H	5.406898	-0.607220	-2.944466
H	6.966634	0.736381	-1.546623
C	1.478046	-2.321434	-0.180972
C	2.106070	-3.430409	0.402463
C	0.590329	-2.521928	-1.246367
C	1.838160	-4.716968	-0.063599
H	2.804087	-3.286559	1.222510
C	0.331091	-3.807010	-1.721471
H	0.083483	-1.662372	-1.675413
C	0.950360	-4.906023	-1.126123
H	2.323112	-5.572407	0.399018
H	-0.373895	-3.951513	-2.534615
H	0.737733	-5.909723	-1.483528
C	-2.258242	-1.884311	0.437992
C	-1.470084	-2.716449	1.250199
C	-3.180810	-2.479603	-0.433233
C	-1.610020	-4.100391	1.204723
H	-0.725844	-2.281362	1.905117
C	-3.310394	-3.868744	-0.488661
H	-3.802253	-1.860026	-1.070651
C	-2.528947	-4.683286	0.330322
H	-0.981132	-4.723633	1.833236
H	-4.030280	-4.312175	-1.171552
H	-2.629133	-5.763978	0.283340

C	-3.387420	0.589274	-0.471082
C	-4.591379	0.997004	0.119164
C	-3.246477	0.702485	-1.864229
C	-5.624825	1.515250	-0.663191
H	-4.727129	0.909164	1.192120
C	-4.283729	1.205584	-2.648405
H	-2.313305	0.394353	-2.329167
C	-5.474582	1.619330	-2.046841
H	-6.550195	1.833402	-0.191074
H	-4.160368	1.283615	-3.725050
H	-6.280285	2.022382	-2.653735

4-L5

(U)B3LYP-D3(BJ) SCF energy: -2353.47116293 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2352.779874 a.u.

(U)B3LYP-D3(BJ) free energy: -2352.893321 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2353.98755944 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2353.296271 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2353.409718 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.081124	0.924587	0.337130
P	1.747523	-0.604505	0.404567
N	0.084121	1.008887	2.364555
C	-0.999873	0.327346	3.053714
C	1.390642	0.626479	2.868625
C	1.900652	-0.713593	2.262726
H	-1.184531	0.760869	4.054104

H	1.403475	0.535076	3.969174
H	2.106990	1.421780	2.617775
H	1.248188	-1.531728	2.586542
H	2.918830	-0.963276	2.584527
H	-0.042989	2.686001	2.258947
H	-0.785108	-0.741548	3.237541
H	-1.591398	3.211343	0.629642
C	-2.303851	0.422377	2.245905
H	-3.106294	-0.169660	2.699014
H	-2.622534	1.471343	2.208645
P	-1.960893	-0.068145	0.476961
C	-0.606481	3.714561	0.690583
O	-0.091344	3.670821	1.993233
C	0.313966	3.037261	-0.335876
C	-0.200369	2.525035	-1.550384
C	1.715837	3.075597	-0.163925
C	0.669354	2.079577	-2.555261
H	-1.274026	2.524377	-1.714530
C	2.571941	2.676292	-1.192126
H	2.099638	3.461569	0.774599
C	2.052820	2.178096	-2.388987
H	0.257995	1.678763	-3.478342
H	3.646252	2.724453	-1.049129
H	2.724160	1.842132	-3.172796
C	-0.812301	5.183028	0.307903
H	-1.239432	5.274293	-0.696800
H	-1.484979	5.658209	1.028663
H	0.148527	5.708046	0.330461
C	3.469268	-0.282628	-0.155775
C	4.357379	0.471351	0.624289
C	3.865508	-0.664681	-1.446077

C	5.610662	0.832844	0.128360
H	4.068460	0.795497	1.618803
C	5.115565	-0.300728	-1.943430
H	3.189692	-1.250125	-2.062779
C	5.992926	0.452250	-1.159026
H	6.287306	1.414469	0.748705
H	5.407048	-0.607392	-2.944459
H	6.967096	0.736117	-1.546851
C	1.478435	-2.320842	-0.180755
C	2.106409	-3.429752	0.402868
C	0.591015	-2.521427	-1.246374
C	1.838737	-4.716340	-0.063235
H	2.804202	-3.285805	1.223090
C	0.332027	-3.806546	-1.721530
H	0.084204	-1.661924	-1.675566
C	0.951239	-4.905488	-1.126001
H	2.323632	-5.571736	0.399520
H	-0.372724	-3.951128	-2.534863
H	0.738804	-5.909212	-1.483449
C	-2.257591	-1.885033	0.437812
C	-1.469375	-2.716966	1.250170
C	-3.179863	-2.480577	-0.433557
C	-1.608993	-4.100943	1.204722
H	-0.725323	-2.281708	1.905188
C	-3.309133	-3.869748	-0.488951
H	-3.801352	-1.861172	-1.071096
C	-2.527649	-4.684083	0.330201
H	-0.980066	-4.724013	1.833366
H	-4.028807	-4.313362	-1.171946
H	-2.627593	-5.764800	0.283256
C	-3.387613	0.588204	-0.471177

C	-4.591618	0.995588	0.119222
C	-3.246847	0.701581	-1.864317
C	-5.625268	1.513659	-0.662983
H	-4.727275	0.907595	1.192175
C	-4.284294	1.204506	-2.648347
H	-2.313670	0.393675	-2.329396
C	-5.475187	1.617922	-2.046635
H	-6.550665	1.831529	-0.190728
H	-4.161049	1.282653	-3.724997
H	-6.281029	2.020856	-2.653421

5-L5

(U)B3LYP-D3(BJ) SCF energy: -1967.30686171 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1966.787850 a.u.

(U)B3LYP-D3(BJ) free energy: -1966.884168 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1967.70233550 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1967.183324 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1967.279642 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.000030	0.000027	-0.018032
P	2.204058	-0.223001	0.144795
N	-0.000078	-0.000304	1.908966
C	-1.163571	0.306848	2.713862
C	1.163413	-0.307277	2.713929
C	2.266107	-0.952314	1.858165
H	-0.918178	1.002544	3.538740
H	0.918114	-1.003105	3.538726

H	1.576216	0.597746	3.204048
H	2.062834	-2.021001	1.723513
H	3.253087	-0.840617	2.320603
H	-1.576615	-0.598131	3.203860
C	-2.266077	0.952190	1.858094
H	-3.253094	0.840720	2.320514
H	-2.062535	2.020831	1.723481
P	-2.204130	0.222992	0.144675
C	3.117162	1.365148	0.324919
C	2.472666	2.398497	1.027732
C	4.394946	1.592639	-0.201518
C	3.107103	3.625253	1.213810
H	1.470822	2.227964	1.413592
C	5.022202	2.827250	-0.021443
H	4.901779	0.808981	-0.754742
C	4.383428	3.843685	0.689083
H	2.601526	4.414756	1.763422
H	6.012148	2.992536	-0.438261
H	4.874364	4.802799	0.829298
C	3.334954	-1.285513	-0.830418
C	4.517438	-1.823374	-0.298750
C	2.997513	-1.573345	-2.159786
C	5.342575	-2.629918	-1.081667
H	4.797381	-1.606961	0.727849
C	3.825163	-2.376018	-2.946062
H	2.076390	-1.168448	-2.571303
C	4.998133	-2.906144	-2.407158
H	6.254330	-3.042636	-0.658674
H	3.551317	-2.591800	-3.974980
H	5.641354	-3.535525	-3.015799
C	-3.335091	1.285576	-0.830372

C	-4.517772	1.823009	-0.298701
C	-2.997446	1.574023	-2.159553
C	-5.342882	2.629766	-1.081426
H	-4.797878	1.606124	0.727755
C	-3.825054	2.376935	-2.945628
H	-2.076192	1.169430	-2.571073
C	-4.998211	2.906643	-2.406721
H	-6.254785	3.042153	-0.658430
H	-3.551035	2.593224	-3.974393
H	-5.641399	3.536205	-3.015210
C	-3.117088	-1.365238	0.324713
C	-2.472409	-2.398671	1.027222
C	-4.394993	-1.592680	-0.201472
C	-3.106762	-3.625492	1.213206
H	-1.470514	-2.228141	1.412951
C	-5.022160	-2.827338	-0.021485
H	-4.901963	-0.808945	-0.754467
C	-4.383182	-3.843884	0.688712
H	-2.601026	-4.415065	1.762572
H	-6.012196	-2.992589	-0.438105
H	-4.874056	-4.803041	0.828853

TS1-L5

(U)B3LYP-D3(BJ) SCF energy: -2353.45331134 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2352.765791 a.u.

(U)B3LYP-D3(BJ) free energy: -2352.879531 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2353.96987889 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2353.282359 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2353.396099 a.u.

