

Density functional study of chiral phosphoric acid-catalyzed direct arylation of trifluoromethyl ketone and diarylation of methyl ketones: reaction mechanism and the important role of CF₃ group

Aiping Fu,^{*a} Wei Meng,^b Hongliang Li,^a Jing Nie,^b and Jun-An Ma^{*b}

^a Institute for Computational Science and Engineering, Laboratory of New Fiber Materials and Modern Textile, the Growing Base for State Key Laboratory, Qingdao University, Qingdao 266071, China

^b Department of Chemistry, Key Laboratory of Systems Bioengineering (the Ministry of Education), State Synergetic Innovation Center of Chemical Science and Engineering, Tianjin University, Tianjin 300072, China

Supplementary Information

* Corresponding author. E-mail: faplh1@eyou.com; Fax: 86-532-85950768; majun_an68@tju.edu.cn

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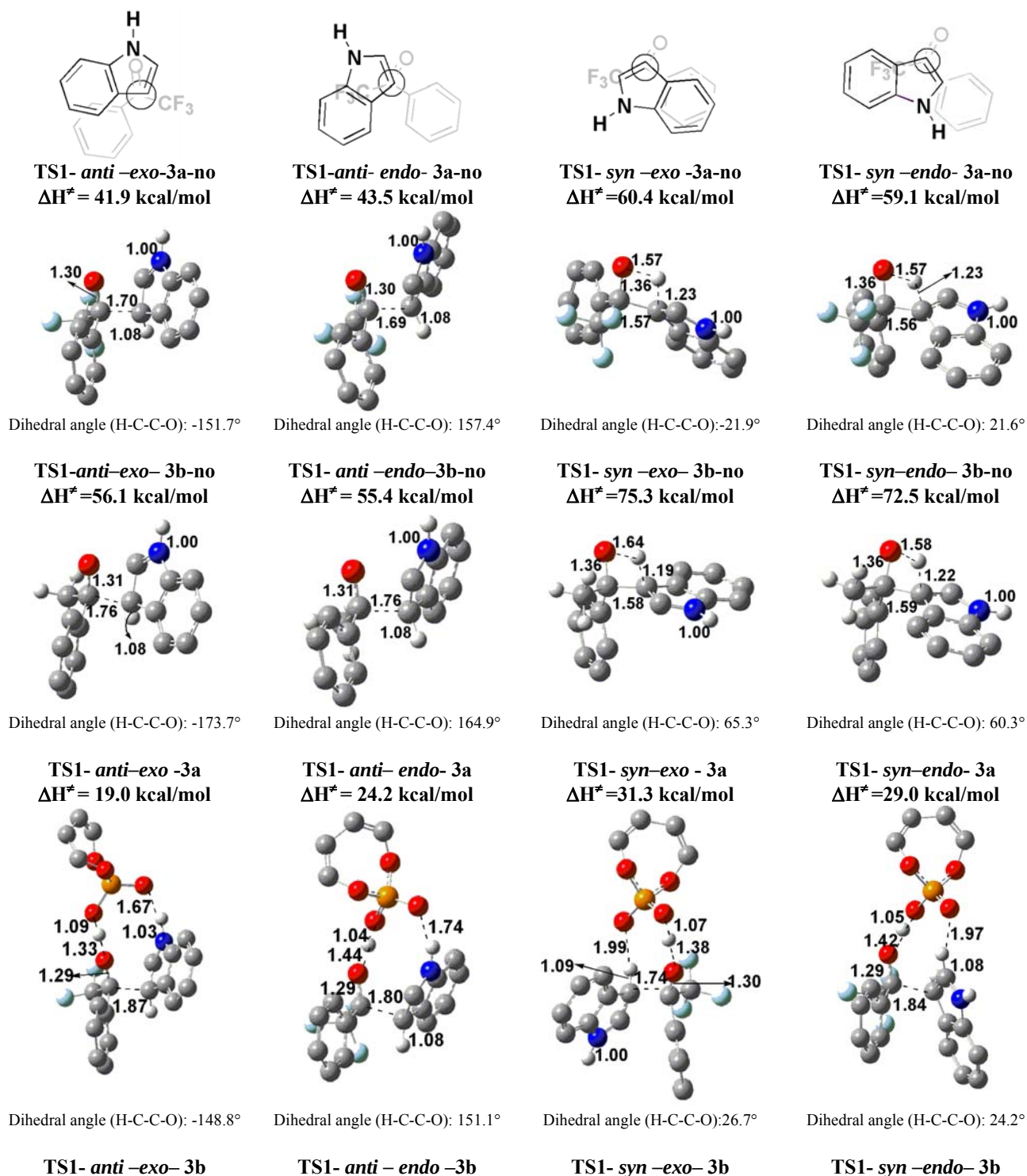
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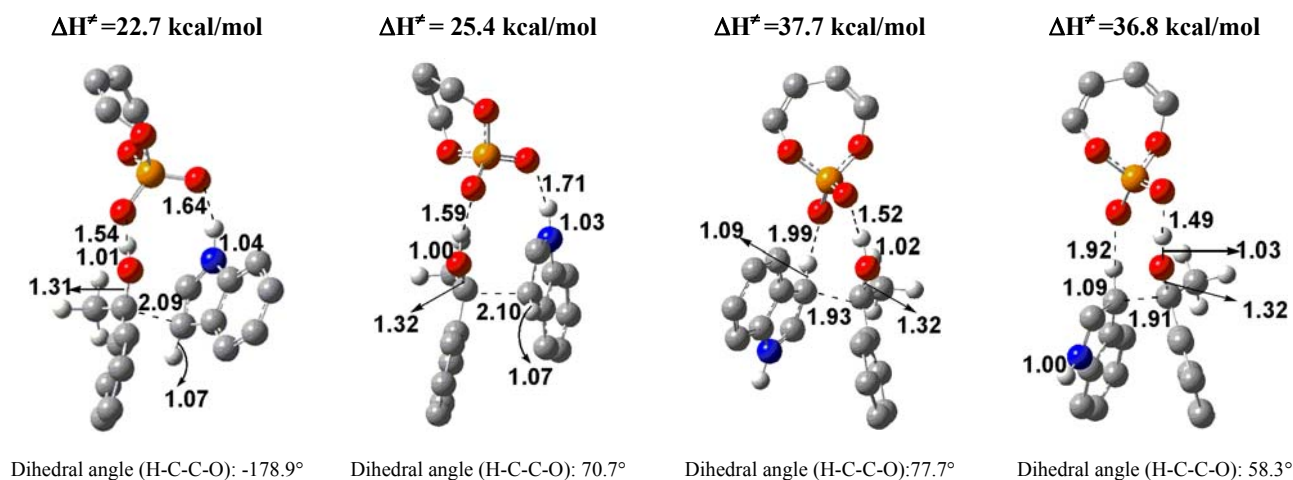
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Fig. S1 BH and HLYP/6-31G (d) computed transition states and activation energies of the C-C bond-forming step for the uncatalyzed and simplified model of chiral phosphoric acid-catalyzed Friedel-Crafts reaction between indole and acetophenone or 2,2,2-trifluoroacetophenone.





Note: Four transition states in the absence of the catalyst depending on the different orientations of the nucleophile and the electrophile for the reactions of indole with **3a** and **3b** has been localized and presented in **Fig. S1**. The notation used for the TSs, for example, “TS1” and “3a” in “TS1-3a-*anti*-exo-no” means the TS of the C-C bond forming step involved in the first Friedel-Crafts stage between **3a** and indole, “*anti*” denotes as the hydrogen atom of the C-H at β position in indole in the opposite direction as the oxygen atom of the carbonyl group, while “*exo*” means the aromatic ring of indole is in the same side with the phenyl group of ketone, “no” means the uncatalyzed process. As shown in **Fig. S1**, when the hydrogen atom of the C-H at β position in indole is in the same direction with the oxygen atom of the carbonyl moiety e.g. “TS1-*syn*-exo” and “TS1-*syn*-endo”, the four-membered-ring transition states for the reaction, in which the formation of the C-C bond and the hydrogen atom transfer take place simultaneously, have been characterized for the uncatalyzed Friedel-Crafts reaction of **3a** and **3b**. In these TSs, the C-C bond being formed is calculated to be 1.56~1.59 Å which indicates a very late transition state for the reaction, and the aromatic C-H bond has increased from 1.07 Å to 1.20~1.23 Å. The O-H bond going to be formed is around 1.57~1.64 Å while the carbonyl bond becomes 1.36 Å. The transition state energy is calculated to be 60~75 kcal/mol which is significantly high to be overcome. When the incoming C-H bond of indole is *anti* to the carbonyl group, whether for the substrate **3a** or **3b**,

the TSs are relatively earlier than the above *syn* ones. For example, in TSs involving **3a**, the lengths of the forming C-C bond are 1.69 Å and 1.70 Å in “*anti*”- TSs, while 1.56 Å and 1.57 Å in “*syn*”. The C=O bond changed to be about 1.30 Å in “*anti*” and about 1.36 Å in “*syn*”. The similar trend of the earlier *anti*-TSs has also been found for the reaction of indole with **3b**. Whether for CF₃ ketone or CH₃ ketone, the activation enthalpy of the *anti*-TSs is 15-20 kcal/mol lower than that of the *syn*-TSs. However, those *anti* barriers are still too high (around 40~60 kcal/mol) which is consistent with the fact that indole and **3a** or **3b** could not react in the absence of the catalyst.

Meanwhile, the corresponding TSs for this C-C bond-forming step of **3a** and **3b** in the presence of the simplified phosphoric acid model have also been illustrated in **Fig. S1**. Similar to the previous computational model in the chiral phosphoric acid-catalyzed Mannich, transfer hydrogenation, and hydrophosphonylation reactions etc.,⁷⁻¹³ the phosphoric acid also acts as a bifunctional catalyst, in which the acid proton of the catalyst activates the carbonyl group of the electrophile-ketone, while the phosphoryl oxygen atom forms hydrogen bond with the N-H moiety (or aromatic C-H) of the nucleophile-indole. Analogous to the uncatalyzed process, the relative orientation of C-H moiety at β-position in indole to the carbonyl group of ketone has great effect on the activation energy. The TSs involving the C-H *syn* to the C=O moiety are still much higher in energy (about 10~15 kcal/mol for CF₃ or CH₃ ketone) than those of the *anti* ones, which suggests the strong hydrogen bond donor ability of the NH moiety in indole. Therefore, the alternative mechanism of *syn*-channel in the phosphoric acid-catalyzed Friedel-Crafts reaction can be safely excluded and we only focus on the TSs of the *anti*-arrangements in the following discussion. Furthermore, as shown in **Fig. S1**, since indole is an unsymmetrical nucleophile, even keeping in the *anti*-conformation, there still have two orientations of the electrophile and nucleophile. We differentiate them as “*exo*” and “*endo*”. In the uncatalyzed process, the energy difference between “*exo*” and “*endo*” is relatively small, while in the presence of phosphoric

acid model, it increases with the “exo” orientation being more favorable than its “endo” counterpart. Hence, in the following description of the full mechanism in the paper, we have only used “**TS1-*anti-exo***” as the reference point. Compared the activation energies of the phosphoric acid-catalyzed reaction with that of the catalyst-free process, we can see that the transition state is stabilized by 22.7 kcal/mol (33.5 kcal/mol) for **3a** (**3b**), which is significant enough to suggest that the reaction could indeed take place at the benign conditions in the presence of the phosphoric acid catalyst.. The calculated FMO energies, which clearly exhibit the lowering of the LUMO of the electrophile and the heightening of the HOMO of the nucleophile when going from the bare **3a** (LUMO: -0.9 eV), **3b** (LUMO:-0.1 eV), and indole (HOMO:-6.4 eV) to the phosphoric acid bonded **3a** (LUMO:-1.2 eV), **3b** (LUMO:-0.6 eV), and indole (HOMO:-6.0 eV) in **IN1a** and **IN1b**, also support the simultaneous activation role of the phosphoric acid catalyst to both of the reaction partners. Moreover, if the structure of “TS1-*anti-exo*-3a” is compared with “TS1-*anti-exo*-3b”, the major difference between the reaction involving **3a** and **3b** is the earlier stage of the C-C bond forming and the complete proton transfer from phosphoric acid to carbonyl group in the latter. The presence of the electron-withdrawing CF₃ group in the substrate can greatly reduce the activation barrier whether for the catalyzed or catalyst-free process, which confirmed that the trifluoroacetophenone can be more reactive than acetophenone in the Friedel-Crafts reaction. The significant lowering of the LUMO ($\pi^* \text{C=O}$) energy from **3b** to **3a** for both the bare (-0.1 eV to -0.9 eV) and the phosphoric acid-bonded system (-0.6 eV in **IN1b** to -1.2 eV in **IN1a**) also suggests the more electrophilic nature of trifluoroacetophenone than acetophenone in the following nucleophilic addition process with indole because of the strong electron-withdrawing character of CF₃ group.

Fig. S2 BH and HLYP/6-31G (d) optimized structures of the intermediates and transition states for the simplified model of chiral phosphoric acid-catalyzed reaction between 2,2,2-trifluoroacetophenone and indole.

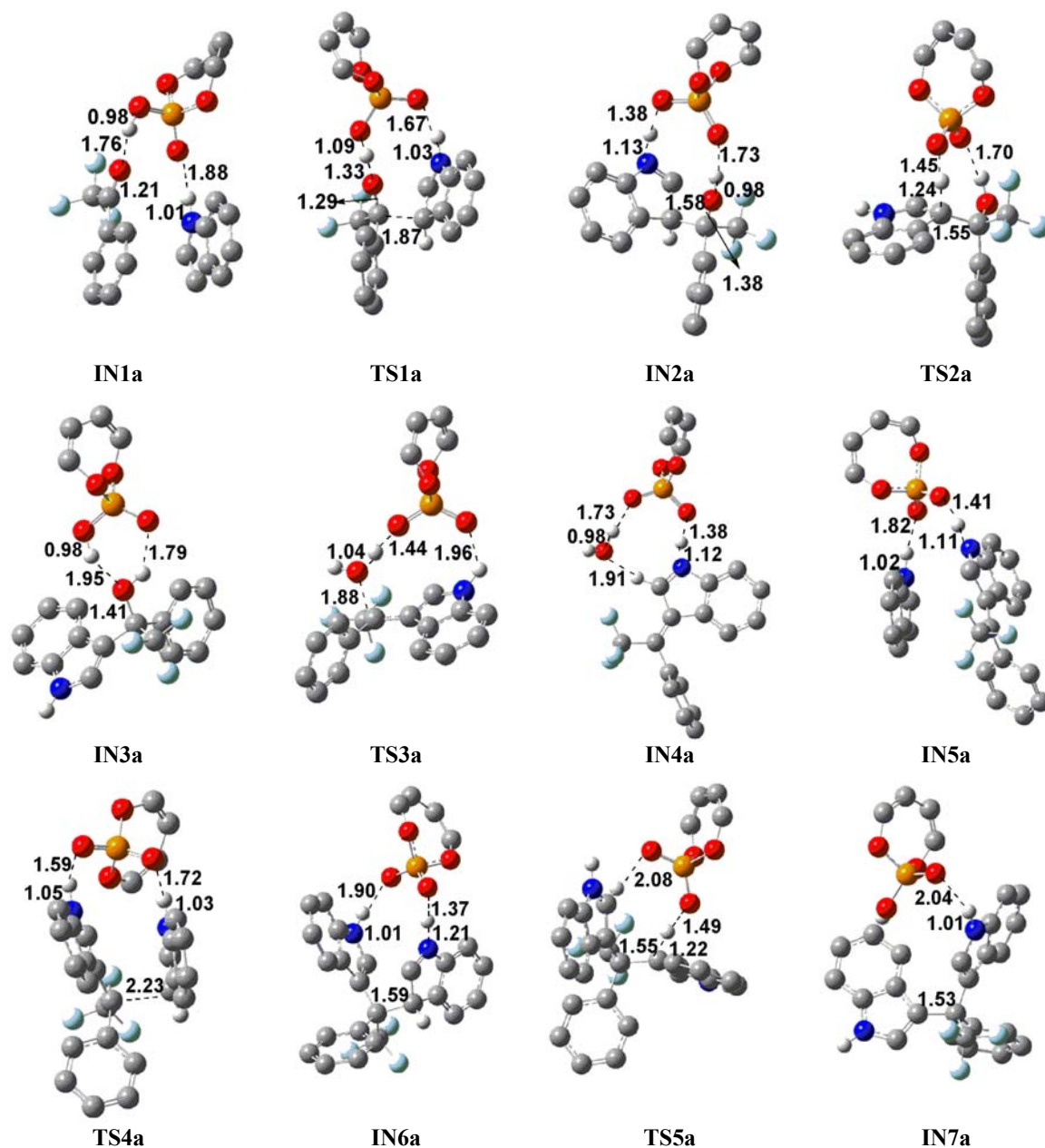


Figure S3. BH and HLYP/6-31G (d) optimized structures of the intermediates and transition states for the simplified model of chiral phosphoric acid-catalyzed reaction between acetophenone and indole.

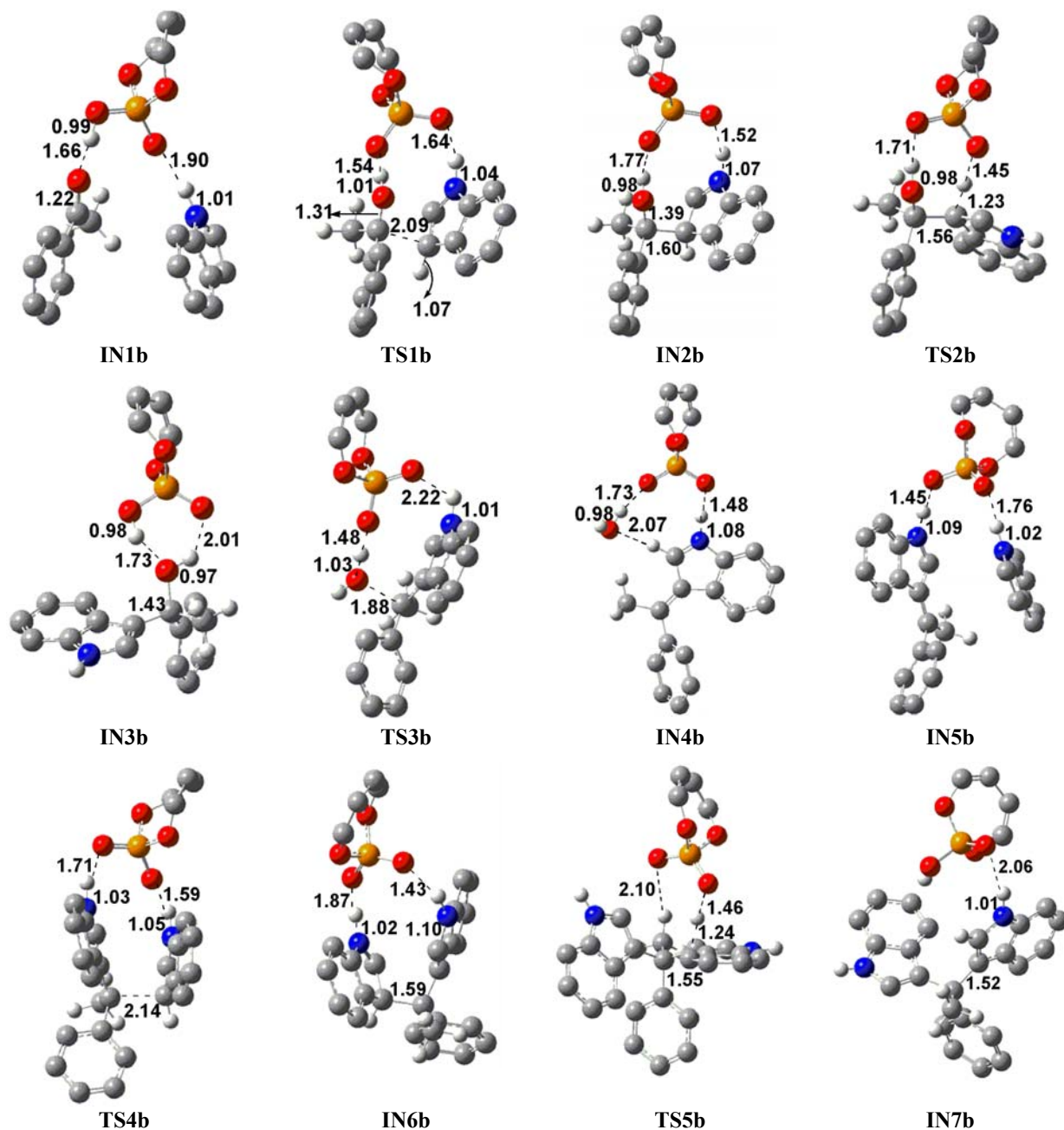


Fig. S4 BH and HLYP/6-31G (d) computed transition states and relative enthalpies for the C-C bond formation step of the simplified model (buta-1,3-diene-1,4-diol-phosphoric acid and biphenyl-phosphoric acid) of the chiral phosphoric acid-catalyzed Friedel-Crafts reaction between indole and 2,2,2-trifluoroacetophenone.