Imaginary frequency: -340.8863 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.342662	-0.568252	-0.164455
P	-0.764872	1.627531	0.099446
N	-0.652695	-0.706218	1.985622
C	0.590722	-0.786023	2.770978
C	-1.568446	0.353280	2.435018
C	-1.091377	1.728777	1.945230
H	0.403740	-1.250914	3.751682
H	-1.674938	0.364441	3.532147
H	-2.553720	0.130765	2.014233
H	-0.149272	2.005023	2.430548
H	-1.827808	2.502223	2.186159
H	-1.103138	-1.635593	2.008836
H	0.941441	0.231058	2.966739
H	-0.940564	-2.047246	-0.632577
C	1.661625	-1.579351	2.019699
H	2.614032	-1.569733	2.561218
H	1.326194	-2.617841	1.922554
P	1.839211	-0.969856	0.257909
C	-1.776429	-3.261950	0.303539
O	-1.321313	-3.333697	1.472396
C	-3.132014	-2.604989	0.105743
C	-3.695829	-2.363065	-1.154900
C	-3.868476	-2.263189	1.246554
C	-4.961958	-1.794682	-1.270185
H	-3.126779	-2.591999	-2.050030
C	-5.131450	-1.678513	1.134638
H	-3.435602	-2.480897	2.217195

C	-5.685851	-1.447022	-0.124338
H	-5.382153	-1.611173	-2.255459
H	-5.688104	-1.417779	2.031037
H	-6.673229	-1.002404	-0.214963
C	-1.374247	-4.350018	-0.685457
H	-1.591352	-4.096196	-1.724964
H	-0.306715	-4.551348	-0.579107
H	-1.928646	-5.262973	-0.425228
C	-2.328262	2.322355	-0.581391
C	-3.402386	1.431461	-0.735576
C	-2.505509	3.670830	-0.918787
C	-4.637460	1.888189	-1.193923
H	-3.272052	0.376736	-0.508662
C	-3.738377	4.121781	-1.392105
H	-1.679007	4.367242	-0.819041
C	-4.807726	3.233800	-1.524784
H	-5.457676	1.185400	-1.299873
H	-3.863002	5.168285	-1.657558
H	-5.767011	3.588050	-1.892192
C	0.483491	2.935045	-0.191371
C	0.588175	4.090157	0.597336
C	1.399973	2.738960	-1.234178
C	1.588950	5.029566	0.345903
H	-0.113318	4.259820	1.409098
C	2.393373	3.681153	-1.491411
H	1.345040	1.827529	-1.822127
C	2.491010	4.826562	-0.699823
H	1.663258	5.919249	0.965442
H	3.107515	3.507425	-2.290078
H	3.274581	5.554478	-0.890643
C	2.665170	-2.409659	-0.531207

C	3.925737	-2.871446	-0.122114
C	1.981820	-3.096596	-1.542369
C	4.489693	-4.000289	-0.713663
H	4.470551	-2.338891	0.652480
C	2.547130	-4.228175	-2.134811
H	0.997034	-2.747598	-1.839269
C	3.800225	-4.680726	-1.721697
H	5.465736	-4.351026	-0.389415
H	2.006516	-4.755514	-2.915965
H	4.240621	-5.561290	-2.181351
C	3.192920	0.277514	0.312973
C	3.207649	1.268040	1.307636
C	4.138888	0.359263	-0.720845
C	4.148834	2.294685	1.283423
H	2.469244	1.250985	2.101819
C	5.080701	1.388070	-0.746572
H	4.145529	-0.392513	-1.503891
C	5.091544	2.358101	0.256278
H	4.137055	3.053345	2.060678
H	5.808989	1.428673	-1.552322
H	5.822180	3.161605	0.233635

TS2-L5

(U)B3LYP-D3(BJ) SCF energy: -2353.46719800 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2352.780223 a.u.

(U)B3LYP-D3(BJ) free energy: -2352.892813 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2353.97909997 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2353.292125 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2353.404715 a.u.

Imaginary frequency: -880.7010 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.125280	-0.966096	0.252786
P	-1.569125	0.773767	0.420374
N	-0.170339	-1.082436	2.361229
C	1.010063	-0.578182	3.047327
C	-1.411073	-0.540684	2.872298
C	-1.720247	0.862687	2.283177
H	1.133962	-1.045090	4.041842
H	-1.418771	-0.467839	3.974466
H	-2.227757	-1.225329	2.603601
H	-0.966032	1.578068	2.628915
H	-2.699287	1.240871	2.599639
H	-0.022188	-2.352716	1.945376
H	0.935521	0.505359	3.238227
H	-0.341655	-4.847019	0.219484
C	2.282924	-0.846573	2.227864
H	3.157128	-0.375296	2.689578
H	2.452332	-1.927062	2.167780
P	2.024033	-0.295610	0.462868
C	-0.747679	-3.914806	0.647197
O	0.323627	-3.224624	1.246851
C	-1.284239	-3.088480	-0.529728
C	-2.631468	-2.761413	-0.730347
C	-0.330974	-2.596587	-1.456023
C	-3.030198	-1.974209	-1.816673
H	-3.381938	-3.116115	-0.032058
C	-0.730412	-1.776651	-2.519084
H	0.706397	-2.901533	-1.354725

C	-2.083418	-1.469713	-2.703442
H	-4.077793	-1.718733	-1.938244
H	0.012782	-1.404794	-3.219576
H	-2.392756	-0.832617	-3.526548
C	-1.819747	-4.307489	1.667425
H	-2.596921	-4.943031	1.226146
H	-1.343128	-4.858836	2.482962
H	-2.299933	-3.419809	2.095686
C	3.343277	-1.158574	-0.474616
C	4.549690	-1.579138	0.101909
C	3.124970	-1.402151	-1.838653
C	5.510371	-2.236500	-0.666777
H	4.741215	-1.393282	1.153943
C	4.089480	-2.048494	-2.611939
H	2.190079	-1.080765	-2.289517
C	5.283167	-2.471272	-2.024533
H	6.438533	-2.563590	-0.206263
H	3.906195	-2.229677	-3.667466
H	6.032512	-2.983770	-2.621186
C	2.605312	1.451726	0.438233
C	3.577791	1.906308	-0.463207
C	1.989234	2.387245	1.285900
C	3.926883	3.257470	-0.510341
H	4.067624	1.203861	-1.129264
C	2.347451	3.731639	1.248487
H	1.206670	2.067301	1.963327
C	3.317199	4.173495	0.346456
H	4.683353	3.590864	-1.215994
H	1.850010	4.438025	1.906342
H	3.588697	5.224683	0.307160
C	-3.326337	0.765685	-0.131231

C	-4.289238	0.026576	0.571579
C	-3.700113	1.381925	-1.334007
C	-5.591309	-0.092688	0.086421
H	-4.020979	-0.474453	1.496426
C	-5.000546	1.259996	-1.822103
H	-2.968103	1.959138	-1.890668
C	-5.951657	0.520466	-1.115312
H	-6.324248	-0.667141	0.646668
H	-5.272817	1.746499	-2.754985
H	-6.965023	0.426563	-1.495218
C	-1.029180	2.445171	-0.106344
C	-1.463930	3.619888	0.522835
C	-0.134772	2.537992	-1.181176
C	-0.999265	4.862454	0.093161
H	-2.167109	3.562391	1.348961
C	0.320113	3.780719	-1.620214
H	0.221428	1.624346	-1.647989
C	-0.106986	4.943608	-0.979018
H	-1.334839	5.767893	0.591728
H	1.028885	3.838262	-2.440718
H	0.259444	5.911984	-1.308125

TS3-L5

(U)B3LYP-D3(BJ) SCF energy: -1968.46390445 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1967.932093 a.u.

(U)B3LYP-D3(BJ) free energy: -1968.027295 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1968.86738266 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1968.335571 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1968.430773 a.u.

Imaginary frequency: -836.0055 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.029541	-1.660820	-0.069260
P	-1.852179	-0.349933	0.158400
N	-0.091108	-1.999295	2.037984
C	0.825342	-1.186278	2.806459
C	-1.471144	-1.884093	2.445709
C	-2.121929	-0.543194	1.999463
H	1.040365	-1.623793	3.800553
H	-1.599405	-1.982773	3.539228
H	-2.041082	-2.710327	1.995566
H	-1.619835	0.297001	2.491278
H	-3.186916	-0.495553	2.253686
H	0.403455	-0.184295	3.017986
C	2.160624	-0.995489	2.072137
H	2.808299	-0.275900	2.585657
H	2.693479	-1.952154	2.024257
P	1.882000	-0.523002	0.280448
H	0.327591	-3.036905	1.022335
H	0.485650	-3.415045	0.163288
C	3.489554	-0.988686	-0.476681
C	4.697093	-0.368707	-0.118593
C	3.511845	-2.036972	-1.405288
C	5.900566	-0.790243	-0.680105
H	4.690688	0.452745	0.592140
C	4.718288	-2.461283	-1.966693
H	2.578845	-2.523296	-1.677176
C	5.912670	-1.838098	-1.605582
H	6.829843	-0.303392	-0.396918

H	4.723265	-3.275861	-2.685583
H	6.851832	-2.165415	-2.043008
C	1.942292	1.313421	0.248291
C	1.310238	2.065372	1.249932
C	2.510685	1.991698	-0.841083
C	1.263798	3.456216	1.175337
H	0.843178	1.563352	2.090521
C	2.465466	3.383544	-0.914271
H	3.002607	1.428787	-1.628545
C	1.843613	4.120965	0.094453
H	0.763267	4.019620	1.957425
H	2.918939	3.891919	-1.761106
H	1.803158	5.204815	0.034173
C	-1.843295	1.455576	-0.136969
C	-2.515174	2.366237	0.691558
C	-1.115854	1.940899	-1.232698
C	-2.464130	3.734859	0.424023
H	-3.080617	2.006874	1.546126
C	-1.072016	3.306471	-1.504393
H	-0.564071	1.241984	-1.854346
C	-1.745460	4.205623	-0.675919
H	-2.986556	4.432111	1.073412
H	-0.491834	3.670219	-2.346594
H	-1.701169	5.271700	-0.880460
C	-3.460501	-0.911366	-0.541360
C	-3.618472	-2.286900	-0.772098
C	-4.526380	-0.048435	-0.829550
C	-4.823685	-2.792046	-1.258936
H	-2.789335	-2.962885	-0.574645
C	-5.727383	-0.553319	-1.329124
H	-4.415599	1.019429	-0.670494

C	-5.880933	-1.924768	-1.540487
H	-4.932602	-3.859642	-1.428691
H	-6.544539	0.126796	-1.554136
H	-6.817169	-2.314929	-1.929709

acetophenone

(U)B3LYP-D3(BJ) SCF energy: -384.91824646 a.u.

(U)B3LYP-D3(BJ) enthalpy: -384.770871 a.u.

(U)B3LYP-D3(BJ) free energy: -384.812231 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -385.04487450 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -384.897499 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -384.938859 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.575665	-1.220969	0.000009
C	0.205867	-0.055539	-0.000058
C	-0.429056	1.194607	-0.000052
C	-1.821070	1.277462	0.000002
C	-2.589530	0.112164	0.000027
C	-1.963977	-1.138455	0.000014
H	-0.065331	-2.178139	0.000060
H	0.158375	2.107006	-0.000162
H	-2.305331	2.249700	0.000066
H	-3.674005	0.177554	0.000078
H	-2.561884	-2.045346	-0.000021
C	1.695647	-0.204307	-0.000014
O	2.212944	-1.311167	-0.000017
C	2.552554	1.050007	0.000041

H	2.346211	1.666251	-0.883030
H	2.346445	1.665958	0.883391
H	3.603349	0.756533	-0.000069

phenylethanol

(U)B3LYP-D3(BJ) SCF energy: -386.11241113 a.u.

(U)B3LYP-D3(BJ) enthalpy: -385.941057 a.u.

(U)B3LYP-D3(BJ) free energy: -385.984024 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -386.24652976 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -386.075176 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -386.118143 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.576908	-1.191310	0.102858
C	0.151644	0.003430	0.181871
C	-0.545753	1.216307	0.109749
C	-1.933137	1.234293	-0.041173
C	-2.647330	0.038694	-0.124265
C	-1.962867	-1.175375	-0.050611
H	-0.041652	-2.133040	0.162653
H	-0.010327	2.158279	0.170307
H	-2.454867	2.185811	-0.097995
H	-3.726919	0.053312	-0.244772
H	-2.508588	-2.113158	-0.111642
C	1.665125	-0.057203	0.369084
O	2.203627	-1.281966	-0.134891
C	2.418196	1.137269	-0.222036
H	2.185179	1.255939	-1.287518

H	2.167481	2.074781	0.284461
H	3.493483	0.968561	-0.115603
H	1.972228	-1.325362	-1.077724
H	1.881147	-0.106021	1.444096

H2

(U)B3LYP-D3(BJ) SCF energy: -1.17562313002 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1.16218413 a.u.

(U)B3LYP-D3(BJ) free energy: -1.17697613 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1.179241 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1.165802 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1.180594 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	0.00000000	0.00000000	0.37142100
H	0.00000000	0.00000000	-0.37142100

6

(U)B3LYP-D3(BJ) SCF energy: -1508.38683883 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1507.764702 a.u.

(U)B3LYP-D3(BJ) free energy: -1507.872661 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1508.78781236 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1508.165676 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1508.273635 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	1.615461	-0.015863	0.264308
N	3.557511	0.100134	-0.095486
C	3.917441	-2.320375	-0.410612
C	4.192378	-0.902223	-0.906550
C	4.238487	1.361023	-0.176658
C	3.747563	2.338954	0.891695
H	5.298343	-0.807846	-0.880573
H	4.372520	3.237161	0.910378
H	3.796620	1.849411	1.870312
H	1.271866	0.739624	3.171008
H	3.920517	-0.854102	-1.985474
N	2.371882	2.778086	0.655346
C	1.349964	1.893258	0.449592
C	1.962207	4.093730	0.501931
C	0.642342	4.059614	0.189382
H	2.637320	4.925948	0.629082
H	-0.065972	4.844932	-0.021169
N	0.282118	2.712119	0.164613
H	4.480174	-3.043405	-1.010984
H	4.247094	-2.396422	0.632789

N	2.508624	-2.723512	-0.473491
C	2.081214	-4.016925	-0.737628
C	1.472768	-1.909801	-0.106559
C	0.737029	-4.035080	-0.550553
H	2.763029	-4.797725	-1.037910
H	0.008552	-4.823396	-0.654594
N	0.382202	-2.743060	-0.169634
C	-1.009597	2.254325	-0.251229
C	-2.069985	2.279662	0.664746
C	-1.185900	1.840294	-1.579868
C	-3.341518	1.925986	0.207813
C	-2.474029	1.484397	-1.988306
C	-3.564502	1.538908	-1.116506
H	-4.176072	1.954294	0.904409
H	-2.628060	1.164701	-3.016268
C	-0.942334	-2.346694	0.204303
C	-1.868080	-2.024950	-0.795749
C	-1.275797	-2.311903	1.566689
C	-3.168794	-1.698387	-0.404805
C	-2.582641	-1.960253	1.910704
C	-3.542891	-1.658575	0.940246
H	-3.901963	-1.460135	-1.169888
H	-2.858689	-1.931040	2.962419

C	-1.831869	2.661270	2.103541
H	-1.072787	2.012294	2.553635
H	-1.465183	3.689977	2.198170
H	-2.753342	2.572962	2.686282
C	-4.955495	1.208544	-1.599836
H	-5.552603	0.737947	-0.812439
H	-5.489684	2.113956	-1.916782
H	-4.929429	0.530044	-2.459026
C	-0.019445	1.778521	-2.532318
H	0.510671	2.736809	-2.578431
H	0.714567	1.032226	-2.201418
H	-0.354332	1.519105	-3.540932
C	-0.249925	-2.638129	2.621428
H	0.221599	-3.609910	2.435110
H	0.552933	-1.892051	2.624631
H	-0.707451	-2.660598	3.614757
C	-1.458171	-2.005175	-2.245868
H	-0.627913	-1.306767	-2.399626
H	-1.115256	-2.987894	-2.589744
H	-2.292351	-1.692006	-2.879789
C	-4.943067	-1.268353	1.344290
H	-4.996022	-0.198480	1.583473
H	-5.660955	-1.461093	0.540471

H	-5.272348	-1.816795	2.233377
H	5.330421	1.250278	-0.005735
H	4.146487	1.870282	-1.164798
H	1.169752	0.789667	3.909617

6b

(U)B3LYP-D3(BJ) SCF energy: -1508.38182394 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1507.759801 a.u.

(U)B3LYP-D3(BJ) free energy: -1507.864497 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1508.78538110 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1508.163358 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1508.268054 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.714352	-0.026099	-0.533030
N	-3.666235	0.172041	-0.059313
C	-4.011865	-2.225769	0.387194
C	-4.322283	-0.786582	0.781515
C	-4.271365	1.461019	0.097422
C	-3.713985	2.475055	-0.896107

H	-5.429447	-0.703514	0.712444
H	-4.298007	3.400263	-0.874472
H	-3.761184	2.048909	-1.904699
H	-4.093583	-0.671217	1.867907
N	-2.327187	2.839223	-0.607788
C	-1.324004	1.915053	-0.497902
C	-1.878859	4.133304	-0.393891
C	-0.551438	4.047640	-0.136353
H	-2.536629	4.987044	-0.446158
H	0.189208	4.799977	0.082875
N	-0.227425	2.691264	-0.202680
H	-4.620659	-2.918645	0.977095
H	-4.254073	-2.359910	-0.674155
N	-2.614336	-2.612974	0.590576
C	-2.211614	-3.833252	1.114784
C	-1.557028	-1.874417	0.134631
C	-0.860978	-3.881369	1.004695
H	-2.914281	-4.545042	1.519882
H	-0.141849	-4.630929	1.294452
N	-0.478805	-2.681687	0.406243
C	1.098725	2.229212	0.076867
C	1.982269	1.987301	-0.981654
C	1.505506	2.142614	1.417462

C	3.318383	1.714906	-0.670816
C	2.848247	1.867057	1.679999
C	3.773988	1.675844	0.648230
H	4.020830	1.547046	-1.483416
H	3.181028	1.812356	2.714468
C	0.872142	-2.374721	0.048501
C	1.705932	-1.764660	0.993132
C	1.331432	-2.741057	-1.224783
C	3.042020	-1.553008	0.646239
C	2.669276	-2.488866	-1.535786
C	3.539850	-1.904025	-0.610981
H	3.704330	-1.096740	1.374852
H	3.042887	-2.769112	-2.518244
C	1.504274	2.036990	-2.409482
H	0.769319	1.246359	-2.597372
H	1.009749	2.988965	-2.633738
H	2.338561	1.907164	-3.104890
C	5.230164	1.435889	0.964714
H	5.820174	1.298675	0.054093
H	5.658559	2.279490	1.519470
H	5.365796	0.542467	1.586559
C	0.512689	2.352769	2.532563
H	0.177229	3.395514	2.585041

H	-0.382336	1.741008	2.375443
H	0.952227	2.088651	3.498669
C	0.406689	-3.401024	-2.215671
H	0.001103	-4.339904	-1.820482
H	-0.451142	-2.758170	-2.440722
H	0.930590	-3.620782	-3.150390
C	1.164602	-1.352144	2.337308
H	0.302599	-0.688068	2.213942
H	0.821533	-2.216538	2.918508
H	1.926913	-0.825732	2.917527
C	4.978312	-1.636008	-0.978570
H	5.075409	-0.679695	-1.508266
H	5.616163	-1.581862	-0.090896
H	5.375465	-2.415192	-1.637928
H	-5.369428	1.429940	-0.080701
H	-4.158704	1.897594	1.119449
H	-1.491179	0.036786	-2.436589
H	-1.578238	-0.724063	-2.306563

6c

(U)B3LYP-D3(BJ) SCF energy: -1508.38811150 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1507.765209 a.u.