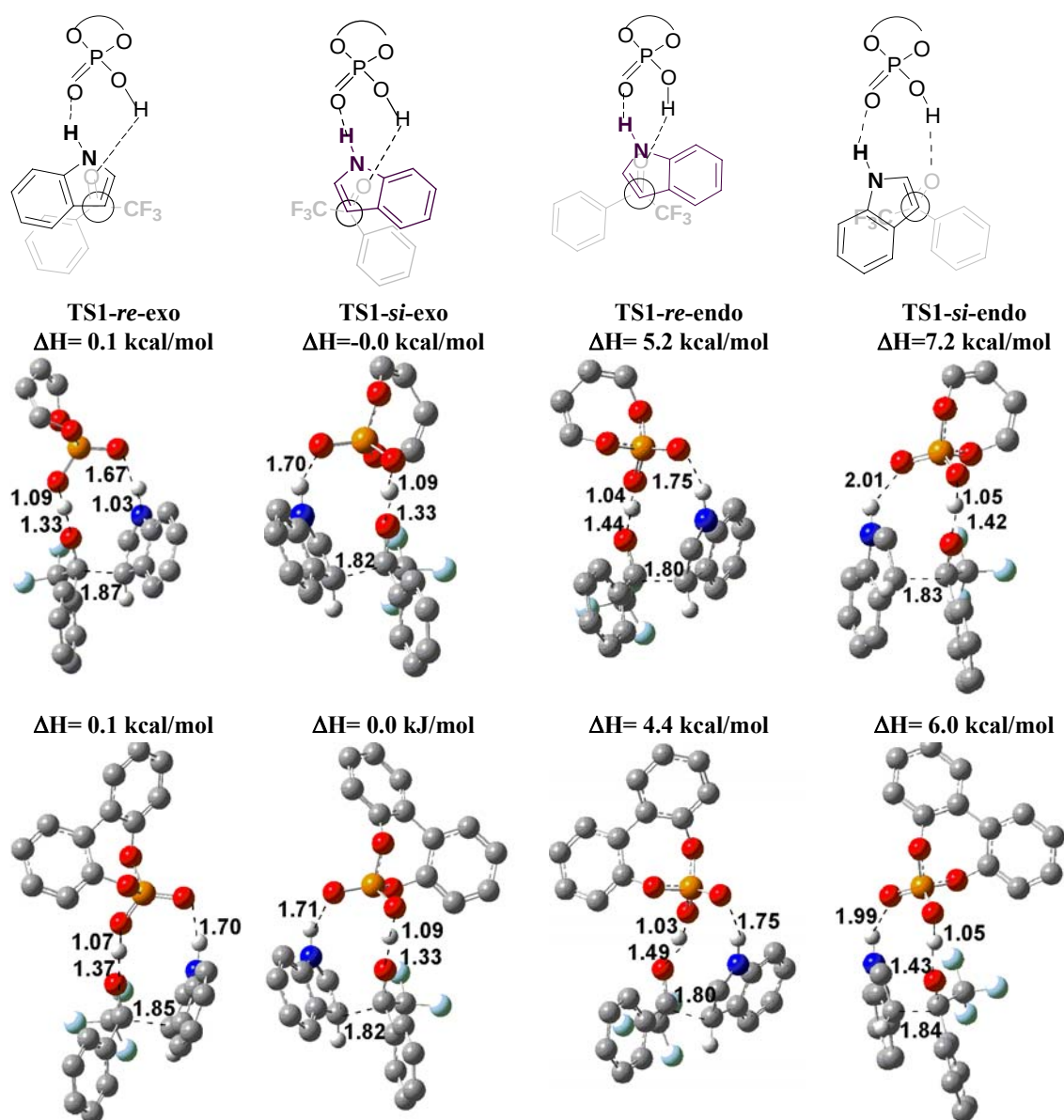
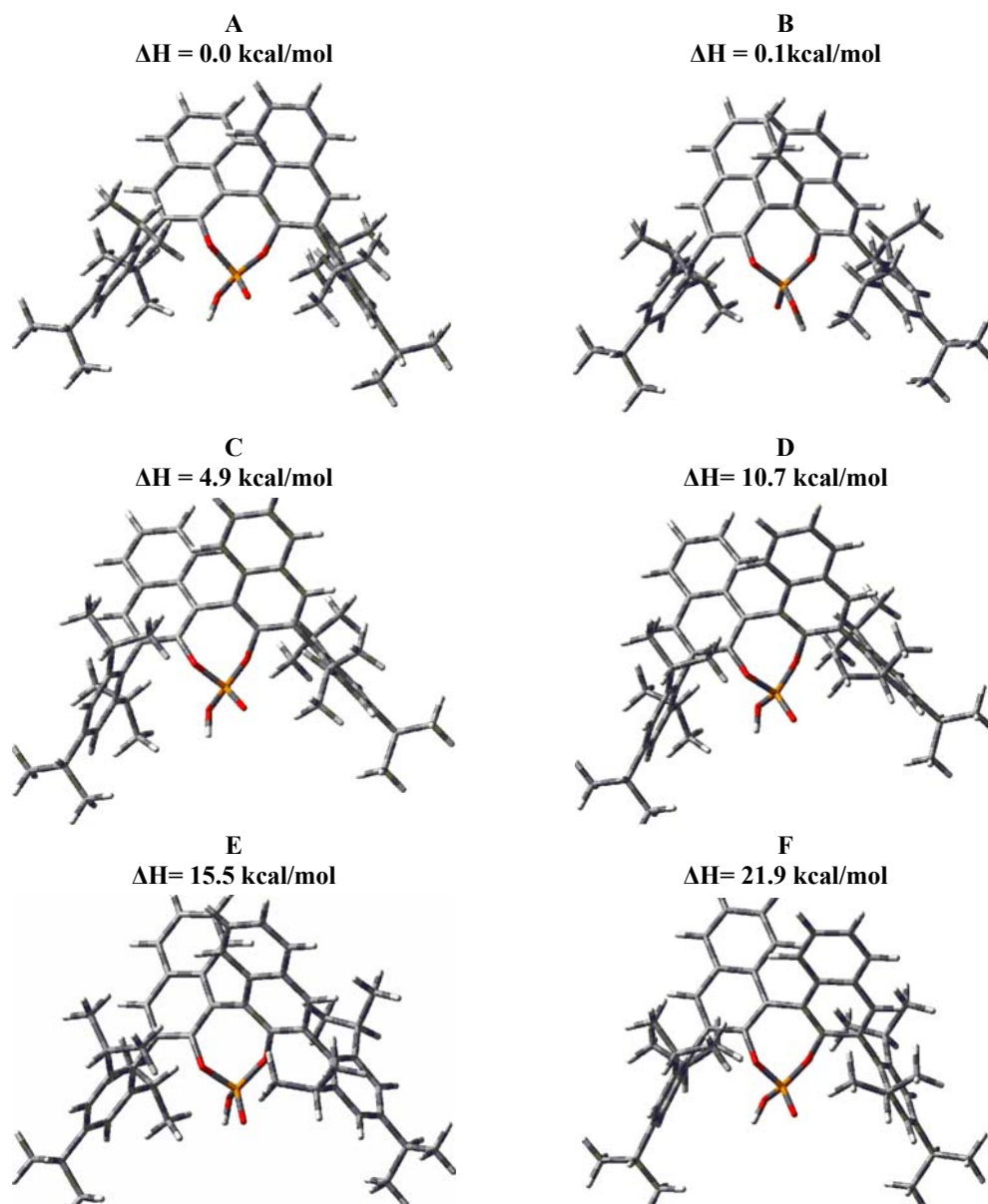


Table S1 Calculated LUMO energies (L_i :eV) and the activation enthalpies ($\Delta H_i^\ddagger$: kcal/mol) of the electrophiles in the first and second C-C bond-formation steps for the F-substituted ketones and common ketones and the correlation between the L_i and H_i .

	ketone		IN1		Cation in IN5		Zwitterion IN5	
	L_i	$\Delta H_i^\ddagger$	L_i	$\Delta H_i^\ddagger$	L_i	$\Delta H_i^\ddagger$	L_i	$\Delta H_i^\ddagger$
CF ₃	-0.93	41.9	-1.2	19	-6.2	0.9	-2.4	15.3
CHF ₂	-0.72	47.8	-0.98	19.1	-6.0	3.7	-2.2	17.6
CH ₂ F	-0.44	54.3	-0.67	19.8	-5.7	5.7	-2.3	19.4
CH ₃	-0.15	56.1	-0.63	22.7	-5.6	11	-2.0	21.2
Correlation between $\Delta H_i^\ddagger$ and L_i	$\Delta H_i^\ddagger = 18.68L_i + 60.36$ $R^2 = 0.9052$		$\Delta H_i^\ddagger = 4.74L_i + 24.27$ $R^2 = 0.3150$		$\Delta H_i^\ddagger = 14.36L_i + 89.70$ $R^2 = 0.7900$		$\Delta H_i^\ddagger = 12.31L_i + 45.77$ $R^2 = 0.5427$	

Note: To understand the relationship between the reactivities and the electrophilicities of the electrophiles, we have calculated the LUMO energies of the zwitterion structures IN5 and the cations in IN5 (Scheme 1) for CF₃, CHF₂ and CH₂F ketones and the common methyl ketone. The computed LUMO energies (L_i :eV) and the activation enthalpies($\Delta H_i^\ddagger$: kcal/mol) for this second C-C bond-formation step are presented in **Table S1**. The linear correlation between $\Delta H_i^\ddagger$ and L_i has been analyzed according to Yu's semiempirical FMO theory.²⁰ As shown in the Table, there is slightly better linear correlation between the activation energies and the LUMO energies for the cations in IN5 than for the zwitterion structures IN5 which can be attributed to the complexity of the phosphoric acid anion interacting with the different cations. The similar analysis has been carried out for the four ketones and their IN1 counterparts. As expected, the LUMO energies of the ketones also have a linear correlation with the corresponding activation energies. The different hydrogen bond abilities of the F-substituted ketones and the common methyl ketone result in the poor linear correlation in IN1, analogues to the case of the zwitterion structures IN5.

Fig. S5 BH and HLYP/6-31G (d) computed geometries and relative enthalpies for different conformers of chiral phosphoric acid catalyst which is determined by the conformation of the isopropyl groups on the 2,4,6-triisopropylphenyl substituents.



Note: we can assume that the conformation of the chiral phosphoric acid catalyst will determine the stability of the related transition states and subsequently the enantioselectivity. Therefore, the different

conformers with respect to the isopropyl groups on the 2,4,6-triisopropylphenyl substituents of catalyst **1** have been investigated first.

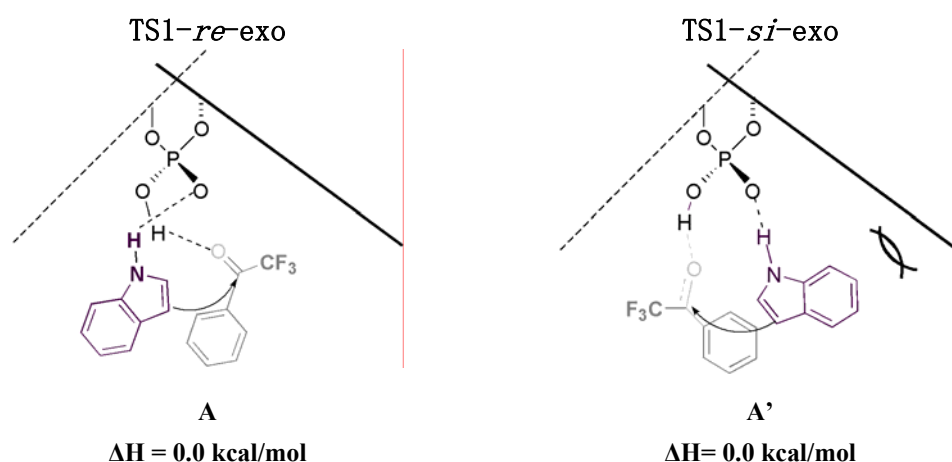
(1) The isopropyl group of the substituent contains two methyls and one H atom and the conformation with the isopropyl H eclipsed to the phenyl double bond is more favorable than the one with the methyl eclipsed to the phenyl double bond because of the significant steric interaction in the latter case.

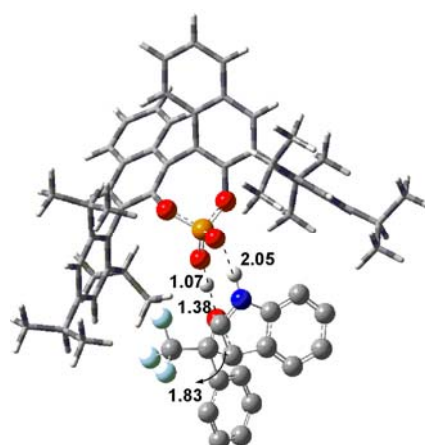
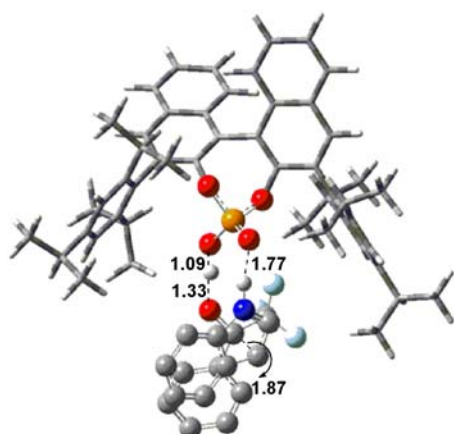
(2) Even all the six isopropyl groups adopt the preferred conformation as mentioned above, there still have different orientations of them. According to the calculations of the different structures for catalyst **1**, we find that the most stable coformation **A** corresponds to the best orientation of the four isopropyl groups which are closer to the binaphthol backbone (2,2',6,6'-positions on the the substituents of 2,4,6-(i-Pr)₃C₆H₂) with all the four isopropyl H pointing to the binaphthol backbone side and the two isopropyl H which are far from the binaphthol backbone (4,4'- positions on the substituents of 2,4,6-(i-Pr)₃C₆H₂), pointing to the same direction. Structure **B** is nearly isoenergetic to **A** with the only difference of the two isopropyl H far from the binaphthol backbone (4,4'- positions) pointing to the opposite direction. Hence, with respect to the catalyst itself, the relative orientation of the isopropyl groups at the 4,4'-positions does not have obvious effect on the stabilization of the catalyst.

(3) From structures **C** to **F**, there are from one to four isopropyl Hs at the 2,2',6,6'-positions on the the substituents of 2,4,6-(i-Pr)₃C₆H₂ pointing to the opposite side of the binaphthol backbone. As shown in **Fig. S5**, because the two methyls of the isopropyl group are closer to the binaphthol core which will result in significant steric hindrance, these structures are greatly destabilized by 4.9, 10.1, 15.5, and 21.9 kcal/mol for conformer **C**, **D**, **E**, and **F** respectively. And as expected, the destabilization energies are proportional to the number of the isopropyl H at 2,2',6,6'-positions that points away from the binaphthol core. Based on the large energy difference between the different conformations, we can assume that conformers **C**, **D**, **E**, or **F** can be safely excluded in the reaction process.

(4) To further verify our above assumption, we have located a transition state in the channel of TS1-*re*-exo which involves the conformer of the catalyst like structure **C** with one isopropyl H at the 2-position of 2,4,6-(i-Pr)₃C₆H₂ substituent pointing away from the binaphthol core. This TS is 5.8 kcal/mol higher in energy than its most stable counterpart in which all the four isopropyl H point to the binaphthol backbone side (like catalyst conformer **A** or **B**) in the TS1-*re*-exo channel. This energy difference between above two TSs is comparative to that between two conformers of the catalyst itself. Therefore, it can be concluded that in the enantio-determining C-C bond formation step, transition states involving the catalyst with the conformation of **C**, **D**, **E**, or **F** should be much higher in energy than the TSs containing conformation **A** or **B** of the catalyst, and those greatly destabilized TSs arising from the unstable conformation of the substituents on the catalyst can be safely excluded. Only TSs containing conformation **A** or **B** of the catalyst should be considered in the following discussion.

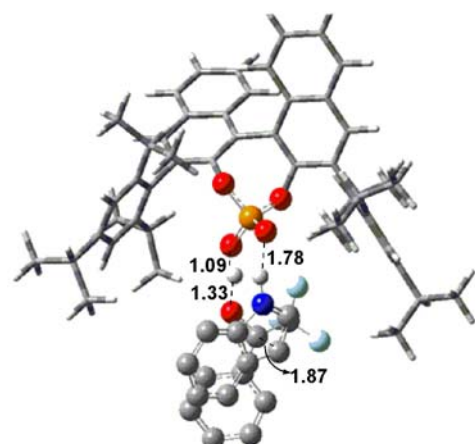
Fig. S6 Different conformers of the transition states arising from the relative orientations of the isopropyl groups at the 4,4'-positions on the 2,4,6-triisopropylphenyl substituents for the two lower-energy channels of the C-C bond formation step of chiral phosphoric-catalyzed Friedel-Crafts reaction (real system) between indole and 2,2,2-trifluoroacetophenone. Relative enthalpies at the ONIOM(BH and HLYP/6-31G(d):HF/3-21G) level are also shown.