(U)B3LYP-D3(BJ) free energy: -1507.870824 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1508.78888289 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1508.165980 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1508.271595 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	1.593212	-0.011223	0.287498
N	3.546500	0.093033	-0.069697
C	3.869383	-2.324979	-0.460600
C	4.163016	-0.896557	-0.913774
C	4.222402	1.357234	-0.173959
C	3.734381	2.348713	0.882676
H	5.270610	-0.819751	-0.886032
H	4.360415	3.246186	0.887552
H	3.786292	1.874546	1.868093
H	4.995065	-0.432168	1.819424
H	3.890732	-0.806762	-1.988807
N	2.358240	2.786348	0.646145
C	1.332917	1.900766	0.464594
C	1.951778	4.099781	0.468136
C	0.629823	4.063402	0.164633

H	2.629910	4.932375	0.575126
H	-0.078011	4.846457	-0.055729
N	0.265745	2.716855	0.169593
H	4.416376	-3.034782	-1.090280
H	4.208533	-2.443802	0.574762
N	2.455062	-2.709121	-0.521231
C	2.012101	-3.990772	-0.815830
C	1.432211	-1.896938	-0.117148
C	0.670688	-4.002233	-0.610623
H	2.682738	-4.769134	-1.146102
H	-0.066119	-4.781258	-0.725153
N	0.332897	-2.718490	-0.188209
C	-1.031141	2.256410	-0.227187
C	-2.077235	2.277684	0.705022
C	-1.227142	1.845660	-1.553889
C	-3.355489	1.925287	0.266453
C	-2.521472	1.492230	-1.944475
C	-3.598670	1.544357	-1.056166
H	-4.179261	1.950177	0.975893
H	-2.691070	1.175767	-2.970967
C	-0.984529	-2.322839	0.210463
C	-1.931618	-2.012700	-0.773424
C	-1.292321	-2.281124	1.578871

C	-3.226948	-1.692928	-0.359786
C	-2.594732	-1.935560	1.945276
C	-3.575738	-1.647279	0.991768
H	-3.976026	-1.464045	-1.112275
H	-2.850923	-1.901756	3.001875
C	-1.815550	2.653467	2.141104
H	-1.050091	2.000332	2.575406
H	-1.444605	3.680847	2.233312
H	-2.727331	2.564635	2.738769
C	-4.997141	1.217754	-1.519971
H	-5.581621	0.740423	-0.727211
H	-5.536291	2.125794	-1.820504
H	-4.984727	0.546638	-2.385192
C	-0.073623	1.782883	-2.521899
H	0.454127	2.741861	-2.579197
H	0.665605	1.038888	-2.197641
H	-0.421284	1.518671	-3.524915
C	-0.245922	-2.593092	2.617707
H	0.245980	-3.551585	2.416526
H	0.540378	-1.828653	2.616814
H	-0.690327	-2.634838	3.616418
C	-1.550085	-1.995903	-2.231426
H	-0.718992	-1.302280	-2.401548

H	-1.220254	-2.980304	-2.583083
H	-2.394798	-1.677503	-2.848545
C	-4.970762	-1.264756	1.420277
H	-5.025243	-0.195659	1.662767
H	-5.701271	-1.459706	0.628485
H	-5.282160	-1.816499	2.313777
H	5.315267	1.251067	-0.005372
H	4.123848	1.845936	-1.170158
H	5.617202	-0.505288	2.234153

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(U)B3LYP-D3(BJ) SCF energy: -1516.01700505 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1515.469774 a.u.

(U)B3LYP-D3(BJ) free energy: -1515.562407 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1516.29734222 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1515.750111 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1515.842744 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.000924	-0.116667	-0.055458

P	-2.217702	0.009442	-0.113864
N	0.001942	1.788223	0.129665
C	1.189053	2.575635	0.379857
C	-1.177661	2.618953	0.036716
C	-2.389967	1.826778	-0.493774
C	-3.308309	-0.759227	-1.437329
C	-4.808602	-0.493994	-1.265335
C	-3.008719	-2.251548	-1.634349
C	-3.147341	-0.207989	1.498840
C	-3.171762	-1.678849	1.933687
C	-2.504562	0.665888	2.585526
H	1.009282	3.334537	1.166745
H	-1.013851	3.481179	-0.639919
H	-1.434101	3.069737	1.017103
H	-2.412887	1.886877	-1.588195
H	-3.336743	2.238635	-0.122814
H	-5.209913	-1.022748	-0.393601
H	-5.362297	-0.846748	-2.144412
H	-5.023990	0.572763	-1.141238
H	-1.936365	-2.424210	-1.770542
H	-3.533300	-2.630961	-2.520200
H	-3.336725	-2.849171	-0.777809
H	-3.727177	-2.310143	1.234126

H	-3.646927	-1.775763	2.917803
H	-2.153013	-2.077674	2.011396
H	-1.443099	0.423373	2.704300
H	-3.009556	0.500889	3.545650
H	-2.573236	1.730585	2.346717
H	-0.412682	-0.575290	-3.501821
H	1.492282	3.155248	-0.515323
C	2.364923	1.691570	0.841566
H	3.334655	2.149167	0.609045
H	2.313022	1.564114	1.929174
P	2.212582	-0.030630	0.142532
C	3.293754	0.007626	-1.387528
C	3.159226	-1.045811	1.410095
C	2.808332	1.114266	-2.335043
H	3.392463	1.094866	-3.263655
H	1.752608	0.979279	-2.589660
H	2.917050	2.107387	-1.890605
C	3.297231	-1.352688	-2.096517
H	3.878189	-1.295664	-3.025457
H	3.736860	-2.140941	-1.478329
H	2.276769	-1.657960	-2.355982
C	2.818490	-2.539582	1.319141
H	3.252594	-3.082009	2.168373

H	1.734785	-2.697497	1.327653
H	3.214138	-2.992174	0.403893
C	4.672998	-0.804200	1.426688
H	5.148818	-1.197350	0.521349
H	4.916773	0.261179	1.500556
H	5.132242	-1.312680	2.283571
H	2.740942	-0.674942	2.356373
H	4.316307	0.247175	-1.068759
H	-2.969742	-0.239251	-2.343800
H	-4.177784	0.134882	1.339033
H	-0.330636	-0.379397	-2.784495

6b-L4

(U)B3LYP-D3(BJ) SCF energy: -1516.01450983 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1515.466427 a.u.

(U)B3LYP-D3(BJ) free energy: -1515.553804 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1516.29856939 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1515.750487 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1515.837864 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.006698	-0.950552	0.652000
P	1.972823	0.068872	-0.024131
N	0.020696	-2.028469	-0.938554
C	-0.908925	-1.688702	-1.997377
C	1.364394	-2.276883	-1.428378
C	2.201005	-0.970514	-1.566444
C	2.186674	1.809724	-0.700710
C	3.605935	2.141506	-1.175812
C	1.634187	2.872186	0.258015
C	3.538890	-0.276364	0.951918
C	3.609322	0.594504	2.212486
C	3.592953	-1.765115	1.325034
H	-1.058190	-2.538161	-2.690769
H	1.354606	-2.786751	-2.407710
H	1.882613	-2.955421	-0.739321
H	1.804065	-0.378817	-2.400643
H	3.259157	-1.170943	-1.783148
H	4.305796	2.201926	-0.335285
H	3.620518	3.114289	-1.683221
H	3.985442	1.391890	-1.878392
H	0.628176	2.608173	0.597334
H	1.588182	3.849064	-0.239346

H	2.264568	2.984134	1.145824
H	3.707962	1.657594	1.975758
H	4.474359	0.308830	2.823847
H	2.708542	0.469099	2.825175
H	2.708164	-2.059578	1.902620
H	4.477907	-1.967519	1.941069
H	3.645715	-2.408775	0.442712
H	-0.548441	-0.853536	-2.633969
C	-2.273616	-1.300185	-1.412037
H	-2.950332	-0.917036	-2.185486
H	-2.733315	-2.195095	-0.976288
P	-2.050240	-0.086838	-0.001789
C	-2.533444	1.543702	-0.802960
C	-3.516643	-0.538051	1.089278
C	-1.551433	1.878454	-1.932203
H	-1.822615	2.833313	-2.399571
H	-0.533500	1.972501	-1.543370
H	-1.542565	1.111710	-2.712140
C	-2.589571	2.684954	0.219675
H	-2.753369	3.643639	-0.288278
H	-3.399205	2.551045	0.942223
H	-1.649829	2.758689	0.779038
C	-3.401100	0.050861	2.502170

H	-4.180965	-0.367332	3.150883
H	-2.428926	-0.176963	2.949174
H	-3.523404	1.138496	2.503457
C	-4.890218	-0.261328	0.467256
H	-5.081320	0.814269	0.381437
H	-4.982824	-0.701043	-0.531546
H	-5.685705	-0.684280	1.093569
H	-3.395714	-1.626246	1.182463
H	-3.530452	1.410258	-1.242239
H	1.533473	1.791254	-1.582952
H	4.400041	-0.048549	0.310837
H	-0.197677	-1.204190	2.329440
H	0.074131	-0.428763	2.272015

6c-L4

(U)B3LYP-D3(BJ) SCF energy: -1516.01825176 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1515.470509 a.u.

(U)B3LYP-D3(BJ) free energy: -1515.561383 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1516.29756012 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1515.749817 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1515.840691 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.005317	0.077366	-0.117655
P	-2.206771	0.068430	0.094637
N	0.015484	-1.641147	0.731756
C	1.213709	-2.391387	1.045975
C	-1.180519	-2.321262	1.183617
C	-2.375258	-1.352270	1.293861
C	-3.111200	1.441247	1.005166
C	-4.625945	1.237349	1.125957
C	-2.756911	2.828745	0.452826
C	-3.320953	-0.419977	-1.329318
C	-3.431314	0.698648	-2.372606
C	-2.779638	-1.704204	-1.971456
H	1.106057	-3.458803	0.771400
H	-1.029375	-2.780653	2.178669
H	-1.447037	-3.163407	0.513212
H	-2.368678	-0.889893	2.287782
H	-3.334106	-1.873386	1.179864
H	-5.119992	1.325687	0.152088
H	-5.063330	1.998165	1.784399
H	-4.873445	0.254340	1.541140

H	-1.671394	2.965434	0.401937
H	-3.172738	3.612803	1.097995
H	-3.159173	2.983108	-0.553501
H	-3.932599	1.587197	-1.978269
H	-4.004866	0.351753	-3.241140
H	-2.437734	1.000518	-2.725779
H	-1.767916	-1.547480	-2.359438
H	-3.424255	-2.008879	-2.805470
H	-2.732630	-2.533568	-1.260177
H	0.114821	-2.913941	-1.398648
H	1.415843	-2.391404	2.135207
C	2.440280	-1.837265	0.293465
H	3.371638	-2.029454	0.840139
H	2.521844	-2.335862	-0.678887
P	2.224096	-0.027857	-0.102323
C	3.138497	0.843241	1.281649
C	3.301609	0.160696	-1.629880
C	2.489645	0.480500	2.625294
H	2.991173	1.015758	3.441345
H	1.428819	0.754150	2.631950
H	2.553813	-0.590908	2.834582
C	3.146228	2.363399	1.078196
H	3.607833	2.860078	1.940703

H	3.705868	2.660060	0.186378
H	2.123549	2.746725	0.976934
C	2.963494	1.433978	-2.417430
H	3.489962	1.437293	-3.380054
H	1.888163	1.501256	-2.613598
H	3.260731	2.338727	-1.877254
C	4.807011	0.027087	-1.371835
H	5.188998	0.874663	-0.791947
H	5.048139	-0.891210	-0.825548
H	5.357571	0.006009	-2.320586
H	2.980514	-0.693538	-2.242322
H	4.173210	0.476555	1.282362
H	-2.674017	1.372924	2.011104
H	-4.317436	-0.625353	-0.916865
H	0.177942	-3.536065	-1.810923

6-L5

(U)B3LYP-D3(BJ) SCF energy: -1968.48529694 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1967.951523 a.u.

(U)B3LYP-D3(BJ) free energy: -1968.054668 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1968.88477379 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1968.351000 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1968.454145 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.000704	-0.009646	0.014570
P	2.202221	0.237013	-0.146628
N	0.001461	0.005038	-1.913416
C	-1.159903	-0.302639	-2.720776
C	1.159141	0.340258	-2.715199
C	2.253368	0.988706	-1.850834
H	-0.912050	-0.994072	-3.548651
H	0.901706	1.045051	-3.528670
H	1.584681	-0.550371	-3.220488
H	2.035541	2.052656	-1.702324
H	3.241849	0.896742	-2.314326
H	-1.575197	0.603503	-3.206869
C	-2.261167	-0.954239	-1.868134
H	-3.246780	-0.848983	-2.334925
H	-2.051263	-2.021420	-1.731349
P	-2.207286	-0.218733	-0.157827
C	3.141995	-1.332152	-0.347478
C	2.528517	-2.356798	-1.089240

C	4.409733	-1.555526	0.204407
C	3.184074	-3.569844	-1.289587
H	1.531816	-2.193101	-1.490344
C	5.058154	-2.776964	0.010051
H	4.892497	-0.778760	0.788024
C	4.450703	-3.783990	-0.740166
H	2.702029	-4.352753	-1.868957
H	6.040050	-2.939169	0.446638
H	4.958045	-4.732793	-0.891675
C	3.314221	1.305935	0.842771
C	4.497676	1.854555	0.324417
C	2.960437	1.588000	2.169072
C	5.307636	2.666521	1.117385
H	4.790149	1.641859	-0.699500
C	3.772932	2.396316	2.965437
H	2.038816	1.173803	2.570148
C	4.946852	2.937367	2.439718
H	6.220343	3.087646	0.704874
H	3.486714	2.607592	3.991916
H	5.578376	3.570913	3.056239
C	-3.346808	-1.267350	0.821294
C	-4.498847	-1.854591	0.275918
C	-3.048222	-1.488706	2.172711

C	-5.332603	-2.644569	1.066927
H	-4.748944	-1.690195	-0.767764
C	-3.884953	-2.273538	2.966712
H	-2.149459	-1.047195	2.595425
C	-5.027593	-2.853786	2.413950
H	-6.220633	-3.096021	0.633172
H	-3.641378	-2.437513	4.012666
H	-5.677348	-3.470212	3.028873
C	-3.113242	1.371734	-0.350756
C	-2.453493	2.408403	-1.033896
C	-4.404087	1.594691	0.144961
C	-3.084818	3.635344	-1.229556
H	-1.443404	2.239237	-1.398375
C	-5.028333	2.829316	-0.044562
H	-4.923039	0.807253	0.681446
C	-4.373513	3.849908	-0.734393
H	-2.567435	4.427862	-1.763630
H	-6.028477	2.991488	0.348444
H	-4.862099	4.809134	-0.881888
H	0.124389	-2.372079	1.060974
H	0.198125	-2.993309	1.471311

6b-L5

(U)B3LYP-D3(BJ) SCF energy: -1968.48836584 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1967.953769 a.u.

(U)B3LYP-D3(BJ) free energy: -1968.049754 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1968.89093003 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1968.356333 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1968.452318 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.066166	-1.768645	0.050074
P	-1.835499	-0.301340	0.130999
N	-0.165122	-1.970313	1.954427
C	0.853485	-1.372682	2.798128
C	-1.508785	-1.750753	2.466348
C	-2.089874	-0.392555	1.985532
H	1.046356	-1.980963	3.701813
H	-1.538986	-1.775118	3.568753
H	-2.175211	-2.555359	2.128267
H	-1.510048	0.427912	2.423893
H	-3.141211	-0.254723	2.266462
H	0.543720	-0.381003	3.183876

C	2.185408	-1.203220	2.051200
H	2.880843	-0.560121	2.601982
H	2.659131	-2.183733	1.922692
P	1.888159	-0.606748	0.301678
H	0.005997	-2.772368	-1.334908
H	-0.116016	-2.014910	-1.629985
C	3.488339	-0.999007	-0.511005
C	4.716484	-0.550103	0.000425
C	3.483214	-1.791822	-1.665086
C	5.911707	-0.892562	-0.628206
H	4.733402	0.078544	0.886177
C	4.680720	-2.135462	-2.296992
H	2.535218	-2.140497	-2.064634
C	5.895244	-1.687142	-1.778570
H	6.856688	-0.540268	-0.223752
H	4.663371	-2.751806	-3.191535
H	6.827953	-1.953619	-2.267913
C	1.932372	1.226891	0.395183
C	1.179653	1.899412	1.371142
C	2.605160	1.987801	-0.573048
C	1.113951	3.290812	1.388266
H	0.633524	1.333569	2.117013
C	2.538093	3.380880	-0.555202

H	3.189409	1.489334	-1.339946
C	1.793585	4.037565	0.425327
H	0.518223	3.790766	2.146284
H	3.070239	3.953243	-1.310498
H	1.735920	5.122205	0.434224
C	-1.793678	1.490967	-0.237400
C	-2.510404	2.437077	0.510157
C	-0.984078	1.929415	-1.293717
C	-2.421964	3.794594	0.201662
H	-3.138938	2.112478	1.334320
C	-0.898955	3.285202	-1.604849
H	-0.400374	1.201339	-1.849136
C	-1.617470	4.219419	-0.857574
H	-2.979935	4.520016	0.787622
H	-0.254408	3.613607	-2.414395
H	-1.542948	5.277533	-1.092717
C	-3.462130	-0.860265	-0.521711
C	-3.702377	-2.244519	-0.542676
C	-4.457031	0.005495	-0.994963
C	-4.918010	-2.748564	-1.002521
H	-2.928848	-2.929490	-0.203190
C	-5.668697	-0.501394	-1.467273
H	-4.283688	1.076608	-0.998420

C -5.905073 -1.876855 -1.467496

H -5.090637 -3.821324 -1.006875

H -6.429859 0.181674 -1.834847

H -6.849785 -2.268370 -1.834243

6c-L5

(U)B3LYP-D3(BJ) SCF energy: -1968.48490439 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1967.950385 a.u.

(U)B3LYP-D3(BJ) free energy: -1968.052755 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1968.88353535 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1968.349016 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1968.451386 a.u.