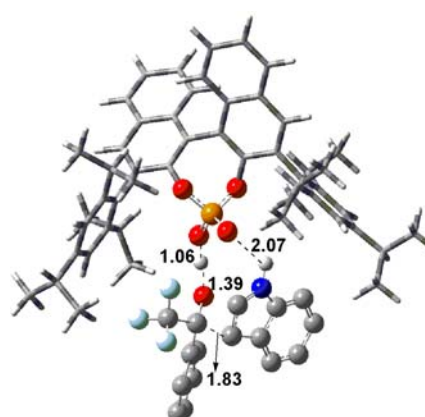


Two isopropyl Hs at 4,4'-positions both point to the bottom face

B
 $\Delta H = 0.1$ kcal/mol

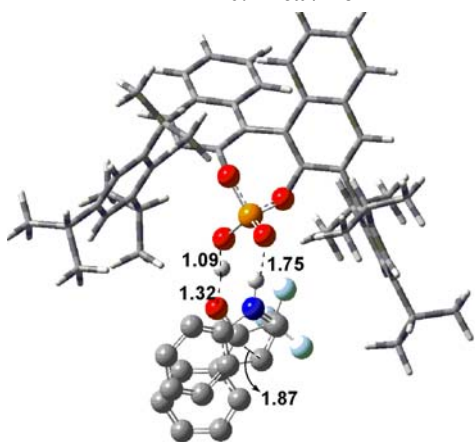


B'
 $\Delta H = 0.4$ kcal/mol

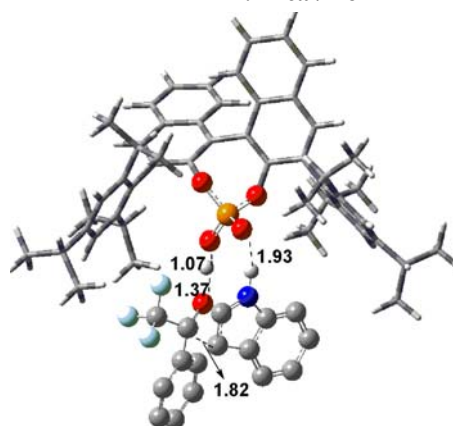


Of the two isopropyl Hs at 4,4'-positions, the right one points to the bottom face while the left one points to the top face

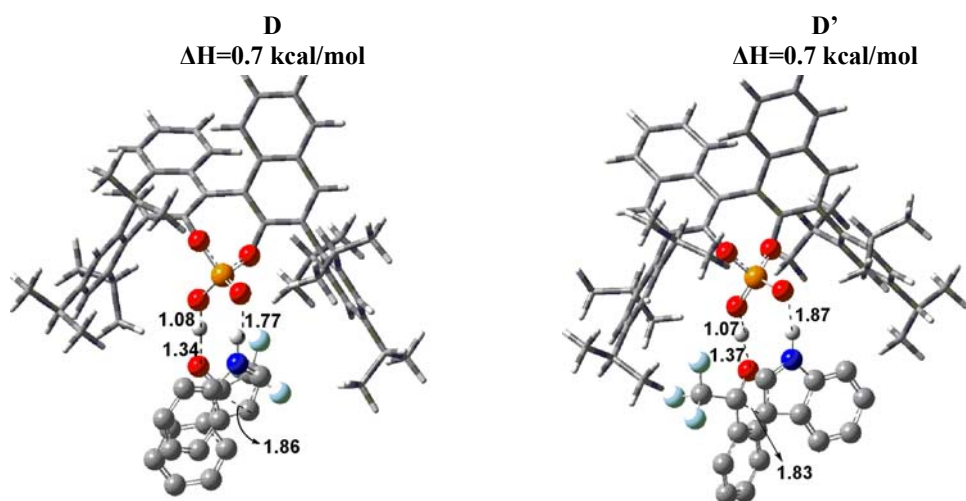
C
 $\Delta H = 0.4$ kcal/mol



C'
 $\Delta H = 1.1$ kcal/mol



Two isopropyl Hs at 4,4'-positions both point to the top face



Of the two isopropyl Hs at 4,4'-positions, the right one points to the top face while the left one points to the bottom face

Note: As shown in **Fig. S6**, the conformational difference of the substituents at the 4,4'-positions of 2,4,6-triisopropylphenyl substituents on BINOLs catalyst also has effect on the stabilization of the transition states when they tried to accommodate the substrates into their chiral pockets. In those TSs, the higher-energy TSs correspond to the structures with larger deviation from the eclipsing conformation of the isopropyl Hs at 4,4'-positions to the phenyl double bond which is required to minish the steric interaction between the steric substituents of the catalyst and the substrates. Obviously, these energy differences are much less than those arising from the unstable conformation of isopropyl groups at 2,2',6,6'-positions. It should also be noted that only the most stable conformers of the TSs corresponding to different reaction channels have been discussed in the paper (**Fig. 3**).

Complete ref 16

a) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, *Gaussian03, Revision D.01*; Gaussian, Inc.; Wallingford CT, **2004**.

b) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision C.01*; Gaussian, Inc., Wallingford CT, **2010**.

Cartesian coordinates and total energies of reported transition states and reactants.

A. Cartesian coordinates and total energies of the reported C-C bond forming transition states for the uncatalyzed Friedel-Crafts reaction between 2,2,2-trifluoroacetophenone and indole at BH and HLYP/6-31G(d) level.

(1) TS1-*anti*-exo-3a-no

C, 0, 0.8758409997, -0.5820686856, 0.354553819
O, 0, 0.5074853474, -1.0482889031, 1.5102267068
C, 0, 1.0044046197, 0.9430490659, 0.2597762047
C, 0, 2.1927015963, -1.2429592044, -0.130004273
F, 0, 3.2193588457, -0.830149141, 0.5951794877
F, 0, 2.1456479787, -2.5809435407, -0.0234449404
F, 0, 2.4959067291, -1.0029693227, -1.4218615997
C, 0, 0.6505191694, 1.6528804533, 1.3980420867
C, 0, 0.7133279076, 3.0365351507, 1.4162872029
C, 0, 1.1257795008, 3.7299353043, 0.2893788882
C, 0, 1.4788676481, 3.0289707602, -0.853519259
C, 0, 1.4199414405, 1.6438122213, -0.869433512
H, 0, 0.3352008793, 1.0817102866, 2.2538800743
H, 0, 0.4404625729, 3.5743167992, 2.3106560081
H, 0, 1.1749656195, 4.8072882289, 0.3007471514
H, 0, 1.807508399, 3.5595690565, -1.7333404894
H, 0, 1.70935378, 1.1185067397, -1.7635197594
C, 0, -3.2494209986, 1.2939771819, -0.8345865106
C, 0, -4.1029545203, 0.5309844488, -0.047926797
C, 0, -3.7034742826, -0.7070280617, 0.4368846569
C, 0, -2.434679322, -1.1175807123, 0.0997880304
C, 0, -1.5561544472, -0.3772732401, -0.6809234249
C, 0, -1.9715003246, 0.8520348932, -1.1557042274
N, 0, -1.7929861588, -2.340196791, 0.4040256695
C, 0, -0.5956445508, -2.3783909282, -0.0867397046
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H, 0, -5.0860453803, 0.9013227576, 0.1902610726
H, 0, -4.3567865068, -1.3094978694, 1.0462818409
H, 0, -1.3133988002, 1.4658871142, -1.7455675197
H, 0, -2.157287966, -3.0249790777, 1.0416168411
H, 0, 0.0440714094, -3.2251251802, 0.0531806457
H, 0, 0.1585565529, -1.2299018773, -1.7677322197

Eelec= -1045.8049185

Eelec+ZPE= -1045.548515

H= -1045.531979

G= -1045.592403

(2) TS1-*anti*-endo-3a-no

C, 0, -0.5501144474, 0.0761896598, 0.5380271369
O, 0, -0.2122712607, -0.5729651639, 1.610948545
C, 0, -2.0007669885, -0.1506736569, 0.0547658491
C, 0, -0.2883108512, 1.5935060695, 0.651714485
F, 0, -1.2422173682, 2.2004661911, 1.3488452762
F, 0, 0.8674515979, 1.8534388225, 1.2478852708
F, 0, -0.2399005746, 2.2037393217, -0.5575878347
C, 0, -2.8068429073, -0.930293207, 0.8725470021
C, 0, -4.1198807061, -1.2031758118, 0.5203063125
C, 0, -4.6447999649, -0.694083936, -0.6562760537
C, 0, -3.8495972387, 0.0939896661, -1.4749866402
C, 0, -2.5372581268, 0.3636734627, -1.1225651134
H, 0, -2.3714166883, -1.2972285116, 1.7862852472
H, 0, -4.7348941802, -1.8076181369, 1.1684793687
H, 0, -5.6659449405, -0.9035537843, -0.9325592021
H, 0, -4.2521467056, 0.5017009932, -2.3887962162
H, 0, -1.9399980058, 0.9917954146, -1.7633023943
C, 0, 3.9914689751, 0.8546693966, -0.7355916482
C, 0, 4.5999892335, -0.2540707913, -0.1592322277
C, 0, 3.8556940097, -1.3734217134, 0.1861706019
C, 0, 2.5045619752, -1.312090818, -0.0666530711
C, 0, 1.8659374095, -0.2157153456, -0.6302176956
C, 0, 2.6238555828, 0.8869437396, -0.9743762903
N, 0, 1.5238041153, -2.3164159164, 0.1171500779
C, 0, 0.3546761039, -1.9032337172, -0.2511560163
C, 0, 0.4076243832, -0.5152395056, -0.7237090187
H, 0, 4.5925776862, 1.7105613249, -0.9943973225
H, 0, 5.661941056, -0.2479490202, 0.0210152313
H, 0, 4.317290441, -2.2409980957, 0.6281108947
H, 0, 2.1588890342, 1.7610415667, -1.3959707852
H, 0, 1.683836323, -3.1758668228, 0.6114876269
H, 0, -0.5199016706, -2.518523093, -0.1671275943
H, 0, -0.0507603009, -0.3360055814, -1.6870468017

Eelec= -1045.8023689
Eelec+ZPE= -1045.545877
H= -1045.529386
G= -1045.589415

(3) TS1-syn-exo-3a-no

C, 0, -0.8522106145, -0.8894447885, 0.4846091971
O, 0, -1.076940633, -1.4548294179, 1.6953444775
C, 0, -1.6050760938, 0.4258100332, 0.2481917034
C, 0, -1.1879380431, -1.8832309424, -0.6405320801
C, 0, -2.3305476179, 0.9272377782, 1.3192693872
C, 0, -3.0336814745, 2.115983967, 1.2007991609
C, 0, -3.0272307151, 2.8133880728, 0.0038377056
C, 0, -2.315989817, 2.3116439479, -1.0760075655
C, 0, -1.608444117, 1.1259660338, -0.9559406567

F, 0, -2.4950532419, -2.0274273938, -0.7970395435
 F, 0, -0.6833372571, -3.0989555863, -0.396188339
 F, 0, -0.6791491792, -1.5139453556, -1.8328439245
 H, 0, -2.3325370187, 0.3506224894, 2.2274461705
 H, 0, -3.5932201055, 2.493197635, 2.0421851141
 H, 0, -3.5776734044, 3.7358739331, -0.0917087905
 H, 0, -2.3143090794, 2.8410342945, -2.0157871997
 H, 0, -1.0642865909, 0.7495119221, -1.8049136993
 C, 0, 2.6634923294, 2.4950249244, -0.3546092356
 C, 0, 3.923655834, 1.8979693102, -0.3622899134
 C, 0, 4.0706983473, 0.5514833588, -0.0865826914
 C, 0, 2.9136242624, -0.15588212, 0.1799640855
 C, 0, 1.6375593016, 0.4118434385, 0.1927967305
 C, 0, 1.5184769761, 1.7706192522, -0.0721786827
 N, 0, 2.7731870116, -1.5147191354, 0.4967135688
 C, 0, 1.5103849014, -1.8138787588, 0.7012221002
 C, 0, 0.6932954346, -0.6510813706, 0.5950689117
 H, 0, 2.5799318989, 3.5475845506, -0.5691116892
 H, 0, 4.7945104728, 2.4929258705, -0.5817340159
 H, 0, 5.0397783645, 0.0799292908, -0.0807888102
 H, 0, 0.5564256651, 2.2492136613, -0.0607276791
 H, 0, 3.5366990957, -2.1555967714, 0.6093490172
 H, 0, 1.1793689492, -2.7961188697, 0.9754479537
 H, 0, 0.3183341582, -0.7338002536, 1.7583442324

Eelec= -1045.7721892
 Eelec+ZPE= -1045.519110
 H= -1045.502442
 G= -1045.563325

(4) TS1-syn-endo-3a-no

C, 0, 0.8040694628, 0.5902454067, 0.725035136
 O, 0, 1.0532188781, 0.8112043382, 2.0399796158
 C, 0, 1.8483880853, -0.2757492741, 0.023308182
 C, 0, 0.6602506969, 1.9226102742, -0.0173064938
 C, 0, 3.0548367979, -0.4778770122, 0.6778795828
 C, 0, 4.0395458874, -1.2666707444, 0.1033907644
 C, 0, 3.824488032, -1.863477255, -1.1287433402
 C, 0, 2.6200481072, -1.6649218085, -1.7870613523
 C, 0, 1.6380351352, -0.8723180265, -1.2153608776
 F, 0, 1.7857972641, 2.6150008543, 0.0282185273
 F, 0, -0.3070862906, 2.6763654873, 0.5163062369
 F, 0, 0.3369999824, 1.7727159964, -1.3178968967
 H, 0, 3.1880162789, -0.0085020114, 1.6371915624
 H, 0, 4.9756352013, -1.4145441633, 0.6183535068
 H, 0, 4.5894901274, -2.4788170557, -1.5750351011
 H, 0, 2.4456383326, -2.1255325035, -2.7465877365
 H, 0, 0.708348311, -0.7152282899, -1.7384713458
 C, 0, -3.7717155144, 0.5102189771, -1.2262342827

C, 0, -4.4133884959, -0.677307716, -0.8749980521
 C, 0, -3.8058107178, -1.5883341878, -0.0315052064
 C, 0, -2.5435948196, -1.2610621308, 0.426971391
 C, 0, -1.8774333905, -0.0778197133, 0.0978752637
 C, 0, -2.5132581834, 0.8253211238, -0.7453627802
 N, 0, -1.7044222499, -1.993799593, 1.2792273921
 C, 0, -0.5829512604, -1.3420205602, 1.4910020186
 C, 0, -0.6054100455, -0.0753799528, 0.8484459238
 H, 0, -4.2703557986, 1.2009108083, -1.8858561384
 H, 0, -5.3954152099, -0.8879300484, -1.2645388473
 H, 0, -4.2931197614, -2.5073198962, 0.2504477569
 H, 0, -2.0383931155, 1.7484301418, -1.0192379137
 H, 0, -1.9470635585, -2.8692115261, 1.7045032167
 H, 0, 0.2053780843, -1.7145848304, 2.11730499
 H, 0, -0.4847052529, 0.5531388913, 1.9022252977

Eelec= -1045.7742103
 Eelec+ZPE= -1045.521246
 H= -1045.504525
 G= -1045.565341

B. Cartesian coordinates and total energies of the reported C-C bond forming transition states for uncatalyzed Friedel-Crafts reaction between acetophenone and indole at BH and HLYP/6-31G(d) level.

(1) TS1-*anti*-exo-3b-no

C, 0, -0.57514656, 1.5924256909, 0.1419280833
 O, 0, 0.0222875653, 1.8361409175, 1.280239587
 C, 0, -1.5685339492, 0.4373346021, 0.1578550759
 C, 0, -1.1831477068, 2.837005381, -0.5244638542
 C, 0, -1.7098918982, -0.2657295531, 1.3460977459
 C, 0, -2.6050026746, -1.3190742175, 1.4428708214
 C, 0, -3.3647443055, -1.6921982856, 0.3452193132
 C, 0, -3.2252064164, -1.0018793469, -0.8497361058
 C, 0, -2.3353698809, 0.0568479698, -0.9399490701
 H, 0, -1.9713128889, 3.1946013087, 0.1333177957
 H, 0, -0.4436950741, 3.6308626504, -0.6012307557
 H, 0, -1.6066781712, 2.6603470356, -1.509825198
 H, 0, -1.1037815534, 0.0493498423, 2.1779333839
 H, 0, -2.7090387069, -1.8515306573, 2.3754234971
 H, 0, -4.0603728879, -2.5132469994, 0.4181339878
 H, 0, -3.8138455292, -1.2836490576, -1.7088616556
 H, 0, -2.2418127895, 0.5834031531, -1.8773576884
 C, 0, 1.5772468564, -2.5655941146, -0.7217248389
 C, 0, 2.6432658598, -2.4460576778, 0.1604812291
 C, 0, 3.0532370284, -1.1983420691, 0.6126271976
 C, 0, 2.3511087855, -0.1108618974, 0.1471481198
 C, 0, 1.2768396279, -0.1984358273, -0.7326371671
 C, 0, 0.8842769516, -1.4487184957, -1.1728379533

N, 0, 2. 5794088425, 1. 2609437105, 0. 3923505103
C, 0, 1. 6803061514, 1. 9940298656, -0. 203104282
C, 0, 0. 7415249671, 1. 1655807096, -0. 9518613631
H, 0, 1. 276050576, -3. 5445437116, -1. 0566599815
H, 0, 3. 1595830847, -3. 3286872523, 0. 4997056124
H, 0, 3. 881058968, -1. 0934684338, 1. 2947682867
H, 0, 0. 0445075058, -1. 5590981727, -1. 8373782256
H, 0, 3. 1907805214, 1. 6083838504, 1. 1076555306
H, 0, 1. 7065784639, 3. 0625324707, -0. 1389011799
H, 0, 0. 510664237, 1. 4632956117, -1. 9651794586

Eelec= -748. 1661752

Eelec+ZPE= -747. 886588

H= -747. 871985

G= -747. 927412

(2) TS1-*anti*-endo-3b-no

C, 0, -0. 5653805576, 0. 1014951424, 0. 80248733
O, 0, -0. 2252401883, -1. 0227894417, 1. 3740487215
C, 0, -2. 0062462705, 0. 1471269134, 0. 267082432
C, 0, -0. 2503496284, 1. 3516859243, 1. 6185271196
C, 0, -2. 8388785629, -0. 9193650078, 0. 5792694304
C, 0, -4. 1612326123, -0. 9355688538, 0. 1593874638
C, 0, -4. 6713423854, 0. 1196048977, -0. 578296277
C, 0, -3. 850039809, 1. 1940376091, -0. 8906252946
C, 0, -2. 5309815652, 1. 205617503, -0. 470287281
H, 0, -0. 8844085612, 1. 3270088091, 2. 502110728
H, 0, 0. 7839378146, 1. 3202734004, 1. 9439945536
H, 0, -0. 4362988089, 2. 2853479369, 1. 0908705224
H, 0, -2. 4181379673, -1. 71624982, 1. 1685751814
H, 0, -4. 7947468097, -1. 7709616624, 0. 4142059594
H, 0, -5. 6989671452, 0. 1101426751, -0. 9052162459
H, 0, -4. 2388176069, 2. 0228188274, -1. 4613232706
H, 0, -1. 907016708, 2. 0502311501, -0. 7218888004
C, 0, 3. 9271289632, 1. 4388474617, -0. 0859339818
C, 0, 4. 5450968161, 0. 2012928482, 0. 0391157163
C, 0, 3. 8169903274, -0. 9735735067, -0. 1010493668
C, 0, 2. 4716977657, -0. 8422748212, -0. 3561667098
C, 0, 1. 8212760798, 0. 3826740789, -0. 4746727885
C, 0, 2. 5648131855, 1. 5406886951, -0. 3419018679
N, 0, 1. 5134469987, -1. 8493976039, -0. 6036463881
C, 0, 0. 3292490451, -1. 3289785739, -0. 7706509475
C, 0, 0. 3791401113, 0. 1254754737, -0. 6881699914
H, 0, 4. 5141718667, 2. 3361185542, 0. 0219033462
H, 0, 5. 6014560718, 0. 148691953, 0. 2438089762
H, 0, 4. 289383796, -1. 9382821003, -0. 01339707
H, 0, 2. 0969658985, 2. 5077208249, -0. 4270071412
H, 0, 1. 6685814881, -2. 8247192201, -0. 4276796619
H, 0, -0. 5319841059, -1. 9342248338, -0. 9714526019