Cartesian coordinates

ATOM X Y Z

Co -0.005129 -0.224879 -0.030748

P 2.188023 0.101748 -0.154857

N -0.003488 -0.329098 -1.951650

C -1.196730 -0.509713 -2.754552

C 1.184143 -0.114120 -2.755219

C 2.271802 0.615894 -1.947304

H	-1.036212	-1.233123	-3.575534
H	0.962234	0.499121	-3.647874
H	1.597987	-1.064854	-3.145813
H	2.061779	1.691607	-1.938229
H	3.270267	0.461361	-2.371809
H	-1.502970	0.434596	-3.247249
C	-2.362508	-1.022917	-1.894119
H	-3.330839	-0.801902	-2.356167
H	-2.281776	-2.106908	-1.756913
P	-2.221236	-0.299073	-0.183925
C	3.306914	-1.354518	-0.061050
C	4.526038	-1.360406	0.628743
C	2.883950	-2.527104	-0.709019
C	5.312960	-2.513691	0.659051
H	4.863186	-0.467060	1.143530
C	3.676742	-3.672612	-0.685868
H	1.926938	-2.536966	-1.219858
C	4.894465	-3.669314	-0.000922
H	6.255448	-2.506155	1.200054
H	3.339692	-4.570463	-1.196759
H	5.509870	-4.564385	0.022708
C	3.110073	1.428618	0.710561
C	4.289109	1.987560	0.192605

C	2.608508	1.910280	1.926805
C	4.950755	3.004533	0.879242
H	4.693685	1.622213	-0.746819
C	3.271956	2.926154	2.617016
H	1.689118	1.488072	2.324576
C	4.443239	3.474503	2.093457
H	5.861771	3.430879	0.468361
H	2.871620	3.291698	3.558445
H	4.959012	4.268003	2.626971
C	-3.436549	-1.251474	0.803480
C	-4.660380	-1.694465	0.278007
C	-3.123733	-1.549744	2.136608
C	-5.550110	-2.418536	1.070811
H	-4.921483	-1.468587	-0.751489
C	-4.015705	-2.269543	2.932649
H	-2.171383	-1.219047	2.543387
C	-5.229502	-2.705761	2.399904
H	-6.493552	-2.758458	0.652588
H	-3.760338	-2.494742	3.964297
H	-5.923062	-3.270984	3.016172
C	-2.988710	1.365012	-0.360441
C	-2.256955	2.336994	-1.065287
C	-4.239149	1.705984	0.170270

C	-2.778861	3.616069	-1.248607
H	-1.275788	2.078313	-1.455195
C	-4.753543	2.992140	-0.006993
H	-4.812266	0.970371	0.724775
C	-4.028498	3.947833	-0.719043
H	-2.206173	4.357362	-1.799518
H	-5.723240	3.245311	0.413287
H	-4.431747	4.947304	-0.856868
H	0.003692	-2.903475	-2.194810
H	0.007274	-3.549742	-2.569490

7-L3

(U)B3LYP-D3(BJ) SCF energy: -1620.34217594 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1619.739374 a.u.

(U)B3LYP-D3(BJ) free energy: -1619.845411 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1620.77230048 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1620.169499 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1620.275536 a.u.

Cartesian coordinates

ATOM X Y Z

Co	-1.131798	-0.116099	-0.368173
N	-3.227673	-0.108420	-0.183329
C	-3.303615	-2.325789	0.874506
C	-3.882259	-1.125678	0.513672
C	-3.951256	0.987536	-0.548956
C	-3.280430	1.978536	-1.479644
H	-3.968982	2.794743	-1.706940
H	-3.026643	1.469205	-2.417539
N	-2.050661	2.571352	-0.958835
C	-0.989574	1.791936	-0.605261
C	-1.805664	3.919025	-0.738700
C	-0.546524	4.006233	-0.237059
H	-2.533781	4.683904	-0.960171
H	0.043799	4.854091	0.071938
N	-0.060963	2.700740	-0.164919
H	-3.894278	-3.061148	1.403165
N	-1.984771	-2.738211	0.633741
C	-1.526257	-4.025658	0.916046
C	-0.972185	-1.962208	0.133970
C	-0.205356	-4.065561	0.592947
H	-2.180559	-4.786908	1.310699
H	0.516963	-4.864460	0.649956
N	0.117709	-2.807698	0.115275

C	1.221700	2.335311	0.359615
C	2.335479	2.366901	-0.490484
C	1.321676	1.948277	1.703670
C	3.581717	2.042206	0.049091
C	2.588475	1.624219	2.197074
C	3.728316	1.677794	1.390210
H	4.456258	2.064527	-0.596317
H	2.683877	1.321594	3.237178
C	1.412639	-2.371142	-0.306185
C	2.334984	-1.954652	0.662863
C	1.707200	-2.330062	-1.677375
C	3.588686	-1.514982	0.231073
C	2.966585	-1.865554	-2.063478
C	3.918231	-1.454239	-1.124435
H	4.316661	-1.197509	0.971582
H	3.209416	-1.825496	-3.123159
C	2.177647	2.704413	-1.950920
H	1.513249	1.983209	-2.441044
H	1.733228	3.695626	-2.095941
H	3.144765	2.684533	-2.461422
C	5.090344	1.361078	1.957762
H	5.556036	2.254195	2.394705
H	5.028151	0.608023	2.750765

H	5.767636	0.985976	1.183605
C	0.095963	1.858031	2.576360
H	-0.489560	2.783640	2.547501
H	-0.568440	1.055666	2.230331
H	0.371729	1.654582	3.615014
C	0.682967	-2.758296	-2.696980
H	0.301079	-3.762895	-2.483345
H	-0.181825	-2.084516	-2.684343
H	1.111001	-2.756820	-3.703688
C	1.965013	-1.947607	2.123845
H	1.069697	-1.337711	2.288298
H	1.736979	-2.953784	2.493707
H	2.778134	-1.534984	2.727254
C	5.257947	-0.922731	-1.571478
H	5.168600	0.110540	-1.931391
H	5.982563	-0.923235	-0.750777
H	5.674415	-1.516429	-2.392828
C	-5.266863	1.204653	-0.214451
H	-5.781220	2.102751	-0.539009
C	-5.271027	-0.932564	0.882161
H	-5.764238	-1.724941	1.438469
C	-5.939775	0.200503	0.539989
H	-6.980349	0.334800	0.824202

7-L4

(U)B3LYP-D3(BJ) SCF energy: -1598.12308820 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1597.514066 a.u.

(U)B3LYP-D3(BJ) free energy: -1597.606687 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1598.44027919 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1597.831257 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1597.923878 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.003091	0.811594	-0.534847
P	1.851130	-0.405157	-0.015245
N	0.064111	1.546090	1.519660
C	-0.992754	1.020487	2.389375
C	1.415393	1.415634	2.077458
C	2.019995	0.028742	1.798960
C	1.975216	-2.280687	0.052991
C	3.180870	-2.838900	0.818373
C	1.869019	-2.900667	-1.346543
C	3.481296	0.119534	-0.801365

C	3.301684	0.196840	-2.326435
C	3.969321	1.475077	-0.271600
H	-1.174860	1.688954	3.247590
H	1.426082	1.610192	3.162931
H	2.029696	2.187374	1.607202
H	1.459540	-0.736459	2.350801
H	3.054899	-0.018418	2.156284
H	4.123654	-2.593147	0.317131
H	3.120712	-3.933193	0.876771
H	3.233734	-2.453990	1.841572
H	1.043041	-2.464373	-1.918652
H	1.702106	-3.982358	-1.273690
H	2.791857	-2.751491	-1.917326
H	2.976432	-0.752951	-2.759767
H	4.247981	0.478125	-2.805516
H	2.552483	0.954557	-2.580275
H	3.220394	2.253954	-0.449489
H	4.886497	1.769454	-0.796516
H	4.196312	1.448287	0.798714
H	-0.652622	0.065638	2.802621
C	-2.296699	0.808318	1.610032
H	-3.060985	0.355904	2.253495
H	-2.680443	1.781246	1.281253

P	-1.979185	-0.184920	0.052269
C	-2.422959	-1.937574	0.580600
C	-3.429087	0.362467	-1.015719
C	-1.674234	-2.341714	1.857112
H	-1.859072	-3.398888	2.084343
H	-0.592515	-2.211770	1.744711
H	-1.994844	-1.756685	2.724166
C	-2.120996	-2.919911	-0.558604
H	-2.333766	-3.949663	-0.244949
H	-2.721237	-2.712943	-1.449296
H	-1.066326	-2.864666	-0.849542
C	-3.188527	0.031035	-2.494973
H	-3.963294	0.494618	-3.118138
H	-2.215471	0.407319	-2.826073
H	-3.220142	-1.048007	-2.681815
C	-4.813064	-0.094715	-0.544374
H	-4.947752	-1.173635	-0.682540
H	-4.985504	0.134085	0.513280
H	-5.597229	0.406242	-1.125640
H	-3.370824	1.454744	-0.920813
H	-3.497355	-1.965866	0.799219
H	1.065305	-2.554483	0.602214
H	4.240284	-0.637225	-0.565334

N	-0.130477	3.913025	-0.018244
H	-0.960963	4.500092	-0.090549
H	0.651475	4.567217	-0.035573
H	-0.106375	2.540008	1.250866
B	-0.052562	2.962756	-1.239685
H	-1.045902	2.179774	-1.198803
H	-0.053095	3.463443	-2.351168
H	0.995999	2.265717	-1.151406

7-L5

(U)B3LYP-D3(BJ) SCF energy: -2050.59584245 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2050.000379 a.u.