H, 0, -0.1235909359, 0.6843447673, -1.4634417944

Eelec= -748.1673581

Eelec+ZPE= -747.887828

H= -747.873209

G= -747.928614

(3) TS1-syn-exo-3b-no

C, 0, -0.8897090027, 1.3381956552, -0.6501598048
O, 0, -0.7492400213, 1.2916817647, -2.0011245556
C, 0, -1.7312406269, 0.2055577813, -0.0675809325
C, 0, -1.4453142909, 2.6895514551, -0.1747508922
C, 0, -2.4717066869, -0.5690224969, -0.9492369103
C, 0, -3.28850348, -1.5864778973, -0.4793425167
C, 0, -3.366884012, -1.8485918472, 0.8791520386
C, 0, -2.625461639, -1.0830976626, 1.7673119718
C, 0, -1.8176930567, -0.0620800254, 1.2944304337
H, 0, -2.4265336991, 2.8090846567, -0.6237423517
H, 0, -0.8190677649, 3.499002954, -0.5478682297
H, 0, -1.5476045982, 2.7769607822, 0.907224391
H, 0, -2.3810239953, -0.3438937495, -1.9982448234
H, 0, -3.8624619674, -2.1779465196, -1.1756450784
H, 0, -3.9973364871, -2.6435172944, 1.2450298034
H, 0, -2.6765409936, -1.2826846093, 2.8263567922
H, 0, -1.2444949611, 0.5263291394, 1.9967246451
C, 0, 2.2497762205, -2.1153230114, -0.9880742654
C, 0, 3.3346122078, -1.9800757781, -0.1164594782
C, 0, 3.4909805091, -0.8478925079, 0.6604902597
C, 0, 2.5117271875, 0.1222637707, 0.5332350052
C, 0, 1.4193727353, 0.0059919247, -0.3203498903
C, 0, 1.2902928039, -1.1273519894, -1.1097693011
N, 0, 2.3962433298, 1.3665387382, 1.173117287
C, 0, 1.3125144423, 1.9993440972, 0.7726964597
C, 0, 0.6312208991, 1.2480505192, -0.2245761182
H, 0, 2.1663859139, -3.0101979026, -1.5825831327
H, 0, 4.0654397438, -2.7691744248, -0.0531715742
H, 0, 4.3312171342, -0.7320422829, 1.3254891953
H, 0, 0.4650320908, -1.2020224288, -1.7951660459
H, 0, 3.0665729894, 1.7358037008, 1.8225370655
H, 0, 1.0558936788, 2.9636095366, 1.1710720276
H, 0, 0.6658643968, 1.7351319521, -1.3084824744

Eelec= -748.1323754

Eelec+ZPE= -747.856250

H= -747.841443

G= -747.897560

(4) TS1-syn-endo-3b-no

C, 0, 0.8759405355, 1.3332025432, 0.0442709312
 O, 0, 1.1707276423, 2.1467600625, 1.0933140092
 C, 0, 1.9185293728, 0.240368486, -0.1967145309
 C, 0, 0.6208817499, 2.1098323233, -1.2505667424
 C, 0, 3.1224332422, 0.3233377696, 0.4885561561
 C, 0, 4.1088113943, -0.6334840775, 0.299165815
 C, 0, 3.9001528339, -1.6891373664, -0.5739372714
 C, 0, 2.6979194976, -1.7812025617, -1.2604360952
 C, 0, 1.7169460021, -0.8207736677, -1.0742387329
 H, 0, 1.5408015423, 2.6319255755, -1.4984028566
 H, 0, -0.1493556516, 2.8596014186, -1.0833738069
 H, 0, 0.3420916601, 1.4821764182, -2.0953533001
 H, 0, 3.2507522951, 1.1527164223, 1.1630420319
 H, 0, 5.0423289813, -0.5540535299, 0.8343910789
 H, 0, 4.6660639034, -2.4342673334, -0.720445027
 H, 0, 2.5256820158, -2.6004304788, -1.9410680424
 H, 0, 0.7846092312, -0.9037665489, -1.6132384717
 C, 0, -3.6851758008, 0.0617450801, -1.4277438165
 C, 0, -4.2324656468, -0.8712773453, -0.5476388293
 C, 0, -3.5636445231, -1.2354807722, 0.6069686604
 C, 0, -2.3386779293, -0.6359717354, 0.8300722982
 C, 0, -1.7660447473, 0.3066427874, -0.0284318659
 C, 0, -2.4614603053, 0.6586110578, -1.17804474
 N, 0, -1.4483218536, -0.8212801244, 1.8981445104
 C, 0, -0.3839111241, -0.0622115732, 1.7419557571
 C, 0, -0.4969872454, 0.7436812626, 0.5807760877
 H, 0, -4.2293914238, 0.3249630149, -2.3197114383
 H, 0, -5.1890616795, -1.3147206134, -0.7686518442
 H, 0, -3.9795705079, -1.9544245661, 1.2938829312
 H, 0, -2.0576767186, 1.3841393314, -1.8621111476
 H, 0, -1.6147239322, -1.4239546841, 2.6822877252
 H, 0, 0.4314774898, -0.0413256114, 2.440248853
 H, 0, -0.3708643003, 1.8072330366, 1.1540777135

Eelec= -748.137045

Eelec+ZPE= -747.860713

H= -747.845964

G= -747.902024

C. Cartesian coordinates and total energies of the reported transition states and intermediates for the simplified model of chiral phosphoric acid-catalyzed diarylation reaction between 2,2,2-trifluoroacetophenone and indole at BH and HLYP/6-31G(d) level.

(1) IN1a

C, 0, -0.3737889146, 4.9388424742, 1.0063173317
 C, 0, -0.4572482265, 3.6965381528, 1.4612122156
 C, 0, 0.1341288196, 5.2997203992, -0.3089346869
 C, 0, -0.0393238071, 4.5717949168, -1.4028184659
 O, 0, 0.0317029117, 2.6107450704, 0.7797510284

O, 0, -0.8178739154, 3.4410056593, -1.4346636282
P, 0, -0.4901792852, 2.1003214659, -0.6420596801
O, 0, 0.4825106219, 1.1901317135, -1.2455247999
O, 0, -1.9342778574, 1.5355413562, -0.4359319494
H, 0, -0.6957986748, 5.7287352521, 1.6653991085
H, 0, -0.8415453394, 3.4384953033, 2.4318317164
H, 0, 0.6787512138, 6.2242329094, -0.4124022099
H, 0, 0.3428918768, 4.8393308507, -2.3714738337
H, 0, -1.9652714322, 0.5599517404, -0.49844459
C, 0, -1.4169367675, -1.9949086418, -1.1826242521
O, 0, -1.7487347125, -1.1779279297, -0.3546908412
C, 0, -1.0369395986, -3.3688216106, -0.8513003594
C, 0, -1.4364462751, -1.5519687258, -2.6573833289
F, 0, -2.3014236751, -2.2968518235, -3.3466779896
F, 0, -1.8125445654, -0.2923327852, -2.7635227077
F, 0, -0.2418139759, -1.6876279694, -3.2190564202
C, 0, -0.9579311131, -3.7021810978, 0.5022277851
C, 0, -0.612152254, -4.9825577491, 0.8807436792
C, 0, -0.346147903, -5.9401147433, -0.0878410891
C, 0, -0.4174690414, -5.6157641894, -1.4341374443
C, 0, -0.7563713273, -4.3333514616, -1.8206743316
H, 0, -1.1507527066, -2.9423378039, 1.2382132849
H, 0, -0.5351442993, -5.2304038397, 1.9256401973
H, 0, -0.0749091844, -6.9407511844, 0.2076422893
H, 0, -0.2042172709, -6.3606301739, -2.1824848528
H, 0, -0.8033539006, -4.0944865136, -2.8672696525
C, 0, 2.4276905639, -3.1386283882, 2.7559784628
C, 0, 1.7563879776, -1.9067717126, 2.7797935501
C, 0, 1.5514764959, -1.1821878477, 1.6248180718
C, 0, 2.031967786, -1.7204690041, 0.4336002735
C, 0, 2.7126623935, -2.9555562201, 0.386731704
C, 0, 2.9067872734, -3.6641120455, 1.5756324653
N, 0, 1.9592152314, -1.2351692613, -0.8423182496
C, 0, 2.5813831744, -2.1146455133, -1.684403963
C, 0, 3.0530925666, -3.1802658286, -0.984574077
H, 0, 2.5768305005, -3.6749033975, 3.6797479949
H, 0, 1.4026730257, -1.5160895519, 3.7207023249
H, 0, 1.0501468201, -0.2277974438, 1.6395082763
H, 0, 3.4277030434, -4.6089520928, 1.5690941736
H, 0, 1.5487195566, -0.3499517382, -1.0972301963
H, 0, 2.6340326851, -1.9074765892, -2.7360449946
H, 0, 3.5792084852, -4.0228013866, -1.3912323396

Eelec= -1843.3654124

Eelec+ZPE= -1843.007152

H= -1842.979254

G= -1843.071653

(2) TS1a

C, 0, -0.2347272927, 4.5284719663, 0.1232373153

C, 0, -0.5531786579, 3.2421207374, 0.1706098285
 C, 0, 0.8907904155, 5.1176084351, 0.833379136
 C, 0, 2.051226883, 4.5080099127, 1.0369070495
 O, 0, 0.0825601685, 2.3460035948, 0.9883748993
 O, 0, 2.3712556598, 3.289433455, 0.5047503316
 P, 0, 1.6195551339, 1.9146259978, 0.8275552498
 O, 0, 2.0552858677, 1.2791565882, 2.089501041
 O, 0, 1.810090461, 1.1424493713, -0.4772508965
 H, 0, -0.8592568909, 5.1732947671, -0.4739136878
 H, 0, -1.3785452173, 2.8099770481, -0.3673723465
 H, 0, 0.788428762, 6.1211539246, 1.2140805772
 H, 0, 2.8713314108, 4.9561211956, 1.5698254149
 H, 0, 1.4955342489, 0.1099103479, -0.6306492206
 C, 0, 1.6681988942, -2.166294356, -1.1932447425
 O, 0, 1.0135424747, -1.1128497422, -0.8389141629
 C, 0, 0.8128929203, -3.2746166273, -1.7812605113
 C, 0, 2.8877202367, -1.8436997027, -2.0818524631
 F, 0, 2.4915274081, -1.5645417353, -3.3146364593
 F, 0, 3.5541756961, -0.784820221, -1.6248089988
 F, 0, 3.7789600645, -2.8431251453, -2.1636643988
 C, 0, -0.5608643984, -3.0710919501, -1.8027994546
 C, 0, -1.4074283568, -4.0401286545, -2.3152022793
 C, 0, -0.8913796225, -5.226289618, -2.810652667
 C, 0, 0.4790215908, -5.4359092319, -2.7936842701
 C, 0, 1.3272239084, -4.4680287229, -2.2817522087
 H, 0, -0.943356332, -2.1449206468, -1.4137412316
 H, 0, -2.4714348967, -3.8665869833, -2.3273334095
 H, 0, -1.5496150176, -5.9809552859, -3.2101216371
 H, 0, 0.8915364556, -6.3527524651, -3.182929614
 H, 0, 2.3876562382, -4.6495442152, -2.2865932775
 C, 0, -0.6643387058, -4.1695494279, 2.1997554021
 C, 0, -0.7567776721, -3.0641331478, 3.0435886543
 C, 0, 0.174734886, -2.0414805377, 2.9850632646
 C, 0, 1.1869380321, -2.1843496033, 2.0577150365
 C, 0, 1.2945388776, -3.2691853667, 1.1937439646
 C, 0, 0.3504761015, -4.2801111198, 1.2615389086
 N, 0, 2.2855425302, -1.3446890795, 1.8254933193
 C, 0, 3.0568061832, -1.8490726046, 0.9095241779
 C, 0, 2.4312458902, -2.9893720087, 0.2980112609
 H, 0, -1.4022397729, -4.951368843, 2.2739737004
 H, 0, -1.5642753607, -3.0049484016, 3.7544205505
 H, 0, 0.1160893674, -1.1777543499, 3.6255002753
 H, 0, 0.3969883534, -5.1281681296, 0.5997720114
 H, 0, 2.3470400547, -0.3681263193, 2.159013513
 H, 0, 3.9413673438, -1.3320598996, 0.5925213454
 H, 0, 3.0412186759, -3.7808391994, -0.1010212904

Eelec= -1843.3304147

Eelec+ZPE= -1842.974581

H= -1842.948947

G= -1843. 032279

(3) IN2a

C, 0, 5. 8786543459, -1. 3192764454, 0. 9280103997
C, 0, 5. 0801034914, -1. 6605893714, -0. 0754128666
C, 0, 5. 9531719485, 0. 0224584122, 1. 4856505267
C, 0, 4. 9138786392, 0. 8407786482, 1. 5954760632
O, 0, 4. 3261919841, -0. 759583208, -0. 770970314
O, 0, 3. 6311795879, 0. 4765984334, 1. 3091875678
P, 0, 3. 0824366319, 0. 055962159, -0. 1493867427
O, 0, 2. 9272569866, 1. 273258482, -1. 0270728188
O, 0, 1. 8852806015, -0. 8010618713, 0. 0444894183
H, 0, 6. 5123938326, -2. 0865584834, 1. 3433836735
H, 0, 5. 0206930029, -2. 6597084008, -0. 4718786964
H, 0, 6. 9062861658, 0. 3805876692, 1. 840961767
H, 0, 4. 9890821768, 1. 8362559825, 1. 9987823775
C, 0, -1. 6293943756, -0. 8679031083, -0. 1389922039
O, 0, -0. 6945977, -0. 7324498691, 0. 8641774971
C, 0, -3. 0201752974, -0. 7872771806, 0. 47953297
C, 0, -1. 4545338118, -2. 2486172996, -0. 8009776305
C, 0, -3. 1425736805, -0. 5827207512, 1. 8469180928
C, 0, -4. 3962592435, -0. 4761612196, 2. 428513707
C, 0, -5. 5395410795, -0. 5732101742, 1. 6534031297
C, 0, -5. 423105257, -0. 783913551, 0. 288247404
C, 0, -4. 1718273833, -0. 8908389283, -0. 2956552289
F, 0, -1. 7817245266, -3. 2244101657, 0. 0259310428
F, 0, -0. 1926131215, -2. 4480396032, -1. 1814884958
F, 0, -2. 2091389837, -2. 372105085, -1. 9033670964
C, 0, -2. 5232625032, 3. 6584573997, 0. 268475037
C, 0, -1. 2913388999, 4. 2855907941, 0. 1374283866
C, 0, -0. 2108652051, 3. 6184715721, -0. 4228087938
C, 0, -0. 4289658945, 2. 3203162738, -0. 8252877324
C, 0, -1. 6463817127, 1. 6650600067, -0. 6912273952
C, 0, -2. 7161795369, 2. 3432596722, -0. 1424260447
N, 0, 0. 4922257645, 1. 4506029629, -1. 4474460405
C, 0, -0. 0579111935, 0. 3287259479, -1. 707975035
C, 0, -1. 47479309, 0. 2642120367, -1. 2288835276
H, 0, 0. 2346276459, -0. 8257537542, 0. 5611445772
H, 0, -2. 2525217913, -0. 5052126707, 2. 4431036813
H, 0, -4. 4759112692, -0. 316492059, 3. 4915812888
H, 0, -6. 5135359853, -0. 4894999544, 2. 1076285924
H, 0, -6. 3054587911, -0. 8690439049, -0. 325044207
H, 0, -4. 1057803319, -1. 0654025525, -1. 3558288371
H, 0, -3. 3483234125, 4. 1995122658, 0. 7014038867
H, 0, -1. 1723724083, 5. 3032156048, 0. 4702453213
H, 0, 0. 7519178351, 4. 0863855205, -0. 5382664682
H, 0, -3. 6765777434, 1. 8732242505, -0. 0259407769
H, 0, 1. 6136077922, 1. 5152465875, -1. 390603848
H, 0, 0. 5088967875, -0. 4769487213, -2. 1326825733

H, 0, -2. 1478769912, 0. 0447856515, -2. 0537420348

Eelec= -1843. 3527267

Eelec+ZPE= -1842. 994369

H= -1842. 969281

G= -1843. 050496

(4) TS2a

C, 0, -0. 8329969708, 5. 4976266596, 0. 8027801446
C, 0, -1. 0579822411, 4. 786030942, -0. 2952219102
C, 0, -0. 9245126154, 4. 9696297581, 2. 1553380791
C, 0, -0. 5845525808, 3. 7304314897, 2. 4864359853
O, 0, -1. 5239032561, 3. 5049324772, -0. 2944570999
O, 0, -0. 0068079185, 2. 8602014836, 1. 6078433907
P, 0, -0. 7714543166, 2. 2215573939, 0. 3413866621
O, 0, -1. 8627051135, 1. 2784880829, 0. 7726167304
O, 0, 0. 2517643502, 1. 662798132, -0. 5827804097
H, 0, -0. 5683509125, 6. 5349750456, 0. 6724413628
H, 0, -0. 966795409, 5. 1969053197, -1. 2864577087
H, 0, -1. 2768584665, 5. 6189634715, 2. 9408705135
H, 0, -0. 6655554303, 3. 3378182155, 3. 4855497693
C, 0, 0. 0294736638, -1. 6971756369, 0. 0942668303
O, 0, 0. 9908699831, -0. 8852074549, -0. 4903874766
C, 0, 0. 227949709, -3. 1143779456, -0. 446257101
C, 0, 0. 2887970967, -1. 652035257, 1. 6066483983
C, 0, 1. 1508477219, -3. 3241621888, -1. 4640999711
C, 0, 1. 3336903422, -4. 5893644064, -1. 9997891772
C, 0, 0. 6026157164, -5. 6640925789, -1. 5237924564
C, 0, -0. 3123920146, -5. 4641089828, -0. 5032486831
C, 0, -0. 4994828604, -4. 2005874139, 0. 0316792705
C, 0, -4. 6813475538, -2. 7067433817, 0. 9284795267
C, 0, -5. 4229184043, -2. 4151621421, -0. 2150156979
C, 0, -4. 8363510837, -1. 7709529875, -1. 2869209633
C, 0, -3. 4954809101, -1. 4610569231, -1. 1656877994
C, 0, -2. 7196938832, -1. 7526934475, -0. 0440071967
C, 0, -3. 3428916744, -2. 3712451142, 1. 0325362883
N, 0, -2. 6714859613, -0. 7976586752, -2. 08543123
C, 0, -1. 4610910216, -0. 6603103854, -1. 6161268289
C, 0, -1. 3771155975, -1. 1448578529, -0. 2693323534
F, 0, 1. 464151367, -2. 1838969706, 1. 8987403097
F, 0, 0. 2833994159, -0. 4001501012, 2. 0503226104
F, 0, -0. 6360612889, -2. 3189294882, 2. 3152233702
H, 0, 0. 7988528072, 0. 0723202981, -0. 3651021332
H, 0, 1. 7291909672, -2. 4934098862, -1. 8233739808
H, 0, 2. 0566565319, -4. 7324530669, -2. 7867919017
H, 0, 0. 7475594985, -6. 6485440083, -1. 9386425485
H, 0, -0. 8833884744, -6. 2929252733, -0. 1169321577
H, 0, -1. 2092346101, -4. 075444872, 0. 8280280466
H, 0, -5. 1645301794, -3. 1967781017, 1. 7574535022
H, 0, -6. 4650789633, -2. 683348163, -0. 2597510719

H, 0, -5.3989571173, -1.517845443, -2.1703901096
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H, 0, -2.9852572822, -0.4194942951, -2.9609091802
H, 0, -0.6826949399, -0.16304824, -2.1620108319
H, 0, -1.5421345826, -0.0414605703, 0.2690312622

Eelec= -1843.3261553
Eelec+ZPE= -1842.969054
H= -1842.943665
G= -1843.026184

(5) IN3a

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C, 0, -3.8433808094, -3.2997232188, -0.8397163763
C, 0, -2.6468306858, -2.628339647, -0.5325950184
C, 0, -2.3600683187, -1.4261672153, -1.1853341754
N, 0, -3.8805020141, -4.4384622922, -0.0765953464
C, 0, -2.7594030376, -4.4986875523, 0.7026393619
C, 0, -1.969072883, -3.4192862998, 0.4610889096
C, 0, -0.6555983966, -3.0595386215, 1.0898817915
C, 0, -0.2685452974, -4.0517123982, 2.1956978094
C, 0, 0.4768943806, -3.0009457157, 0.0609332747
C, 0, 0.5957746283, -4.0079621371, -0.8914121063
C, 0, 1.6288066316, -3.9906440893, -1.8111992709
C, 0, 2.5588224902, -2.9628434433, -1.7945902145
C, 0, 2.4459873803, -1.957255972, -0.8509859601
C, 0, 1.4133262138, -1.974806964, 0.0750261255
F, 0, 0.8517884406, -3.6498263982, 2.7940543943
F, 0, -1.2051325189, -4.1447051461, 3.1349298349
F, 0, -0.0594649735, -5.281180733, 1.7241202458
O, 0, -0.843337662, -1.8244137749, 1.7482159718
H, 0, -3.0508822067, -0.0086028134, -2.6120918431
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H, 0, -1.4486783829, -0.8920727268, -0.9761438203
H, 0, -4.6176772255, -5.1118920466, -0.0717988191
H, 0, -2.6134123466, -5.3179560029, 1.3776514226
H, 0, -0.1295407816, -4.8030232416, -0.9174935304
H, 0, 1.703133368, -4.7776466048, -2.5441201208
H, 0, 3.3618333865, -2.9456608821, -2.5136662205
H, 0, 3.1616874945, -1.1514921408, -0.8289763037
H, 0, 1.3517931769, -1.1752877141, 0.7932726079
H, 0, -0.0359725989, -1.5017428508, 2.1755585588
C, 0, -1.327415407, 4.1477861859, 3.7095175883
C, 0, -1.754648157, 2.9274235686, 4.0010328527
C, 0, -0.0432134969, 4.4409391178, 3.0909524026
C, 0, 0.5435561279, 3.6722798288, 2.1846048905

O, 0, -0.979766095, 1.8046101043, 3.8503030586
O, 0, -0.051915653, 2.5591326987, 1.6439854897
P, 0, -0.4306884973, 1.2454489585, 2.4619869251
O, 0, 0.6350934391, 0.2615164172, 2.6745917425
O, 0, -1.6608892504, 0.7332797209, 1.6354227815
H, 0, -1.97551291, 4.9717313601, 3.9606311612
H, 0, -2.7083335135, 2.7154751759, 4.4502270796
H, 0, 0.4674963194, 5.3470446553, 3.3741422332
H, 0, 1.4957983187, 3.8910043829, 1.735844802
H, 0, -1.6315566222, -0.2384483466, 1.520252347

Eelec= -1843.3683617

Eelec+ZPE= -1843.007547

H= -1842.980952

G= -1843.067909

(6) TS3a

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C, 0, 0.3867512547, 2.5027038236, -1.2116488791
C, 0, 1.4472976417, 1.7881577861, -0.6314021685
C, 0, 2.489433822, 2.5087281745, -0.0510062779
N, 0, -0.4894004476, 1.5861470407, -1.7742487416
C, 0, -0.0414983729, 0.3595940829, -1.5900119615
C, 0, 1.1586718186, 0.3759508116, -0.8711563334
C, 0, 1.7116569167, -0.7805595498, -0.2870710237
C, 0, 1.6853898323, -2.0808762171, -1.0884678709
C, 0, 2.8906330768, -0.6442106382, 0.6254247656
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C, 0, 5.2668503027, -0.742798771, 0.9934228184
C, 0, 5.0948423194, -0.2614619913, 2.2801523439
C, 0, 3.8194569944, 0.0292122596, 2.7394187916
C, 0, 2.7221559505, -0.1545708142, 1.9172179306
F, 0, 2.0396749185, -3.1168793512, -0.3304065178
F, 0, 0.5029916319, -2.3597436698, -1.6088450703
F, 0, 2.5573076188, -1.9974824557, -2.0917383119
H, 0, 3.2224077467, 4.450153137, 0.4149399417
H, 0, 1.3187978339, 5.6495891655, -0.5691924608
H, 0, -0.523710049, 4.3972556347, -1.6555825023
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H, 0, -1.4760607516, 1.7073325604, -1.9814965875
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H, 0, 4.3244500837, -1.3103156075, -0.8295850185
H, 0, 6.2537905555, -0.9708443686, 0.6261176904
H, 0, 5.9482835342, -0.1151204579, 2.9218123548
H, 0, 3.6757199854, 0.4033284633, 3.7396879228
H, 0, 1.7330986347, 0.072565211, 2.2700550723
O, 0, 0.4062587325, -1.3615070923, 0.9372760882
H, 0, -0.5619457347, -1.2472052504, 0.5717430825

H, 0, 0.5041734934, -2.2776913297, 1.2159634408
C, 0, -5.4495937427, -0.3743096931, 2.003762969
C, 0, -4.203052408, 0.0805525737, 2.0690614591
C, 0, -6.1816560619, -0.5846115189, 0.7642689592
C, 0, -5.6166683168, -0.9984941234, -0.3634402224
O, 0, -3.4901968533, 0.5233082777, 0.9997557621
O, 0, -4.3106797989, -1.380764269, -0.4399324741
P, 0, -3.0714175405, -0.3496559179, -0.3070874079
O, 0, -2.9863423488, 0.5833826627, -1.4534658674
O, 0, -1.8941169007, -1.2228170211, 0.022395183
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H, 0, -3.6845717327, 0.2150822499, 3.004094923
H, 0, -7.2450012319, -0.4046007976, 0.755511977
H, 0, -6.1608346201, -1.1364795932, -1.2825342276

Eelec= -1843.3160588

Eelec+ZPE= -1842.958246

H= -1842.932172

G= -1843.017003

(7) IN4a

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C, 0, -0.8291882504, -0.7029131181, -0.2607411485
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C, 0, -1.1476411429, -3.0480102894, -0.5942452282
N, 0, 0.2059467604, 0.2117226611, 0.0026424359
C, 0, 1.3386440446, -0.3839043977, 0.1011200942
C, 0, 1.1522027919, -1.8383560984, -0.0799353619
C, 0, 2.1017778699, -2.7859336331, -0.0444919071
C, 0, 3.5799394668, -2.5070310085, 0.1044977783
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C, 0, 0.9344340863, -6.2138234095, 0.9572722579
C, 0, 1.1885987253, -6.9465015535, -0.1920092233
C, 0, 1.7496170097, -6.3269097689, -1.2975903261
C, 0, 2.0596959107, -4.9775593921, -1.2579336407
F, 0, 3.8981918687, -1.2251267253, 0.1770662703
F, 0, 4.0398651369, -3.1021731031, 1.2001473665
F, 0, 4.2364610371, -3.018003961, -0.9384737836
H, 0, -3.1670926224, -3.5905001972, -1.0136523802
H, 0, -4.0468811074, -1.3069834472, -0.8891930823
H, 0, -2.5068917007, 0.6095586313, -0.4061117463
H, 0, -0.7888891906, -4.0587610653, -0.655540631
H, 0, 2.2391866981, 0.1805876287, 0.3192100624
H, 0, 1.0291030418, -4.2893379209, 1.8877098814
H, 0, 0.5058387757, -6.6925960697, 1.8222180826
H, 0, 0.9542820434, -7.9979077305, -0.2242433293
H, 0, 1.950928979, -6.8934484025, -2.1917517405

H, 0, 2. 5019647122, -4. 4998209107, -2. 1152612698
C, 0, -0. 7771069695, 6. 8864371386, -0. 4675856524
C, 0, -0. 1715953681, 6. 011426458, -1. 26159956
C, 0, -1. 542248687, 6. 5137610919, 0. 7123202307
C, 0, -1. 2311984072, 5. 4957701299, 1. 506513477
O, 0, -0. 3037678793, 4. 6621948558, -1. 1259719958
O, 0, -0. 0947967968, 4. 758254663, 1. 3800053847
P, 0, 0. 2740675585, 3. 8078351574, 0. 1221165285
O, 0, -0. 5788524817, 2. 5654860298, 0. 1625599105
O, 0, 1. 7437516398, 3. 6614550814, 0. 0748192154
H, 0, -0. 6958666749, 7. 9313216432, -0. 7222250129
H, 0, 0. 408247269, 6. 2995903201, -2. 1222860144
H, 0, -2. 4112713876, 7. 0982144275, 0. 9702589203
H, 0, -1. 8173432805, 5. 2261152212, 2. 3691489515
H, 0, -0. 0146946736, 1. 3048521337, 0. 096256268
O, 0, 3. 3818988812, 1. 6437359929, 0. 7998661077
H, 0, 2. 8182811404, 2. 4266002581, 0. 6436852607
H, 0, 4. 1688390852, 1. 811593855, 0. 2828255474

Eelec= -1843. 338094

Eelec+ZPE= -1842. 982820

H= -1842. 954665

G= -1843. 047852

(8) IN5a

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C, 0, -2. 0351919116, -1. 1806151451, 0. 2481960232
C, 0, -2. 5208528556, -1. 9660318633, 1. 281216186
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C, 0, -1. 7579469962, -2. 5376918021, -1. 9003131046
C, 0, -1. 5737659633, -2. 5830061435, -3. 4029492925
C, 0, -1. 9639008536, -3. 8719369458, -1. 2926550435
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F, 0, -2. 7506669049, -2. 8474613429, -3. 9813754628
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H, 0, -2. 5200200054, 0. 3708805424, 3. 7408929417
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C, 0, 2.7000912114, 5.9971839427, -0.4993789519
C, 0, 2.8394743367, 4.6829411186, -0.6240078507
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P, 0, 0.5073805672, 3.5630100779, -0.0547958466
O, 0, -0.5574129899, 3.136448115, -1.0295392503
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C, 0, 2.006287911, -0.6784374337, -2.9468576412
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C, 0, 2.2039651524, -2.6765044229, -1.594742806
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C, 0, 1.8471058115, -0.9704073174, 1.5837187676
C, 0, 2.0388958163, -2.1662395692, 0.9605908199
H, 0, 2.2651622184, -2.663462735, -3.7236484279
H, 0, 1.9978617367, -0.2276820687, -3.9264054974
H, 0, 1.7674294091, 1.1931880073, -1.9198342037
H, 0, 2.3395208977, -3.744234681, -1.5175719205
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H, 0, 1.7633469902, -0.7512892469, 2.6310458896
H, 0, 2.1655294996, -3.1182813809, 1.4406888889

Eelec= -2130.5610698

Eelec+ZPE= -2130.094418

H= -2130.061558

G= -2130.164136

(9) TS4a

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C, 0, -0.4674369691, 2.0191154801, -1.7428456466
C, 0, -1.4850517323, 1.2984570705, -1.097812208
C, 0, -2.6735970558, 1.9661387018, -0.8040345498
N, 0, 0.6221917062, 1.1830289108, -1.8986425784
C, 0, 0.3553115899, -0.0019935562, -1.3829431625

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C, 0, -1.0093019394, -2.5458002707, -0.533985924
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C, 0, -3.73930266, -0.9807330815, -1.3372205359
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F, 0, -1.4475684963, -2.9285019742, -1.7305491984
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H, 0, -3.7284453607, 3.8064739742, -0.9468973146
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H, 0, 0.2147994702, 3.8583305946, -2.6158524729
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H, 0, 1.5944351577, 1.4358565157, -2.1296197254
H, 0, 1.1128930162, -0.7587099269, -1.3910101449
H, 0, -3.2973128358, -1.8523208504, 1.8916031917
H, 0, -5.7073792646, -2.0619546082, 1.7737642211
H, 0, -6.9057937065, -1.5977718915, -0.3357409268
H, 0, -5.6187991247, -0.9237358658, -2.3387129643
H, 0, -3.1905675273, -0.6894897758, -2.215337561
C, 0, -2.2539740381, 2.3654593815, 2.8472684228
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C, 0, 0.0449237455, 2.4296018845, 2.0928772767
C, 0, -0.033068348, 1.055470271, 1.9613020932
C, 0, -1.1924338471, 0.3218265927, 2.2338886795
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N, 0, 0.9730144068, 0.1569527152, 1.6060049458
C, 0, 0.5128863405, -1.0691926982, 1.6778042515
C, 0, -0.8815301416, -1.0616180509, 1.9077004699
H, 0, -3.1168498667, 2.8994042251, 3.2103124644
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H, 0, 0.9537860765, 2.9590246885, 1.8618729434
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H, 0, 1.9445630733, 0.429319411, 1.3110462302
H, 0, 1.1552205164, -1.9051545341, 1.4853611328
H, 0, -1.3854747048, -1.9251628458, 2.2930237713
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O, 0, 5.4191181756, 0.6197088333, -0.7266493351
P, 0, 3.8023580735, 0.5977999209, -0.6821424588
O, 0, 3.2950712838, 1.3331007196, -1.8617232242
O, 0, 3.3366259219, 0.8937304376, 0.7062333464
H, 0, 5.1941304406, -3.0857599195, 0.9242397371

H, 0, 3. 3507378756, -2. 9206566683, -0. 4665675539
H, 0, 6. 7195936321, -1. 3602336491, 1. 5983688403
H, 0, 6. 9484361719, 0. 7774156999, 0. 6010698693

Eelec= -2130. 5377472
Eelec+ZPE= -2130. 068308
H= -2130. 037218
G= -2130. 131734

(10) IN6a

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C, 0, 0. 2529042705, -2. 0749138005, 1. 0778042521
C, 0, -1. 0139208408, -1. 879236815, 0. 4933495436
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C, 0, -0. 3828841021, -0. 0227010748, 1. 601052049
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C, 0, -5. 2833876279, -2. 280532706, 0. 0938607515
C, 0, -4. 2246049139, -1. 4947702131, 0. 5048103797
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C, 0, 0. 3563022571, 2. 0884318027, -0. 9444872307
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C, 0, 5.556467105, 1.4503107203, 0.3690218645
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O, 0, 3.1920720775, -0.4432163813, 0.9629611607
O, 0, 2.7277466437, -0.1011855342, -1.5837574503
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Eelec= -2130.5576839
Eelec+ZPE= -2130.088465
H= -2130.057109
G= -2130.153682

(11) TS5a

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C, 0, 1.7542383926, -3.0632759905, -2.1564728616
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C, 0, 1.1083700489, -4.5214132042, 0.611919259
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Eelec=-2130.5297814

Eelec+ZPE=-2130.062634

H=-2130.031398

G=-2130.127330

(12) IN7a

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 C, 0, 2.7261762494, -2.1427412764, -0.9326829349

N, 0, 3. 0737766195, -0. 0024163657, 1. 8865010417
 C, 0, 2. 1774530693, -0. 8671762399, 2. 4312655904
 C, 0, 1. 8817505035, -1. 8757812877, 1. 5606633599
 C, 0, 0. 879845148, -2. 9853172108, 1. 8714744634
 C, 0, 1. 2794882208, -3. 6159185431, 3. 2249840782
 C, 0, 0. 9125062353, -4. 1117596276, 0. 8179377572
 C, 0, -0. 1964814218, -4. 3919280312, 0. 0303150492
 C, 0, -0. 1596599653, -5. 3967683811, -0. 925974755
 C, 0, 0. 9855997553, -6. 1512856485, -1. 1031394518
 C, 0, 2. 0985328028, -5. 8841361297, -0. 3209310817
 C, 0, 2. 0655044658, -4. 8723373385, 0. 6218872879
 F, 0, 0. 5636311983, -4. 7171415983, 3. 4862125116
 F, 0, 2. 5602019957, -3. 9721766743, 3. 2759709269
 F, 0, 1. 0813757547, -2. 786932747, 4. 2544688413
 C, 0, -1. 5089261863, 0. 5874244475, -0. 1264574294
 C, 0, -2. 8015677199, 0. 7389956567, 0. 4001899103
 C, 0, -3. 2677341346, -0. 114202435, 1. 3736758819
 C, 0, -2. 411799904, -1. 117555949, 1. 8176310547
 C, 0, -1. 1014830441, -1. 2851702084, 1. 3229796377
 C, 0, -0. 6630153445, -0. 4112117124, 0. 3194770909
 N, 0, -2. 6192629123, -2. 0834729281, 2. 75965487
 C, 0, -1. 48931186, -2. 8423701591, 2. 8828604635
 C, 0, -0. 5201438371, -2. 3998560953, 2. 0344277142
 H, 0, 3. 60963956, -1. 9741000367, -2. 8557868891
 H, 0, 4. 8991805214, 0. 0558320296, -2. 3300005554
 H, 0, 4. 7246248647, 1. 0979891825, -0. 086547992
 H, 0, 2. 1768357427, -3. 0259322434, -1. 1992542623
 H, 0, 3. 2662192269, 0. 9176356984, 2. 2486549093
 H, 0, 1. 7998130797, -0. 6955266006, 3. 4190471303
 H, 0, -1. 0989473656, -3. 8212140578, 0. 1541662512
 H, 0, -1. 0335945992, -5. 5869579726, -1. 5281141373
 H, 0, 1. 0140029322, -6. 9358970702, -1. 8419670158
 H, 0, 3. 0021100249, -6. 4579092027, -0. 4498004569
 H, 0, 2. 9502239743, -4. 6662594705, 1. 1950596424
 H, 0, -1. 1732174301, 1. 2519135127, -0. 9061099785
 H, 0, -3. 4368702548, 1. 5275634683, 0. 0316428305
 H, 0, -4. 2605281226, -0. 0093949403, 1. 7809941152
 H, 0, 0. 3190964661, -0. 5107778778, -0. 1064818246
 H, 0, -3. 4426203592, -2. 1876692613, 3. 3152994678
 H, 0, -1. 4614289967, -3. 6501293707, 3. 5850736146
 H, 0, -0. 3512158369, 1. 6606970853, 1. 4987704806
 C, 0, 2. 1138047518, 5. 5332643288, -0. 1205950595
 C, 0, 1. 3526569058, 5. 5525645717, 0. 9681368789
 C, 0, 2. 5561517494, 4. 416336759, -0. 9479502394
 C, 0, 2. 211385991, 3. 1374224441, -0. 8860081886
 O, 0, 0. 7622408073, 4. 491695407, 1. 5999580893
 O, 0, 1. 3100151365, 2. 605627846, 0. 0091390914
 P, 0, 1. 3537367651, 3. 004286807, 1. 5619663547
 O, 0, 2. 6546047042, 2. 8602130421, 2. 2124632773

O, 0, 0. 1734113809, 2. 1609296047, 2. 1451189442
H, 0, 2. 4617871683, 6. 5038822571, -0. 4329296352
H, 0, 1. 0998877406, 6. 4718385065, 1. 4636014863
H, 0, 3. 2628573374, 4. 6617881231, -1. 723277124
H, 0, 2. 6008743918, 2. 3852241314, -1. 5462460894

Eelec= -2130. 5766093
Eelec+ZPE= -2130. 106286
H= -2130. 074027
G= -2130. 172602

(13) product a-single arylation

C, 0, -2. 1161462451, 1. 9841315088, -1. 5470934986
C, 0, -3. 3383356718, 1. 3292381247, -1. 3426584952
C, 0, -3. 4518478286, 0. 2977601171, -0. 4367289435
C, 0, -2. 3069527672, -0. 0684635989, 0. 2630237857
C, 0, -1. 0708572408, 0. 5730088566, 0. 072394291
C, 0, -0. 9863910787, 1. 6194121747, -0. 849341405
N, 0, -2. 1210442363, -1. 0424836744, 1. 2098483388
C, 0, -0. 8173074917, -1. 0298604186, 1. 622360767
C, 0, -0. 1309925153, -0. 064299799, 0. 9557216381
C, 0, 1. 3224327973, 0. 2917127363, 1. 0636351552
C, 0, 1. 976271565, -0. 38156162, 2. 2788839623
C, 0, 2. 0935869113, -0. 0927755149, -0. 2048992726
C, 0, 2. 0265788858, -1. 3894225683, -0. 7054155609
C, 0, 2. 7320826267, -1. 743739018, -1. 8409922328
C, 0, 3. 5103017115, -0. 8054631902, -2. 5021684207
C, 0, 3. 5709449298, 0. 4894459361, -2. 019725961
C, 0, 2. 8668474221, 0. 8424948454, -0. 8779430353
F, 0, 3. 2412541251, 0. 0389611747, 2. 3951636232
F, 0, 1. 358181334, -0. 0744919795, 3. 4123207562
F, 0, 2. 0050745605, -1. 711818481, 2. 1923985518
O, 0, 1. 3927938164, 1. 6761438009, 1. 3165110449
H, 0, -2. 0642781366, 2. 7897815485, -2. 2612472308
H, 0, -4. 2055009254, 1. 639982107, -1. 9025762956
H, 0, -4. 3920240853, -0. 2052950574, -0. 2760706043
H, 0, -0. 0534577668, 2. 13366264, -1. 0014408338
H, 0, -2. 8280926873, -1. 6514438537, 1. 564832131
H, 0, -0. 4799587372, -1. 7205644508, 2. 3691511251
H, 0, 1. 4116073472, -2. 1210031979, -0. 2108460146
H, 0, 2. 6679160532, -2. 753023718, -2. 2142360634
H, 0, 4. 0561985198, -1. 0811415832, -3. 3898230639
H, 0, 4. 1618155416, 1. 2320061486, -2. 5312133269
H, 0, 2. 9052154601, 1. 8610763427, -0. 5329468235
H, 0, 2. 3081168069, 1. 9081436616, 1. 4882979123