(U)B3LYP-D3(BJ) free energy: -2050.101131 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2051.03175460 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2050.436291 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2050.537043 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Co	0.086088	-1.525041	0.196537
P	1.833342	-0.085199	-0.053462

N	0.230433	-1.832083	-1.953278
C	-0.799225	-1.166071	-2.760009
C	1.603122	-1.570116	-2.403633
C	2.100044	-0.204706	-1.909010
H	-0.993420	-1.717764	-3.693953
H	1.691729	-1.622077	-3.501382
H	2.234076	-2.363930	-1.991256
H	1.521241	0.602368	-2.371679
H	3.150662	-0.052720	-2.177630
H	-0.423750	-0.182080	-3.057918
C	-2.109528	-0.999546	-1.982479
H	-2.818135	-0.379338	-2.542563
H	-2.572246	-1.980757	-1.828332
P	-1.811501	-0.339352	-0.249952
C	3.517611	-0.487474	0.585674
C	3.872333	-1.843879	0.669405
C	4.452600	0.481403	0.976511
C	5.141750	-2.219294	1.107960
H	3.141748	-2.604938	0.412403
C	5.718013	0.102470	1.426811
H	4.192223	1.533593	0.935123
C	6.068742	-1.246983	1.487882
H	5.400847	-3.272973	1.165741

H	6.430289	0.864884	1.731031
H	7.054694	-1.539523	1.838296
C	1.693277	1.722313	0.223032
C	2.353570	2.676223	-0.565730
C	0.856373	2.161497	1.257904
C	2.180392	4.038836	-0.322642
H	3.009249	2.355397	-1.370100
C	0.687254	3.522389	1.505859
H	0.316760	1.427034	1.848888
C	1.347566	4.462961	0.714509
H	2.695240	4.768611	-0.941785
H	0.021554	3.848007	2.299101
H	1.205871	5.524228	0.898551
C	-1.985629	1.486044	-0.422207
C	-1.262905	2.172557	-1.410800
C	-2.726612	2.237627	0.502499
C	-1.296128	3.562651	-1.488111
H	-0.652823	1.621637	-2.117862
C	-2.757443	3.630474	0.427577
H	-3.289088	1.731648	1.280247
C	-2.046043	4.298209	-0.569186
H	-0.722534	4.071964	-2.256908
H	-3.341944	4.193322	1.150569

H	-2.066970	5.382837	-0.624516
C	-3.390067	-0.795929	0.573538
C	-4.640163	-0.416594	0.059172
C	-3.340517	-1.567155	1.741532
C	-5.815324	-0.803969	0.699652
H	-4.691715	0.195897	-0.836706
C	-4.518291	-1.953797	2.385255
H	-2.376672	-1.876977	2.133863
C	-5.755295	-1.573892	1.865096
H	-6.777699	-0.505411	0.292894
H	-4.466695	-2.554049	3.289159
H	-6.672008	-1.875678	2.364165
N	0.034446	-4.449314	-0.933526
H	0.820192	-5.094521	-1.008350
H	0.076606	-2.864481	-1.887137
H	-0.794841	-5.035145	-1.024823
B	0.037533	-3.761711	0.454098
H	-0.002001	-4.470840	1.443446
H	1.075924	-3.047020	0.558405
H	-0.967053	-2.996016	0.516486

TS4-L3

(U)B3LYP-D3(BJ) SCF energy: -2006.46650436 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2005.695501 a.u.

(U)B3LYP-D3(BJ) free energy: -2005.817825 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2007.00851923 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2006.237516 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2006.359840 a.u.

Imaginary frequency: -1160.9570 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	0.848340	-0.100517	0.189470
N	2.493934	0.147441	-1.187163
C	2.262008	-2.219797	-1.533260
C	2.920429	-0.958688	-1.851860
C	3.181013	1.292048	-1.284148
C	2.773913	2.383826	-0.321470
H	3.317100	3.304859	-0.545035
H	3.062648	2.065937	0.686127
H	2.281830	-1.701977	2.999038
N	1.351174	2.696391	-0.321836
C	0.365352	1.780174	-0.019147
C	0.845965	3.961251	-0.586782

C	-0.495502	3.873269	-0.452659
H	1.481545	4.798499	-0.830099
H	-1.273297	4.613316	-0.546241
N	-0.779094	2.547008	-0.114950
H	2.697695	-3.072681	-2.052796
H	2.273248	-2.153458	-0.041941
N	0.806356	-2.284196	-1.674233
C	0.149487	-3.315554	-2.329989
C	-0.055717	-1.512839	-0.947160
C	-1.164417	-3.216154	-2.007323
H	0.672239	-4.019659	-2.958694
H	-2.017670	-3.818149	-2.275714
N	-1.275739	-2.105628	-1.168538
C	-2.138896	2.135719	0.059131
C	-2.614037	1.779210	1.328967
C	-3.003090	2.250957	-1.043931
C	-3.995223	1.632837	1.492765
C	-4.373593	2.107639	-0.826609
C	-4.891488	1.831969	0.441669
H	-4.378178	1.378428	2.477893
H	-5.052660	2.218194	-1.669614
C	-2.465214	-1.862687	-0.409854
C	-3.606484	-1.383522	-1.062063

C	-2.490236	-2.240565	0.945161
C	-4.801449	-1.314328	-0.339148
C	-3.699009	-2.122015	1.632423
C	-4.867667	-1.677944	1.005585
H	-5.697300	-0.960995	-0.843366
H	-3.736089	-2.418153	2.678674
C	-1.677224	1.584693	2.491859
H	-1.070466	0.682821	2.352078
H	-0.975565	2.420512	2.587755
H	-2.236067	1.486178	3.427288
C	-6.382353	1.745422	0.653985
H	-6.886539	2.648678	0.290346
H	-6.815660	0.894630	0.115173
H	-6.629396	1.625961	1.712913
C	-2.470279	2.521837	-2.430806
H	-2.235945	3.580961	-2.591262
H	-1.547882	1.960249	-2.610425
H	-3.207616	2.228735	-3.183776
C	-1.276765	-2.826446	1.620592
H	-0.916788	-3.708083	1.076258
H	-0.431026	-2.133636	1.645240
H	-1.518784	-3.130673	2.643724
C	-3.554382	-0.972920	-2.511796

H	-2.633730	-0.424397	-2.728757
H	-3.577047	-1.839846	-3.184253
H	-4.407210	-0.334710	-2.760351
C	-6.157848	-1.585638	1.782412
H	-6.157592	-0.714147	2.449452
H	-7.021905	-1.489232	1.117654
H	-6.309353	-2.471508	2.409543
C	4.308673	1.433700	-2.088060
H	4.835903	2.380919	-2.135862
C	4.078657	-0.890669	-2.657633
H	4.410468	-1.780683	-3.183533
C	4.763208	0.308132	-2.783513
H	5.642639	0.373731	-3.419084
C	2.835451	-1.812381	2.053826
O	1.872904	-1.803005	1.018321
C	3.801579	-0.638502	1.970223
C	3.708560	0.412535	2.889662
C	4.788778	-0.570853	0.978830
C	4.583855	1.500495	2.833194
H	2.944374	0.372165	3.662582
C	5.661365	0.513476	0.912612
H	4.863601	-1.361764	0.239762
C	5.565804	1.552473	1.842909

H	4.498082	2.303319	3.560876
H	6.411672	0.550878	0.128533
H	6.250204	2.395205	1.793935
C	3.557954	-3.163759	2.089545
H	4.262885	-3.216556	2.927141
H	2.820982	-3.966542	2.192823
H	4.114752	-3.334863	1.161925

TS4-L4

(U)B3LYP-D3(BJ) SCF energy: -1598.10691221 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1597.499732 a.u.

(U)B3LYP-D3(BJ) free energy: -1597.593358 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1598.42847663 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1597.821296 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1597.914922 a.u.

Imaginary frequency: -129.6137 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	0.040458	-0.302117	-0.405146
P	-2.164310	0.255867	-0.013615

N	0.001418	-1.208943	1.561887
C	0.899705	-0.517145	2.487347
C	-1.358874	-1.434135	2.060589
C	-2.279970	-0.232092	1.786302
C	-2.619417	2.074472	0.061428
C	-3.954735	2.376799	0.752492
C	-2.545239	2.720200	-1.328230
C	-3.592186	-0.569432	-0.912556
C	-3.227867	-0.688076	-2.401682
C	-3.924856	-1.953553	-0.339274
H	0.985344	-1.054801	3.447512
H	-1.362298	-1.659895	3.139627
H	-1.743542	-2.316304	1.541915
H	-1.932691	0.637124	2.359686
H	-3.304379	-0.441722	2.112145
H	-4.799674	1.970945	0.185356
H	-4.105218	3.460835	0.828883
H	-3.997799	1.961771	1.764325
H	-1.590945	2.502414	-1.819841
H	-2.651624	3.808835	-1.249074
H	-3.350790	2.358741	-1.976961
H	-2.994446	0.282061	-2.851401
H	-4.064919	-1.125912	-2.959593

H	-2.353848	-1.336052	-2.524284
H	-3.061042	-2.620873	-0.417343
H	-4.744833	-2.399056	-0.915574
H	-4.244003	-1.907429	0.706702
H	0.487162	0.474185	2.713911
B	0.152059	-2.918980	-1.119555
H	0.476990	-3.440122	-2.179470
H	0.459424	-1.692391	-1.340891
H	-1.050614	-3.013303	-0.930467
N	0.919992	-3.423689	0.138801
H	0.590191	-4.357830	0.378957
H	1.910902	-3.541881	-0.072906
H	0.421927	-2.124391	1.248184
C	2.289157	-0.377409	1.850294
H	2.940092	0.251040	2.468871
H	2.750236	-1.369518	1.788555
P	2.147779	0.263262	0.091156
C	2.678983	2.053042	0.272128
C	3.577003	-0.621689	-0.741362
C	4.967822	-0.168570	-0.284253
H	5.740246	-0.821706	-0.708714
H	5.185601	0.852246	-0.617814
H	5.071124	-0.195371	0.806435

C	3.428829	-0.618116	-2.268981
H	2.447067	-1.001084	-2.561648
H	3.547605	0.386204	-2.689214
H	4.196368	-1.257608	-2.722167
C	1.676835	2.785786	1.175141
H	0.663627	2.722808	0.758484
H	1.650602	2.369564	2.187116
H	1.942420	3.846874	1.257492
C	2.765053	2.740004	-1.096434
H	1.817067	2.641863	-1.639699
H	2.974706	3.810019	-0.974775
H	3.554753	2.315371	-1.722279
H	-4.473176	0.076380	-0.804704
H	-1.810464	2.499796	0.672788
H	3.420521	-1.656570	-0.408228
H	3.666291	2.077736	0.751208

TS4-L5

(U)B3LYP-D3(BJ) SCF energy: -2050.58047468 a.u.