Eelec= -1045. 8835422
Eelec+ZPE= -1045. 624895
H= -1045. 607717
G= -1045. 669769

(14) Product a-diarylation

C, 0, 1. 9650512581, 0. 3187238925, -2. 8322456795
 C, 0, 3. 0337003925, 1. 2194897439, -2. 9170138603
 C, 0, 3. 5134344177, 1. 8455560701, -1. 7896301837
 C, 0, 2. 9050801914, 1. 5448382221, -0. 5758077515
 C, 0, 1. 8422033385, 0. 6258510627, -0. 4521282127
 C, 0, 1. 3705163332, 0. 0189826865, -1. 6263666937
 N, 0, 3. 1667017939, 2. 0433339004, 0. 6696685451
 C, 0, 2. 3116791622, 1. 4787421339, 1. 5687335112
 C, 0, 1. 4817343176, 0. 5923983299, 0. 9498683265
 C, 0, 0. 3820400457, -0. 1951376352, 1. 6638219378
 C, 0, 0. 967857905, -0. 748496836, 2. 9813311744
 C, 0, -0. 0605769431, -1. 4338174041, 0. 8569966253
 C, 0, -1. 3999762281, -1. 68120477, 0. 5880240309
 C, 0, -1. 7882891236, -2. 8106039946, -0. 1184744879
 C, 0, -0. 8432011567, -3. 7204999753, -0. 5563903877
 C, 0, 0. 4967848024, -3. 4887879228, -0. 2863711437
 C, 0, 0. 8835682411, -2. 3571446455, 0. 4086554467
 F, 0, 0. 1111152933, -1. 5718720083, 3. 5914310797
 F, 0, 2. 0950657677, -1. 431409878, 2. 7994024941
 F, 0, 1. 25608682, 0. 2141098058, 3. 8688997703
 C, 0, -2. 1444975999, 3. 0001202617, -0. 7271733693
 C, 0, -3. 1535043411, 3. 5880644045, 0. 0453198823
 C, 0, -3. 336310099, 3. 2247596655, 1. 3606853373
 C, 0, -2. 4830594913, 2. 2603794045, 1. 8856537615
 C, 0, -1. 4534631108, 1. 6589610325, 1. 1355662354
 C, 0, -1. 3007701641, 2. 046855949, -0. 2003881746
 N, 0, -2. 4515358917, 1. 712300727, 3. 1386857681
 C, 0, -1. 4428287876, 0. 7926084337, 3. 2023733826
 C, 0, -0. 7895988197, 0. 7168403937, 2. 0096098827
 H, 0, 1. 5986524001, -0. 1508146745, -3. 7306787875
 H, 0, 3. 4796688213, 1. 4298511145, -3. 8754811219
 H, 0, 4. 3277625868, 2. 5506591077, -1. 8427317274
 H, 0, 0. 5479473228, -0. 6715167936, -1. 5976808914
 H, 0, 3. 8719921297, 2. 7145203612, 0. 8910817576
 H, 0, 2. 3599811318, 1. 7540962599, 2. 6021998774
 H, 0, -2. 1491178396, -0. 9878188347, 0. 9247563372
 H, 0, -2. 8344279115, -2. 9747662213, -0. 3210337448
 H, 0, -1. 144450002, -4. 5995535675, -1. 1031016636
 H, 0, 1. 2465488233, -4. 1862568824, -0. 6235393479
 H, 0, 1. 929001123, -2. 1853464973, 0. 5899881138
 H, 0, -2. 0254231749, 3. 2997918566, -1. 7557216457
 H, 0, -3. 7969226394, 4. 3320095976, -0. 39589591
 H, 0, -4. 1139390544, 3. 6678175667, 1. 9624861426
 H, 0, -0. 5345348452, 1. 6136045129, -0. 81631723
 H, 0, -3. 0478192321, 1. 9625270545, 3. 8992879586
 H, 0, -1. 2690099631, 0. 2579669894, 4. 1133396357

Eelec= -1333. 1000736
Eelec+ZPE= -1332. 731264
H= -1332. 708758
G= -1332. 782240

(15) Indole

C, 0, -1. 6824089979, 1. 2887970236, 0. 1257312631
C, 0, -2. 1018961913, -0. 0483943107, 0. 1257655232
C, 0, -1. 1939837437, -1. 0819468434, 0. 0383082095
C, 0, 0. 1531823729, -0. 7479974203, -0. 0498481219
C, 0, 0. 5982292933, 0. 5892165552, -0. 0516199206
C, 0, -0. 3467574246, 1. 6141927283, 0. 0381792621
N, 0, 1. 2625405372, -1. 5469347594, -0. 146707591
C, 0, 2. 3831009952, -0. 7569251406, -0. 2080297668
C, 0, 2. 0257892407, 0. 5500369707, -0. 1536550597
H, 0, -2. 419818805, 2. 0718897942, 0. 1954631402
H, 0, -3. 1539408161, -0. 2726697257, 0. 1954154077
H, 0, -1. 5181889043, -2. 110451052, 0. 038332203
H, 0, -0. 0333478442, 2. 6460651047, 0. 0388728902
H, 0, 1. 2582739556, -2. 544940734, -0. 1671444376
H, 0, 3. 3562980318, -1. 2018362702, -0. 2869389908
H, 0, 2. 6946673004, 1. 3886430798, -0. 1825470105

Eelec= -363. 591965
Eelec+ZPE= -363. 457081
H= -363. 450055
G= -363. 487266

(16) Phosphoric Model

C, 0, -2. 184172809, 0. 7231236658, 0. 0980156913
C, 0, -1. 1293026487, 1. 4925077135, -0. 1311366374
C, 0, -2. 2081693289, -0. 7196748376, -0. 0895314409
C, 0, -1. 174413829, -1. 5163727893, 0. 1396330132
O, 0, 0. 0397650627, 1. 0347169054, -0. 6835924237
O, 0, 0. 0043934829, -1. 0658974729, 0. 6842173111
P, 0, 1. 0033466462, -0. 0760957049, -0. 0662599458
O, 0, 1. 9249350046, -0. 6281861803, -1. 0464216818
O, 0, 1. 6937712643, 0. 6026984243, 1. 1935245748
H, 0, -3. 0840561964, 1. 2102521404, 0. 4370294859
H, 0, -1. 1225280187, 2. 5572520224, 0. 0191078337
H, 0, -3. 1242689121, -1. 1792392428, -0. 4234097139
H, 0, -1. 1873272697, -2. 5817122805, -0. 0044321747
H, 0, 2. 6471205518, 0. 6261176364, 1. 0830591082

Eelec= -797. 4587043
Eelec+ZPE= -797. 358680
H= -797. 349738
G= -797. 391806

D. Cartesian coordinates and total energies of the reported transition states and intermediates for the simplified model of chiral phosphoric acid-catalyzed diarylation reaction between acetophenone and indole at BH and HLYP/6-31G(d) level.

(1) IN1b

C, 0, -5.71715811, -0.6718449788, 1.2824795363
C, 0, -4.4756103354, -0.8302617619, 1.7190302696
C, 0, -6.0800283251, 0.1056693575, 0.1070896277
C, 0, -5.3433542179, 0.1917798505, -0.99156013
O, 0, -3.3983803289, -0.1836199224, 1.1686614893
O, 0, -4.197114646, -0.5363250606, -1.1894157318
P, 0, -2.8672216507, -0.393018516, -0.3233710275
O, 0, -1.9545897477, 0.6909447522, -0.6926169399
O, 0, -2.3056072999, -1.8416576209, -0.4428712187
H, 0, -6.5045192339, -1.1434691092, 1.8478345905
H, 0, -4.2138456155, -1.4127221902, 2.5843175811
H, 0, -7.0148191239, 0.6425322988, 0.1164425848
H, 0, -5.6176369723, 0.7732010347, -1.8535029293
C, 0, 1.261462699, -1.6606571236, -0.8032533025
O, 0, 0.3127350132, -2.1372261307, -0.2016952504
C, 0, 2.6299778039, -2.1289750317, -0.4822223201
C, 0, 1.0621849777, -0.6249121291, -1.8698758728
C, 0, 2.781405316, -3.1585221563, 0.445685988
C, 0, 4.0399004401, -3.6269854015, 0.7682130181
C, 0, 5.1608377287, -3.0690484664, 0.1685679094
C, 0, 5.0203871422, -2.043296165, -0.752738712
C, 0, 3.7596246855, -1.5745988844, -1.0786501554
H, 0, -1.3202548651, -1.9074775708, -0.3883109213
H, 0, 1.4222903776, -0.9994080717, -2.8258374142
H, 0, 0.0134095278, -0.3686989378, -1.9449637555
H, 0, 1.6207360654, 0.2756758394, -1.6312392713
H, 0, 1.9002919073, -3.5767390427, 0.9003516702
H, 0, 4.150729414, -4.4241988687, 1.4848026246
H, 0, 6.1435472413, -3.4332947673, 0.421302055
H, 0, 5.890573574, -1.6062602654, -1.2137687045
H, 0, 3.6627651581, -0.7723586628, -1.7895524582
C, 0, 3.6530833465, 2.3122590524, 1.589403714
C, 0, 2.6955712702, 1.3103985968, 1.8060768499
C, 0, 1.4695585145, 1.3469247611, 1.1768880087
C, 0, 1.21768804, 2.4111396077, 0.3135515355
C, 0, 2.1672491811, 3.4294596816, 0.0809276658
C, 0, 3.3991561232, 3.3656936919, 0.7385762939
N, 0, 0.1119162334, 2.6915786145, -0.4388793832
C, 0, 0.334706505, 3.8464860378, -1.1350445598
C, 0, 1.5706906246, 4.3362873536, -0.8505414741
H, 0, 4.6005827537, 2.2544026408, 2.1008845762
H, 0, 2.9217820504, 0.4989623351, 2.4790421085
H, 0, 0.7271192623, 0.5836087793, 1.3472116293
H, 0, 4.1415662418, 4.1325183572, 0.5810097813

H, 0, -0.7051279194, 2.1049266567, -0.5063855742
H, 0, -0.4212877252, 4.2354496708, -1.7902873364
H, 0, 2.0048198981, 5.2328228653, -1.2502136645

Eelec= -1545.7529738
Eelec+ZPE= -1545.371424
H= -1545.345289
G= -1545.455723

(2) TS1b

C, 0, -5.6404208484, -0.8037859058, 1.3553844971
C, 0, -4.4185214517, -0.528834852, 1.7963278319
C, 0, -6.1817593691, -0.309706489, 0.0986327174
C, 0, -5.4600482899, -0.140292212, -1.0026160494
O, 0, -3.5723818394, 0.3438139082, 1.1818316406
O, 0, -4.1570198954, -0.5250899134, -1.1115951766
P, 0, -2.9326918709, 0.142073187, -0.2916933105
O, 0, -2.5916965722, 1.4951118903, -0.8072223842
O, 0, -1.861019562, -0.9068355018, -0.269057234
H, 0, -6.2652040396, -1.4248535717, 1.9775802038
H, 0, -4.0296067933, -0.9139396048, 2.7240039406
H, 0, -7.2320299454, -0.0699492248, 0.0478356006
H, 0, -5.8696754577, 0.2422912624, -1.9221899055
H, 0, -0.4339769324, -0.8486690582, 0.3016789138
C, 0, 1.3247679673, -1.3672166965, -0.3293503364
O, 0, 0.5396057817, -0.8372711659, 0.5730534387
C, 0, 2.7088307819, -1.6029314078, 0.1640720489
C, 0, 0.7127352143, -2.4289307696, -1.2123142712
C, 0, 3.0725032846, -1.1426340224, 1.4262813498
C, 0, 4.3435088699, -1.3855444464, 1.9195306246
C, 0, 5.2681186677, -2.0799315165, 1.1569567771
C, 0, 4.9153077109, -2.5362840244, -0.1050560626
C, 0, 3.6442429079, -2.3017319013, -0.5966380569
H, 0, 0.7227484158, -3.3632653774, -0.6532049879
H, 0, -0.3180084767, -2.1863146488, -1.4370493092
H, 0, 1.2678828339, -2.5815001872, -2.1299447266
H, 0, 2.3499343121, -0.6057010922, 2.0135705271
H, 0, 4.6101267269, -1.0299770351, 2.9013639582
H, 0, 6.2573098443, -2.2674849203, 1.5419325992
H, 0, 5.6279987824, -3.0798504604, -0.70351464
H, 0, 3.3864228674, -2.6670677067, -1.5767258379
C, 0, 3.5174437051, 2.7322132844, 0.4621711907
C, 0, 2.3789577062, 3.4838586388, 0.7583256208
C, 0, 1.143470341, 3.1465554202, 0.2361981315
C, 0, 1.0957785817, 2.0386311962, -0.5904878974
C, 0, 2.2191656853, 1.2620189419, -0.8898638721
C, 0, 3.4501713741, 1.6159697015, -0.3534398081
N, 0, 0.0102385264, 1.5018033457, -1.2775611474
C, 0, 0.3992629444, 0.4633964953, -1.9798193687
C, 0, 1.7483997592, 0.1487661126, -1.7016046976

H, 0, 4. 4661851521, 3. 0271673033, 0. 8799087085
H, 0, 2. 4646814114, 4. 3437648262, 1. 4020294982
H, 0, 0. 258173604, 3. 7186350465, 0. 4575209529
H, 0, 4. 3332319297, 1. 036346179, -0. 5652195976
H, 0, -0. 9980814913, 1. 715391231, -1. 1264214966
H, 0, -0. 3127066555, -0. 0881389805, -2. 5628667101
H, 0, 2. 3669908016, -0. 4083122777, -2. 3808678879

Eelec= -1545. 7157724
Eelec+ZPE= -1545. 332757
H= -1545. 309166
G= -1545. 387204

(3) IN2b

C, 0, -0. 7254754041, 5. 6537520268, -0. 7842460455
C, 0, -0. 8077299957, 4. 5209759859, -0. 0969385245
C, 0, 0. 4194046848, 6. 026010182, -1. 6012971414
C, 0, 1. 1476105038, 5. 1610107505, -2. 2969440863
O, 0, 0. 2213820454, 3. 6338937371, 0. 0137462878
O, 0, 0. 8325607554, 3. 8408061016, -2. 4224044865
P, 0, 0. 8281854658, 2. 7697662568, -1. 2118718824
O, 0, 2. 2287858246, 2. 4104807075, -0. 8159120064
O, 0, -0. 0882875593, 1. 6660582161, -1. 6198398205
H, 0, -1. 5578834098, 6. 336489102, -0. 720488999
H, 0, -1. 6670034645, 4. 2511200998, 0. 4934903233
H, 0, 0. 6971883684, 7. 0666706398, -1. 6561045083
H, 0, 2. 0023468517, 5. 4504367755, -2. 8845773066
C, 0, -0. 7082525617, -1. 6277277404, -1. 1824895238
O, 0, -1. 0318319097, -0. 5648831409, -0. 3497617979
C, 0, -1. 4013316419, -2. 8764724794, -0. 6610252505
C, 0, -1. 1407643828, -1. 3378074431, -2. 6216700043
C, 0, -2. 2019123263, -2. 8108680526, 0. 471498329
C, 0, -2. 8367363325, -3. 9474048895, 0. 9498146902
C, 0, -2. 6789977142, -5. 1634103445, 0. 3064124075
C, 0, -1. 8834382525, -5. 2368450791, -0. 8270654163
C, 0, -1. 2520242466, -4. 1011909768, -1. 3059019156
H, 0, -0. 8088554724, 0. 2851885499, -0. 7766233193
H, 0, -2. 2245504294, -1. 2850526525, -2. 6494163418
H, 0, -0. 7561974058, -0. 3789210261, -2. 955284854
H, 0, -0. 8213612087, -2. 1140298471, -3. 3117333655
H, 0, -2. 3189425209, -1. 865189147, 0. 9680305065
H, 0, -3. 4557100652, -3. 8791573221, 1. 8300388852
H, 0, -3. 1725356397, -6. 0458161598, 0. 680447827
H, 0, -1. 75693529, -6. 1761322412, -1. 3410425209
H, 0, -0. 642157656, -4. 179086498, -2. 1927744721
C, 0, 1. 8752766453, -2. 9407729233, 2. 4416127174
C, 0, 2. 6231873251, -1. 8107682571, 2. 7464571679
C, 0, 2. 7865305509, -0. 7929141977, 1. 8167701636
C, 0, 2. 1684518421, -0. 9678746023, 0. 5995865025
C, 0, 1. 4032075142, -2. 080784877, 0. 273739261

C, 0, 1. 2549771943, -3. 0883024246, 1. 2051729349
N, 0, 2. 2068762719, -0. 1128876287, -0. 5237474526
C, 0, 1. 5447742873, -0. 6136230843, -1. 4976161431
C, 0, 0. 8671301546, -1. 8807337753, -1. 1191400861
H, 0, 1. 7688119956, -3. 7183447918, 3. 1799053747
H, 0, 3. 086398769, -1. 7229511687, 3. 7150766011
H, 0, 3. 3654624099, 0. 0887015263, 2. 0335613374
H, 0, 0. 6694617202, -3. 9648434777, 0. 9888632063
H, 0, 2. 4561728428, 0. 931422786, -0. 5545814209
H, 0, 1. 4325213604, -0. 0668470139, -2. 4133856431
H, 0, 1. 1106335063, -2. 68842318, -1. 8043321882

Eelec= -1545. 7283074
Eelec+ZPE= -1545. 343798
H= -1545. 320119
G= -1545. 398187

(4) TS2b

C, 0, 2. 538957698, 4. 720974858, 0. 9166268465
C, 0, 1. 7955699984, 3. 9041599799, 1. 6572713222
C, 0, 3. 3237740988, 4. 2872491247, -0. 229476433
C, 0, 2. 9482524837, 3. 3247012806, -1. 0673163589
O, 0, 1. 7865132536, 2. 5510668235, 1. 491529833
O, 0, 1. 7315286001, 2. 7160445227, -1. 0167314796
P, 0, 1. 1876660091, 1. 786257734, 0. 1925689446
O, 0, 1. 8666164848, 0. 4419003229, 0. 1722168752
O, 0, -0. 2959824509, 1. 8102791169, 0. 1476033627
H, 0, 2. 5602693794, 5. 7626111847, 1. 1944993842
H, 0, 1. 2040415578, 4. 2399905239, 2. 4920988018
H, 0, 4. 2632003505, 4. 7776592322, -0. 4287885066
H, 0, 3. 5482045271, 3. 0100814815, -1. 9045116607
C, 0, -1. 0745964228, -1. 4784696421, -0. 1889229981
O, 0, -1. 5010706589, -0. 5086618231, 0. 7218336592
C, 0, -1. 9564553428, -2. 7112925886, 0. 0135852862
C, 0, -1. 1859541279, -0. 9601781019, -1. 6199419922
C, 0, -2. 9843282738, -2. 6929450438, 0. 9510522895
C, 0, -3. 788563957, -3. 8093410992, 1. 1421748453
C, 0, -3. 5818937393, -4. 9603189294, 0. 3989828568
C, 0, -2. 5635923208, -4. 9855272347, -0. 5433871294
C, 0, -1. 7609866989, -3. 8714906101, -0. 7339804969
C, 0, 2. 6932885222, -3. 8589851551, -2. 1165604222
C, 0, 3. 4223519202, -4. 4879974764, -1. 1061935741
C, 0, 3. 1376987662, -4. 2455008055, 0. 2257531106
C, 0, 2. 0958584693, -3. 3752665367, 0. 4881105322
C, 0, 1. 3401684043, -2. 7402245809, -0. 4965455264
C, 0, 1. 6640474748, -2. 9785456466, -1. 8263722751
N, 0, 1. 6099081014, -2. 9401758025, 1. 7315674922
C, 0, 0. 6232336102, -2. 0970555743, 1. 5737673866
C, 0, 0. 4012915599, -1. 8139131381, 0. 1885513313
H, 0, -1. 1335302443, 0. 371044499, 0. 4949645812

H, 0, -2.2149821047, -0.6636106978, -1.7961853957
H, 0, -0.5505107796, -0.0925339166, -1.763554166
H, 0, -0.926456224, -1.7208266333, -2.3484773109
H, 0, -3.1531383306, -1.7957114904, 1.5183169122
H, 0, -4.5826461745, -3.7722755904, 1.8706246293
H, 0, -4.2088738182, -5.8247744139, 0.5453697283
H, 0, -2.3950537986, -5.8708017145, -1.1351981952
H, 0, -0.9807255473, -3.9160364902, -1.4746477495
H, 0, 2.9441515805, -4.0556880444, -3.145627681
H, 0, 4.2214034606, -5.1617848182, -1.3655563784
H, 0, 3.7050130224, -4.7096003985, 1.0155245512
H, 0, 1.1355167866, -2.4848857778, -2.6226118968
H, 0, 2.0011681848, -3.1987561999, 2.61849704
H, 0, 0.1076419075, -1.6477219203, 2.4024354639
H, 0, 1.0090618029, -0.7662097889, 0.1625065607

Eelec= -1545.6996829

Eelec+ZPE= -1545.318923

H= -1545.295474

G= -1545.373911

(5) IN3b

C, 0, -3.0545709932, -1.0535147091, -0.2059063787
C, 0, -3.8194003272, -1.8516794987, 0.6546937718
C, 0, -3.2290482582, -2.80176562, 1.4595630582
C, 0, -1.8468402591, -2.9352248131, 1.3853505989
C, 0, -1.057952467, -2.1439940067, 0.5307418095
C, 0, -1.6856733959, -1.1911957519, -0.2763786167
N, 0, -1.0017047577, -3.7818452573, 2.0548011143
C, 0, 0.2859145023, -3.5415711665, 1.6535099009
C, 0, 0.3100501902, -2.5523710117, 0.7227014768
C, 0, 1.5164258656, -1.9706615383, 0.0427604673
C, 0, 2.8159201717, -2.6022329821, 0.5414093304
C, 0, 1.4328240164, -2.130305989, -1.4774651361
C, 0, 1.0885005709, -3.3644238694, -2.0215899951
C, 0, 1.0678092432, -3.5570027521, -3.3912790319
C, 0, 1.3899699809, -2.5139278863, -4.2465089228
C, 0, 1.7314499342, -1.2830015867, -3.7155663004
C, 0, 1.7547904289, -1.0905115802, -2.3409825679
H, 0, -3.5478040531, -0.3201054024, -0.8225317232
H, 0, -4.8888972264, -1.7204066287, 0.6877679796
H, 0, -3.8170172748, -3.4172010612, 2.1218237981
H, 0, -1.1094834199, -0.5756220258, -0.9463125199
H, 0, -1.2763148547, -4.4616514275, 2.732237523
H, 0, 1.0948200117, -4.1063289586, 2.0742676702
H, 0, 3.6623785681, -2.1226306078, 0.0562724066
H, 0, 2.9101470522, -2.4660172039, 1.6148534821
H, 0, 2.8586673456, -3.6611558264, 0.3052085755
H, 0, 0.8195280323, -4.175743387, -1.3646326342

H, 0, 0.7931693209, -4.5201017211, -3.7910504174
 H, 0, 1.3703426837, -2.6603186198, -5.3144404444
 H, 0, 1.9809894427, -0.4620252082, -4.3685204992
 H, 0, 2.023047653, -0.1204323234, -1.9583700907
 C, 0, 0.9140140373, 5.6525426569, 0.9232229806
 C, 0, 1.1279154927, 4.5696098968, 1.6572182903
 C, 0, 1.3574664216, 5.8089335435, -0.4538784238
 C, 0, 1.4053074973, 4.8241246174, -1.339937235
 O, 0, 1.8935503083, 3.513920695, 1.2316677323
 O, 0, 0.9340814064, 3.5607359132, -1.0862541369
 P, 0, 1.5414327219, 2.5621535787, -0.0007933408
 O, 0, 2.7077396558, 1.7710109726, -0.4034786866
 O, 0, 0.2679996873, 1.7371110538, 0.3845772885
 H, 0, 0.3850468484, 6.4689224595, 1.3877545187
 H, 0, 0.7883747196, 4.4547925624, 2.6711413873
 H, 0, 1.6585040049, 6.7885864163, -0.7882219902
 H, 0, 1.7405079339, 4.9451646724, -2.354473844
 O, 0, 1.5363447047, -0.5931217193, 0.4140686548
 H, 0, 0.4801962513, 0.7796987846, 0.4694230967
 H, 0, 2.318421581, -0.1393976832, 0.0737270237

Eelec= -1545.7397433
 Eelec+ZPE= -1545.355111
 H= -1545.330633
 G= -1545.412091

(6) TS3b

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 C, 0, 2.6683311143, -0.2870038208, 1.5811698481
 C, 0, 1.725342736, -0.3129667544, 0.5661276459
 C, 0, 1.1635043793, -1.5033493315, 0.0675354923
 C, 0, 1.6121446717, -2.7128616224, 0.5996299175
 N, 0, 1.1887373748, 0.7418500819, -0.1493032384
 C, 0, 0.3322773314, 0.2794118209, -1.0538197521
 C, 0, 0.2398473289, -1.1013550741, -0.985897808
 C, 0, -0.7733993872, -1.8063335841, -1.7042450211
 C, 0, -1.1878789688, -1.2494477822, -3.0434894409
 C, 0, -0.8694117044, -3.291449935, -1.5633021899
 C, 0, -0.5158351376, -4.1005272226, -2.6390437559
 C, 0, -0.5595867939, -5.4810006161, -2.5247636041
 C, 0, -0.9774410482, -6.0676898623, -1.342551212
 C, 0, -1.3420691808, -5.2670142267, -0.2701606028
 C, 0, -1.2813881508, -3.8887111204, -0.374424603
 H, 0, 2.8950494382, -3.6299940948, 2.0261660757
 H, 0, 3.8011078011, -1.5189445268, 2.8981281017
 H, 0, 3.073024837, 0.6451704932, 1.939664926
 H, 0, 1.2381876431, -3.651675022, 0.2337412936
 H, 0, 1.1538929207, 1.713539266, 0.1153873005
 H, 0, -0.2372145204, 0.9700275748, -1.6360651976

H, 0, -2.0357618533, -1.7936829885, -3.445483304
H, 0, -1.449917329, -0.2017424707, -2.96615483
H, 0, -0.3592118203, -1.3455068281, -3.7404064391
H, 0, -0.1918719093, -3.6599439344, -3.5667889124
H, 0, -0.2733197282, -6.0938208079, -3.3636829449
H, 0, -1.0220623731, -7.1411311818, -1.2570567234
H, 0, -1.6728675545, -5.7158404024, 0.652147649
H, 0, -1.5620396654, -3.266790022, 0.4566359389
O, 0, -2.3238031932, -1.3285169802, -0.747362247
H, 0, -2.3966308794, -0.3013266051, -0.7613530046
H, 0, -3.1270930582, -1.6587062544, -1.1615322228
C, 0, -2.9096267623, 4.2760329317, 2.1852614566
C, 0, -2.8225972815, 2.9512935924, 2.2672351433
C, 0, -2.9956110116, 5.1372590269, 1.0133439216
C, 0, -3.0769867935, 4.8005769532, -0.2689552976
O, 0, -2.7970570341, 2.0459103826, 1.255263209
O, 0, -3.116859607, 3.538360203, -0.7774208934
P, 0, -2.1601337745, 2.3535212032, -0.2136993977
O, 0, -0.7585546149, 2.8116149369, -0.0955799142
O, 0, -2.5083768875, 1.1500269852, -1.0420020619
H, 0, -2.9201992119, 4.7837993959, 3.1361484532
H, 0, -2.7914791959, 2.4599246433, 3.22463973
H, 0, -2.997996129, 6.196990212, 1.2104389705
H, 0, -3.1521240157, 5.5448504369, -1.042922053

Eelec= -1545.7009933

Eelec+ZPE= -1545.318261

H= -1545.294108

G= -1545.374097

(7) IN4b

C, 0, -2.8837018094, -2.7305784927, -0.4897961757
C, 0, -2.7740208654, -1.5763688037, -1.2592449836
C, 0, -1.8122554648, -0.6220074256, -0.9694846709
C, 0, -0.9801444959, -0.8839713261, 0.0978298048
C, 0, -1.0515702368, -2.0410962829, 0.8771744746
C, 0, -2.0343235323, -2.9751654912, 0.5799065974
N, 0, 0.0338438089, -0.0599222891, 0.6004406111
C, 0, 0.5841588446, -0.5982720644, 1.6383488903
C, 0, -0.0178531231, -1.8877373267, 1.9166797131
C, 0, 0.3476380157, -2.6737599427, 2.959902621
C, 0, 1.3175015356, -2.2311342073, 4.0109575546
C, 0, -0.1698118673, -4.0491215686, 3.1227112723
C, 0, -0.7803187028, -4.448509948, 4.3102908019
C, 0, -1.2239943664, -5.7500846724, 4.4672128754
C, 0, -1.0330070291, -6.6777759281, 3.4549996474
C, 0, -0.406215168, -6.2957525125, 2.2789420547
C, 0, 0.015265845, -4.9882422631, 2.1094423773
H, 0, -3.6470015858, -3.4530730979, -0.7278074249
H, 0, -3.4487806003, -1.4190635776, -2.0841891376

H, 0, -1. 7123132054, 0. 2889836105, -1. 5350926899
H, 0, -2. 1464821996, -3. 8738516694, 1. 1584173697
H, 0, 0. 2837901578, 0. 9059130365, 0. 1826283791
H, 0, 1. 3928242426, -0. 1115395124, 2. 1624567494
H, 0, 1. 6925094567, -1. 2231404669, 3. 8840671395
H, 0, 0. 8378545862, -2. 295930258, 4. 9867637187
H, 0, 2. 1546225135, -2. 926892749, 4. 0429737449
H, 0, -0. 9315557889, -3. 7356749802, 5. 1041177926
H, 0, -1. 7130348965, -6. 0405610243, 5. 3824442345
H, 0, -1. 3674112769, -7. 6941440547, 3. 5837382755
H, 0, -0. 2453750429, -7. 0145840245, 1. 49232418
H, 0, 0. 4994891831, -4. 6913749357, 1. 1938362297
O, 0, 2. 7475386011, 0. 7377951653, 3. 4735110997
H, 0, 2. 4936419607, 1. 5040044621, 2. 925844022
H, 0, 3. 6673555642, 0. 6017708429, 3. 2461590384
C, 0, 2. 8965497597, 5. 8963555634, -0. 6945536209
C, 0, 3. 382899049, 4. 660905991, -0. 6619342333
C, 0, 1. 4756954818, 6. 2073369244, -0. 7120003457
C, 0, 0. 5561431751, 5. 4973745155, -0. 0684752626
O, 0, 2. 612276017, 3. 5445135927, -0. 7643811651
O, 0, 0. 8526978907, 4. 4743796726, 0. 77807289
P, 0, 1. 5179339509, 3. 0641513459, 0. 3324648563
O, 0, 0. 5281988763, 2. 2311956239, -0. 425678062
O, 0, 2. 1562149768, 2. 4782706808, 1. 5332062645
H, 0, 3. 6042884007, 6. 7100248129, -0. 7156540235
H, 0, 4. 4387831405, 4. 4484243253, -0. 6338255916
H, 0, 1. 1411030444, 7. 0658158463, -1. 272753808
H, 0, -0. 4951358216, 5. 7301488841, -0. 1046640855

Eelec= -1545. 7285611

Eelec+ZPE= -1545. 347632

H= -1545. 321633

G= -1545. 407900

(8) IN5b

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C, 0, -2. 4639320005, -0. 2573118354, 4. 3721964074
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C, 0, -1. 7779895758, -1. 3020430026, 1. 8880755125
C, 0, -2. 0920989542, -2. 1689157244, 2. 925239526
N, 0, -1. 5457138371, 0. 752647903, 0. 9387856804
C, 0, -1. 3168141733, -0. 0911921835, -0. 011021448
C, 0, -1. 4259010471, -1. 4499103345, 0. 4669302992
C, 0, -1. 2196627764, -2. 5422689817, -0. 3099976693
C, 0, -1. 0271390988, -2. 4623932851, -1. 7894314477
C, 0, -1. 1195381144, -3. 8970408899, 0. 2698212291
C, 0, -0. 1244631716, -4. 1726635685, 1. 2064758886
C, 0, 0. 011572435, -5. 450965384, 1. 719743291
C, 0, -0. 8516223693, -6. 4596040607, 1. 31924189

C, 0, -1.8427726466, -6.191778403, 0.3877395425
 C, 0, -1.9659622873, -4.921541274, -0.1483565995
 H, 0, -2.6702866113, -2.2981471822, 4.971599207
 H, 0, -2.7242093903, 0.1251491792, 5.3450366605
 H, 0, -2.1984060307, 1.6936097765, 3.4804368198
 H, 0, -2.0721844904, -3.2348682912, 2.7890320121
 H, 0, -1.4299620833, 1.8314879346, 0.8374552674
 H, 0, -1.0249571844, 0.2465531792, -0.987316254
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 H, 0, -1.6435352108, -3.2127382954, -2.2791809597
 H, 0, -1.2648253699, -1.4941950322, -2.2092741687
 H, 0, 0.5523680615, -3.3885104005, 1.5038003992
 H, 0, 0.7927356712, -5.6586285615, 2.4325144623
 H, 0, -0.7484569525, -7.452095573, 1.7264973618
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 H, 0, -2.7383735382, -4.7207789892, -0.8731555994
 C, 0, 2.2146022861, -1.2354610711, -3.3593678673
 C, 0, 1.7294183923, 0.0735527069, -3.2121862048
 C, 0, 1.654196929, 0.6737285455, -1.9724399001
 C, 0, 2.068712398, -0.071814774, -0.8689472922
 C, 0, 2.5539575818, -1.3934327346, -0.992930088
 C, 0, 2.6278546253, -1.9682578281, -2.266729487
 N, 0, 2.0962400535, 0.2659678299, 0.453427528
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 H, 0, 1.3067654667, 1.6886074493, -1.8555590334
 H, 0, 3.012531235, -2.9686257424, -2.393340282
 H, 0, 1.8419856989, 1.1830795937, 0.8220957546
 H, 0, 2.7122939456, -0.7094234479, 2.2260175633
 H, 0, 3.299146118, -2.7739574416, 0.6165536358
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 C, 0, 1.5191220785, 5.1284027448, -1.1367485494
 C, 0, 0.3942600537, 6.9551087034, 0.0604999463
 C, 0, -0.1287082602, 6.3018089498, 1.0912077641
 O, 0, 0.5776250835, 4.1983080965, -0.8140334023
 O, 0, 0.334375763, 5.0984667801, 1.5299397317
 P, 0, 0.2314805285, 3.7137570952, 0.7022465773
 O, 0, -1.195435857, 3.2471991342, 0.6435545221
 O, 0, 1.2637281749, 2.7927096258, 1.2267451705
 H, 0, 2.1782426101, 7.0800652652, -1.1982552731
 H, 0, 2.3059138183, 4.7391931249, -1.761165084
 H, 0, 0.0270111256, 7.9495869586, -0.1380352514
 H, 0, -0.9085651004, 6.7102802156, 1.7117678945

Eelec= -1832.9472009

Eelec+ZPE= -1832.456292

H= -1832.425285

G= -1832.524126

(9) TS4b

C, 0, -2.309838592, 3.4142851493, -0.260451
C, 0, -1.1252860523, 3.9755535875, -0.7459599511
C, 0, -0.131880655, 3.1772529031, -1.2718451496
C, 0, -0.3610767555, 1.8094233957, -1.3005458642
C, 0, -1.5454824275, 1.2176893445, -0.8289976819
C, 0, -2.5299556637, 2.0521202799, -0.2953931866
N, 0, 0.4696972698, 0.8092984007, -1.7607256837
C, 0, -0.1240005084, -0.3669733647, -1.5941898527
C, 0, -1.3981277437, -0.2167643607, -1.0424573619
C, 0, -2.2660072972, -1.3004256268, -0.7054385446
C, 0, -2.1283783659, -2.5886328798, -1.4975763581
C, 0, -3.7287990191, -0.9631316396, -0.5184898078
C, 0, -4.5327928332, -1.3142046714, 0.5587981953
C, 0, -5.8906158268, -1.0252472835, 0.5614481379
C, 0, -6.4772958228, -0.3923451391, -0.5183839211
C, 0, -5.6914077533, -0.0466141555, -1.6066244305
C, 0, -4.3376344291, -0.3262904008, -1.6043948294
H, 0, -3.0679186308, 4.0593851916, 0.1534688704
H, 0, -0.9859585198, 5.0435425965, -0.7052475483
H, 0, 0.7908882657, 3.5897629939, -1.6447917655
H, 0, -3.4454109638, 1.6485610677, 0.0971498631
H, 0, 1.4779031563, 0.8782138855, -1.9645924016
H, 0, 0.4139932064, -1.2591060762, -1.8483744375
H, 0, -2.6023634563, -3.417827036, -0.980804927
H, 0, -2.6450131848, -2.4623940021, -2.446941143
H, 0, -1.1004290021, -2.8500168014, -1.7147463731
H, 0, -4.1211602383, -1.805027826, 1.4193995921
H, 0, -6.4857409417, -1.3016024504, 1.4166893317
H, 0, -7.5318634543, -0.1704895769, -0.5139954778
H, 0, -6.1291291765, 0.4476075408, -2.458602362
H, 0, -3.7362910117, -0.0392075691, -2.4506835653
C, 0, -1.5330845835, 1.1951668416, 3.2951589569
C, 0, -0.1871893243, 1.4847897974, 3.0632703634
C, 0, 0.6042700684, 0.6438326754, 2.3034416253
C, 0, -0.0065106324, -0.4873827974, 1.7924641374
C, 0, -1.3590245671, -0.7886113792, 1.9861761493
C, 0, -2.1326157608, 0.0706944064, 2.756898923
N, 0, 0.5639003086, -1.5228465296, 1.0531100576
C, 0, -0.3402880165, -2.4386424352, 0.8100027624
C, 0, -1.6200701726, -1.9991317764, 1.2160680061
H, 0, -2.1183961689, 1.8672569913, 3.9010393879
H, 0, 0.2427798482, 2.3766867017, 3.4878934136
H, 0, 1.6457807238, 0.846064792, 2.1151917607
H, 0, -3.176556456, -0.1259242092, 2.9344294428
H, 0, 1.5235307543, -1.5223060089, 0.6296732316
H, 0, -0.07907007, -3.3270123797, 0.2675110487
H, 0, -2.4047874359, -2.7030284891, 1.4155345752
C, 0, 6.6208006337, -0.7433451352, 0.5284235788

C, 0, 6. 0013187794, -1. 4542524011, -0. 4067576029
C, 0, 6. 2946069864, 0. 6399821919, 0. 8397404418
C, 0, 5. 0642218812, 1. 1384572781, 0. 7999278971
O, 0, 5. 0766086333, -0. 9296988772, -1. 2557411598
O, 0, 3. 9514210199, 0. 3839216959, 0. 5850415972
P, 0, 3. 6131184125, -0. 4034700354, -0. 8099674702
O, 0, 3. 1515487845, 0. 5420114594, -1. 8564926732
O, 0, 2. 7424151434, -1. 5476066855, -0. 3968514573
H, 0, 7. 4169652074, -1. 2230628682, 1. 0755603194
H, 0, 6. 2430100265, -2. 4822415769, -0. 6197413917
H, 0, 7. 0932695206, 1. 3077439288, 1. 1221244796
H, 0, 4. 8465348835, 2. 1719363476, 1. 0135082329