(U)B3LYP-D3(BJ) enthalpy: -2049.986708 a.u.

(U)B3LYP-D3(BJ) free energy: -2050.088306 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -2051.01908373 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -2050.425317 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -2050.526915 a.u.

Imaginary frequency: -31.9827 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-0.015701	-0.749400	0.009478
P	-2.181241	-0.171136	0.105361
N	-0.045105	-0.490880	2.164600
C	1.189767	0.035926	2.754694
C	-1.262212	0.139100	2.690583
C	-2.485956	-0.388751	1.935055
H	1.266469	-0.215062	3.825880
H	-1.184898	1.226150	2.556593
H	-1.381347	-0.049242	3.770599
H	-3.402391	0.113130	2.262894
H	-2.604020	-1.462552	2.111387
H	1.169835	1.130605	2.680767
B	0.068726	-3.508491	0.778705
H	-0.573387	-4.382093	0.209532
H	1.271005	-3.695298	0.708576
H	-0.203654	-2.474016	0.055845

N	-0.340973	-3.257875	2.256937
H	-1.303356	-3.544330	2.430833
H	0.226953	-3.830722	2.877167
H	-0.112384	-1.534705	2.352673
C	2.409633	-0.516880	2.007049
H	3.345473	-0.086701	2.380877
H	2.468485	-1.603428	2.137424
P	2.175038	-0.276911	0.177104
C	3.643908	-1.085078	-0.560672
C	4.866155	-0.420003	-0.732603
C	3.523574	-2.426873	-0.952800
C	5.956649	-1.090549	-1.285695
H	4.961884	0.622289	-0.442946
C	4.620551	-3.095080	-1.497431
H	2.577567	-2.942023	-0.813732
C	5.835665	-2.428786	-1.667212
H	6.900115	-0.568367	-1.420160
H	4.521914	-4.135351	-1.794443
H	6.686195	-2.949086	-2.099116
C	2.468799	1.514376	-0.116821
C	2.989355	2.396514	0.839204
C	2.090273	2.027365	-1.369426
C	3.117127	3.758470	0.555753

H	3.297801	2.027611	1.811883
C	2.228744	3.383468	-1.658197
H	1.680418	1.353074	-2.117829
C	2.736689	4.255243	-0.690889
H	3.516663	4.430008	1.310638
H	1.936497	3.760719	-2.634321
H	2.836522	5.314588	-0.909421
C	-3.565302	-1.085622	-0.669604
C	-3.480349	-2.488957	-0.629234
C	-4.646213	-0.482697	-1.325259
C	-4.481939	-3.267948	-1.204944
H	-2.616444	-2.967499	-0.174041
C	-5.641026	-1.269131	-1.909677
H	-4.710094	0.598269	-1.389661
C	-5.566020	-2.660606	-1.843999
H	-4.406259	-4.350987	-1.167162
H	-6.474307	-0.791166	-2.417711
H	-6.341938	-3.270048	-2.298882
C	-2.520490	1.620589	-0.110346
C	-3.685780	2.251057	0.354308
C	-1.508571	2.406710	-0.679061
C	-3.837684	3.632083	0.236704
H	-4.477308	1.661867	0.808900

C	-1.653010	3.790315	-0.786548
H	-0.593862	1.931629	-1.020920
C	-2.820626	4.404066	-0.332423
H	-4.745875	4.108389	0.595653
H	-0.848304	4.381611	-1.214171
H	-2.938338	5.481052	-0.413809

TS5-L3

(U)B3LYP-D3(BJ) SCF energy: -1621.48874422 a.u.

(U)B3LYP-D3(BJ) enthalpy: -1620.872527 a.u.

(U)B3LYP-D3(BJ) free energy: -1620.974867 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -1621.91866632 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -1621.302449 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -1621.404789 a.u.

Imaginary frequency: -1313.9546 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.552013	-0.210561	-1.087985
N	-3.416491	-0.221125	-0.143873
C	-3.036831	-2.582256	-0.001311

C	-3.862340	-1.425403	0.307132
C	-4.246950	0.839411	-0.133055
C	-3.749403	2.056638	-0.882600
H	-4.435706	2.896228	-0.749617
H	-3.717616	1.808745	-1.951903
H	-2.305841	-1.594520	-2.077793
N	-2.419604	2.489523	-0.479865
C	-1.308943	1.682985	-0.592214
C	-2.150546	3.681977	0.177971
C	-0.832628	3.658775	0.482055
H	-2.907279	4.431670	0.350013
H	-0.197194	4.375392	0.977236
N	-0.334755	2.443072	0.007798
H	-3.509498	-3.534705	0.231810
H	-2.786121	-2.217103	-1.377089
N	-1.645204	-2.625815	0.372932
C	-1.020402	-3.790705	0.807615
C	-0.736126	-1.677955	-0.032380
C	0.312497	-3.585560	0.697798
H	-1.578575	-4.648136	1.150193
H	1.149640	-4.228192	0.915647
N	0.482176	-2.292117	0.200685
C	1.008876	2.051662	0.318009

C	2.027452	2.263125	-0.617893
C	1.272608	1.589407	1.615178
C	3.347229	2.076226	-0.199554
C	2.606952	1.434854	1.993938
C	3.656152	1.698938	1.109812
H	4.151891	2.241883	-0.911881
H	2.830780	1.095039	3.002125
C	1.777528	-1.804103	-0.159610
C	2.770369	-1.740362	0.830629
C	2.074252	-1.515459	-1.506054
C	4.078731	-1.432941	0.445783
C	3.388920	-1.176413	-1.831414
C	4.409063	-1.146460	-0.877253
H	4.852021	-1.395732	1.208987
H	3.625536	-0.956457	-2.870291
C	1.700245	2.680998	-2.028051
H	1.096318	1.915535	-2.528201
H	1.115626	3.608131	-2.047847
H	2.613118	2.836411	-2.610238
C	5.090129	1.595523	1.566381
H	5.749584	1.280068	0.752647
H	5.457935	2.564610	1.929135
H	5.197199	0.879192	2.387306

C	0.140754	1.248905	2.550818
H	-0.485803	2.120372	2.774099
H	-0.509862	0.495482	2.090261
H	0.524586	0.853645	3.495954
C	1.037312	-1.601525	-2.594051
H	0.411280	-2.492041	-2.492634
H	0.347519	-0.747093	-2.565367
H	1.516316	-1.615709	-3.578245
C	2.453200	-1.978830	2.287080
H	1.471800	-1.572526	2.547574
H	2.440062	-3.044734	2.545511
H	3.205775	-1.499129	2.919859
C	5.818411	-0.781694	-1.273229
H	5.897527	0.286445	-1.515871
H	6.528508	-0.991528	-0.467077
H	6.142185	-1.335700	-2.161973
C	-5.528111	0.786857	0.393410
H	-6.159589	1.669922	0.393681
C	-5.169171	-1.550562	0.825418
H	-5.508324	-2.520549	1.176071
C	-5.994123	-0.441707	0.889673
H	-6.992936	-0.520627	1.309588

NH2-BH2

(U)B3LYP-D3(BJ) SCF energy: -82.04135885 a.u.

(U)B3LYP-D3(BJ) enthalpy: -81.989121 a.u.

(U)B3LYP-D3(BJ) free energy: -82.015727 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -82.08003005 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -82.027792 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -82.054398 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	-0.612255	0.000000	0.000134
H	-1.167813	-0.844837	0.000465
H	-1.167816	0.844834	-0.001206
B	0.780232	0.000000	0.000009
H	1.360128	-1.047113	-0.000794
H	1.360128	1.047113	0.000554

NH3-BH3

(U)B3LYP-D3(BJ) SCF energy: -83.21722354 a.u.

(U)B3LYP-D3(BJ) enthalpy: -83.142236 a.u.

(U)B3LYP-D3(BJ) free energy: -83.169469 a.u.

(U)B3LYP-D3(BJ) SCF energy in solution: -83.27369637 a.u.

(U)B3LYP-D3(BJ) enthalpy in solution: -83.198709 a.u.

(U)B3LYP-D3(BJ) free energy in solution: -83.225942 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.000000	0.000000	0.730656
H	0.523152	-0.795479	1.097056
H	-0.950481	-0.055323	1.097056
H	0.427329	0.850803	1.097056
B	0.000000	0.000000	-0.936657
H	1.170591	0.069424	-1.240824
H	-0.525172	-1.048473	-1.240824
H	-0.645418	0.979049	-1.240824