Eelec= -1832. 913674

Eelec+ZPE= -1832. 420535

H= -1832. 391500

G= -1832. 481668

(10) IN6b

C, 0, -2. 3759554654, -0. 9098104583, 3. 4347070479
C, 0, -2. 6835718653, 0. 456777759, 3. 4069203341
C, 0, -2. 668336646, 1. 1569249711, 2. 2230433565
C, 0, -2. 3381951778, 0. 4605789289, 1. 0647725008
C, 0, -2. 0121960645, -0. 9107642577, 1. 06218446
C, 0, -2. 0424714956, -1. 5963834696, 2. 28758655
N, 0, -2. 2410263829, 0. 9356955232, -0. 214028014
C, 0, -1. 8136647606, -0. 0775586083, -1. 0143301093
C, 0, -1. 6611925964, -1. 2379717929, -0. 3075817942
C, 0, -0. 9340075107, -2. 4669068304, -0. 8350215097
C, 0, -1. 3871000482, -2. 8181119395, -2. 2601542729
C, 0, -1. 2129984255, -3. 6946953209, 0. 0409076179
C, 0, -0. 2428826391, -4. 4569707939, 0. 6786932264
C, 0, -0. 5844935123, -5. 5701374419, 1. 4382506029
C, 0, -1. 9061762221, -5. 9471475617, 1. 5717462493
C, 0, -2. 8889330865, -5. 1950416238, 0. 9430069775
C, 0, -2. 5446883373, -4. 0870237375, 0. 1944443557
H, 0, -2. 3993141798, -1. 4362255368, 4. 3754148153
H, 0, -2. 9298299293, 0. 9649441337, 4. 3250133062
H, 0, -2. 8831082999, 2. 2115546837, 2. 1817843766
H, 0, -1. 8121719817, -2. 6447460709, 2. 3470499183
H, 0, -2. 012570995, 1. 9092154767, -0. 3905863739
H, 0, -1. 6099762915, 0. 116444414, -2. 0499418179
H, 0, -0. 8128657108, -3. 655522246, -2. 6513344619
H, 0, -2. 4315497369, -3. 106209535, -2. 2540928041
H, 0, -1. 2787848317, -1. 979501859, -2. 9368862861
H, 0, 0. 8006321486, -4. 2021457606, 0. 6156293836
H, 0, 0. 1934275058, -6. 1366876788, 1. 9241157282
H, 0, -2. 1715031113, -6. 8099158408, 2. 160519238
H, 0, -3. 9271201697, -5. 4665849872, 1. 0448203952
H, 0, -3. 3239772206, -3. 4953509259, -0. 256685037

C, 0, 1. 8041027555, -0. 4510400234, -4. 1385038057
C, 0, 2. 1691691314, 0. 7723922178, -3. 5903314451
C, 0, 2. 036359213, 1. 0122702254, -2. 2299365206
C, 0, 1. 5139391778, -0. 0173668666, -1. 4775470257
C, 0, 1. 1057978086, -1. 2365347645, -1. 9988027345
C, 0, 1. 2742884832, -1. 4677052778, -3. 351003104
N, 0, 1. 3431307405, -0. 0412216634, -0. 0764445409
C, 0, 0. 8874332485, -1. 173429888, 0. 3016967935
C, 0, 0. 6110929321, -2. 0940769209, -0. 856282117
H, 0, 1. 9329507761, -0. 6171998537, -5. 1953493281
H, 0, 2. 5701774824, 1. 5430718191, -4. 2271334658
H, 0, 2. 3167162811, 1. 9486075142, -1. 7781934443
H, 0, 1. 003314044, -2. 409341165, -3. 7970001291
H, 0, 1. 4077185187, 0. 9008221505, 0. 4796650488
H, 0, 0. 6679254532, -1. 369193404, 1. 3356872917
H, 0, 1. 2135449945, -2. 9963552528, -0. 7973114229
C, 0, 0. 5413214023, 6. 3775962137, -0. 7639314144
C, 0, 1. 1890064212, 5. 3460186712, -1. 2967805707
C, 0, -0. 0079539321, 6. 5445996982, 0. 5744523129
C, 0, 0. 0393538717, 5. 7153438386, 1. 6112884037
O, 0, 1. 5139696158, 4. 1649971265, -0. 7081308053
O, 0, 0. 6399799865, 4. 4961037394, 1. 6589225106
P, 0, 0. 5827641685, 3. 4423516437, 0. 4281032503
O, 0, -0. 7974855473, 3. 2942388544, -0. 0827855435
O, 0, 1. 405089083, 2. 2764580194, 0. 8827859383
H, 0, 0. 4086935169, 7. 2159884017, -1. 4284270328
H, 0, 1. 556011598, 5. 3903391978, -2. 3080430478
H, 0, -0. 521887304, 7. 4744233884, 0. 7562193483
H, 0, -0. 3956868816, 5. 9784057465, 2. 5600166405

Eelec= -1832. 9315252

Eelec+ZPE= -1832. 437469

H= -1832. 408220

G= -1832. 499443

(11) TS5b

C, 0, 2. 0658449687, -3. 1644922507, -3. 3068027837
C, 0, 3. 1760885712, -2. 408653174, -3. 7026443679
C, 0, 3. 5388364502, -1. 2753044111, -3. 009366339
C, 0, 2. 7681491311, -0. 9154739682, -1. 909336332
C, 0, 1. 6502389883, -1. 6625147505, -1. 4791701818
C, 0, 1. 3072571974, -2. 8070279418, -2. 2130195381
N, 0, 2. 8961662325, 0. 1515706987, -1. 0644378214
C, 0, 1. 9116625616, 0. 1116081381, -0. 1214711442
C, 0, 1. 1147883331, -0. 9785904413, -0. 3223600657
C, 0, -0. 0855412061, -1. 3240121, 0. 5477015956
C, 0, 0. 2254382944, -0. 9322439339, 2. 0111868608
C, 0, -0. 3598814705, -2. 8332039352, 0. 5339803865
C, 0, -1. 5856318209, -3. 3887742261, 0. 1925609633
C, 0, -1. 7932139172, -4. 7620528337, 0. 2415520468

C, 0, -0.7746811356, -5.6079287057, 0.6367318997
 C, 0, 0.4582167668, -5.068364531, 0.9762194397
 C, 0, 0.6603921713, -3.7026183657, 0.922265498
 C, 0, -2.2042536152, -0.2505377255, -3.6220619433
 C, 0, -3.5628493939, 0.0186200921, -3.4526057311
 C, 0, -4.1176509084, 0.0743201581, -2.1897131801
 C, 0, -3.2621998217, -0.1573351278, -1.128172685
 C, 0, -1.9003580384, -0.4274107693, -1.2630189726
 C, 0, -1.3636923276, -0.4642408751, -2.5447973719
 N, 0, -3.5560706186, -0.1697071506, 0.2394483364
 C, 0, -2.4813172496, -0.4271295395, 0.9427897178
 C, 0, -1.3246964125, -0.5106682465, 0.1057178075
 H, 0, 1.8004584233, -4.0456389929, -3.8685182784
 H, 0, 3.7515324737, -2.715740469, -4.5609172828
 H, 0, 4.3892341603, -0.6835445908, -3.3091466788
 H, 0, 0.4582322527, -3.4053935061, -1.9334601348
 H, 0, 3.5904272403, 0.8670076808, -1.1266919123
 H, 0, 1.8362627005, 0.8919019235, 0.616862687
 H, 0, -0.5656897764, -1.2637660833, 2.6802478174
 H, 0, 1.1391161918, -1.4162049997, 2.3355823166
 H, 0, 0.3603919035, 0.1387513708, 2.1233547056
 H, 0, -2.3950544066, -2.7633343542, -0.1428202721
 H, 0, -2.7548499545, -5.1633222924, -0.0361066751
 H, 0, -0.9330710333, -6.6734657133, 0.6748069582
 H, 0, 1.2668434622, -5.7144845839, 1.2779439536
 H, 0, 1.6305680046, -3.3028747759, 1.1660575854
 H, 0, -1.7968049379, -0.2873990298, -4.6188105059
 H, 0, -4.1851842858, 0.1888842145, -4.3152316049
 H, 0, -5.1625160397, 0.2912249537, -2.0398508893
 H, 0, -0.3194436297, -0.6593354323, -2.6994308036
 H, 0, -4.4371734381, 0.1052965287, 0.6334363665
 H, 0, -2.5142446892, -0.4322801737, 2.0151258419
 H, 0, -1.0984216563, 0.6880398637, 0.325727216
 C, 0, 0.3996100678, 5.5936484244, 2.9684320641
 C, 0, -0.4118976706, 4.6019330462, 3.3128665965
 C, 0, 0.8145524699, 5.9915849942, 1.6307117251
 C, 0, 0.6387198113, 5.381074894, 0.4607135211
 O, 0, -1.0476500458, 3.7614226604, 2.4471777919
 O, 0, 0.0227783999, 4.2060248988, 0.1886366823
 P, 0, -0.2234492677, 3.0054137529, 1.2619532869
 O, 0, 1.0535010277, 2.4615199622, 1.7641106051
 O, 0, -1.2360841533, 2.1108347701, 0.6034397772
 H, 0, 0.7962469144, 6.1792329827, 3.7819959057
 H, 0, -0.6585784365, 4.3966977613, 4.3405919276
 H, 0, 1.3477804493, 6.9264584037, 1.5676243948
 H, 0, 0.991641738, 5.8385798269, -0.4478557828

Eelec=-1832.9033499

Eelec+ZPE=-1832.412762

H=-1832.383450

G= -1832. 475154

(12) IN7b

C, 0, 0. 4536071827, -0. 7437223951, -3. 8924196081
C, 0, 0. 8273432708, 0. 5987171628, -4. 0358364886
C, 0, 1. 6102084652, 1. 2146203774, -3. 0842690334
C, 0, 2. 0127263199, 0. 4582101867, -1. 9876648084
C, 0, 1. 6710319965, -0. 9034508046, -1. 825885865
C, 0, 0. 863705121, -1. 4933061406, -2. 8111190442
N, 0, 2. 7629332937, 0. 8397113869, -0. 9111163891
C, 0, 2. 8705544583, -0. 2233339839, -0. 0622620584
C, 0, 2. 2522466606, -1. 3265036108, -0. 5697557383
C, 0, 2. 191236815, -2. 6586785072, 0. 1754054424
C, 0, 3. 6246886814, -3. 0466080619, 0. 6054737232
C, 0, 1. 6722465424, -3. 7910143568, -0. 723761315
C, 0, 0. 4985882601, -4. 4826724149, -0. 4533622943
C, 0, 0. 0698675087, -5. 5168071803, -1. 2751498391
C, 0, 0. 8129172443, -5. 8860330381, -2. 3814099297
C, 0, 1. 9892297662, -5. 2064680942, -2. 662911453
C, 0, 2. 40926449, -4. 1734086475, -1. 8451853055
C, 0, -1. 7897232602, -0. 328160255, 1. 3047986439
C, 0, -2. 1370133642, -0. 4759320877, 2. 6570435115
C, 0, -1. 3767679165, -1. 2557209708, 3. 4989500949
C, 0, -0. 2544512178, -1. 8804631455, 2. 9634494626
C, 0, 0. 1260929961, -1. 7441451352, 1. 611977093
C, 0, -0. 6763231779, -0. 9560030122, 0. 7771589285
N, 0, 0. 6692633788, -2. 6827731694, 3. 5684730212
C, 0, 1. 6242788351, -3. 0354094179, 2. 6499567128
C, 0, 1. 3467800734, -2. 4956147862, 1. 4320272947
H, 0, -0. 1655820689, -1. 2022938006, -4. 6466114854
H, 0, 0. 5019821079, 1. 1532475767, -4. 9017522063
H, 0, 1. 9047024274, 2. 2478586018, -3. 1757528554
H, 0, 0. 5550392305, -2. 519112564, -2. 7302873587
H, 0, 2. 8954237914, 1. 7971443215, -0. 6293347657
H, 0, 3. 3781006396, -0. 1055457832, 0. 8758200572
H, 0, 3. 6385910993, -4. 0327507404, 1. 0626779634
H, 0, 4. 2892102505, -3. 0688941375, -0. 2499810527
H, 0, 4. 0228430721, -2. 3305770567, 1. 3177562561
H, 0, -0. 0936292583, -4. 213890616, 0. 4034940017
H, 0, -0. 848461304, -6. 0323862328, -1. 0429556939
H, 0, 0. 4821452149, -6. 6904393074, -3. 018540725
H, 0, 2. 577941547, -5. 4766337184, -3. 5250466298
H, 0, 3. 3099168055, -3. 639789808, -2. 0993082287
H, 0, -2. 4087900877, 0. 2766615359, 0. 6623142246
H, 0, -3. 0112738366, 0. 025664345, 3. 0384574976
H, 0, -1. 6373842167, -1. 373299657, 4. 538635642
H, 0, -0. 4314640639, -0. 8321677139, -0. 2629330088
H, 0, 0. 6894453904, -2. 916564992, 4. 5389885158
H, 0, 2. 4438950017, -3. 6576840314, 2. 9499700531

H, 0, -0.0808792616, 1.1577879676, 1.6658554249
 C, 0, -0.8928052105, 5.53965574, -0.2823726306
 C, 0, -0.5365993598, 5.356891432, 0.984556225
 C, 0, -0.9393161475, 4.6013737608, -1.3982458373
 C, 0, -0.7436891386, 3.2897762501, -1.4007061816
 O, 0, -0.1213742828, 4.198683878, 1.5827522933
 O, 0, -0.4624955764, 2.5322808988, -0.2863941796
 P, 0, 0.618775998, 3.0167041934, 0.7934685271
 O, 0, 1.9268494502, 3.3867061491, 0.2568724279
 O, 0, 0.5802747273, 1.849489378, 1.8328943915
 H, 0, -1.1884556445, 6.5489046408, -0.5164992192
 H, 0, -0.5717239365, 6.157245916, 1.7006759314
 H, 0, -1.167500853, 5.0310588785, -2.3595714368
 H, 0, -0.7982759299, 2.682883797, -2.2850456956

Eelec= -1832.9446971
 Eelec+ZPE= -1832.450678
 H= -1832.420391
 G= -1832.514195

(13) product b-single arylation

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 C, 0, -3.3748962381, 0.7466342995, 0.0941242822
 C, 0, -2.2014649791, 0.342242437, 0.722404705
 C, 0, -0.9457756847, 0.8839815639, 0.3941067768
 C, 0, -0.8729610322, 1.868529021, -0.5943222007
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 C, 0, -0.6654909093, -0.635748438, 2.015643949
 C, 0, 0.025442029, 0.2375582536, 1.2376400923
 C, 0, 1.510586552, 0.4701325335, 1.2284013372
 C, 0, 2.1952591913, -0.1936153012, 2.4240671904
 C, 0, 2.1305693167, -0.050655051, -0.0736258328
 C, 0, 2.03184539, -1.3997869251, -0.404091918
 C, 0, 2.6165102905, -1.8948761245, -1.5551002324
 C, 0, 3.3106087788, -1.0467082359, -2.4063546764
 C, 0, 3.4043566583, 0.2972114117, -2.0946496769
 C, 0, 2.817531674, 0.7907644124, -0.9370833998
 O, 0, 1.6835954937, 1.8749316605, 1.3392418508
 H, 0, -1.9872987195, 3.0289226685, -1.9871693289
 H, 0, -4.1605405956, 2.0512445491, -1.3891057871
 H, 0, -4.3291263185, 0.3202535096, 0.3602325804
 H, 0, 0.0755327209, 2.3076525242, -0.8495976801
 H, 0, -2.7141358922, -1.1258482686, 2.1541149904
 H, 0, -0.3131663393, -1.3042910984, 2.7769349039
 H, 0, 3.2611908096, 0.025140347, 2.4025768414
 H, 0, 1.7778966428, 0.1947872212, 3.3483243341
 H, 0, 2.0891582741, -1.273759333, 2.4107003933
 H, 0, 1.4752534095, -2.0649591581, 0.2366031986

H, 0, 2. 5256887479, -2. 9428930994, -1. 7923387649
H, 0, 3. 7646006356, -1. 4309963323, -3. 3054445799
H, 0, 3. 9299878956, 0. 9702651301, -2. 7531908185
H, 0, 2. 8787809973, 1. 8428749243, -0. 7186441198
H, 0, 2. 6178683402, 2. 0499533881, 1. 4649793707

Eelec= -748. 253537
Eelec+ZPE= -747. 971404
H= -747. 956174
G= -748. 013253

(14) Product b-diarylation

C, 0, 2. 7667872424, 1. 0378111704, -2. 8133796116
C, 0, 3. 5653690359, 2. 1757606697, -2. 9834263576
C, 0, 3. 8292867862, 3. 0137183501, -1. 9240406521
C, 0, 3. 2767856668, 2. 6880504424, -0. 6897334747
C, 0, 2. 47493733, 1. 5457575669, -0. 4834193313
C, 0, 2. 2269130941, 0. 7166425052, -1. 5874230661
N, 0, 3. 3733522526, 3. 3446272468, 0. 5048078701
C, 0, 2. 6644264394, 2. 6562886056, 1. 4503635364
C, 0, 2. 091858157, 1. 5446598302, 0. 9124297449
C, 0, 1. 2037978364, 0. 584239673, 1. 7036083812
C, 0, 1. 825186769, 0. 3788097112, 3. 1032217889
C, 0, 1. 1666606692, -0. 8099853221, 1. 0590729159
C, 0, -0. 0198380708, -1. 4797531776, 0. 7907895326
C, 0, -0. 011689849, -2. 7647702203, 0. 2634983336
C, 0, 1. 1842957119, -3. 4079696575, 0. 0028302064
C, 0, 2. 3775828305, -2. 7534397993, 0. 2728006402
C, 0, 2. 3653747321, -1. 4727619747, 0. 7936715672
C, 0, -2. 0978856519, 2. 3929311255, -1. 1933388858
C, 0, -3. 2354614683, 2. 8328811692, -0. 5054323246
C, 0, -3. 3210298019, 2. 7193083399, 0. 8643950602
C, 0, -2. 2393042944, 2. 154302069, 1. 5314747902
C, 0, -1. 080730974, 1. 7066745133, 0. 8659673044
C, 0, -1. 0290749743, 1. 8353168449, -0. 5260649112
N, 0, -2. 062784176, 1. 9175288259, 2. 8668908823
C, 0, -0. 8352838966, 1. 3388226836, 3. 0589496309
C, 0, -0. 1847569145, 1. 182519814, 1. 8737745601
H, 0, 2. 5726834006, 0. 3986272357, -3. 6594520469
H, 0, 3. 9757591692, 2. 3986756484, -3. 9550014209
H, 0, 4. 4397794685, 3. 8946978192, -2. 0448380935
H, 0, 1. 6200340507, -0. 1651639226, -1. 4865955491
H, 0, 3. 8771967935, 4. 1916218669, 0. 6634856354
H, 0, 2. 6128556639, 3. 0292802953, 2. 4545420797
H, 0, 1. 2566716064, -0. 3565718196, 3. 6656182163
H, 0, 2. 8432142389, 0. 0171630347, 3. 0158310316
H, 0, 1. 8428918605, 1. 3039971213, 3. 6721915536
H, 0, -0. 9609190503, -0. 9976890457, 0. 9878466988
H, 0, -0. 9481227073, -3. 2588554294, 0. 0585203433

H, 0, 1.1903479507, -4.4054057019, -0.4065345438
H, 0, 3.3193822991, -3.2390376855, 0.0724503663
H, 0, 3.3010742211, -0.9703029946, 0.9776407705
H, 0, -2.057817703, 2.494159645, -2.2657834006
H, 0, -4.0556042338, 3.2656339104, -1.0554105484
H, 0, -4.1947762513, 3.05375967, 1.4011757356
H, 0, -0.164725645, 1.5107633489, -1.0761214606
H, 0, -2.71318855, 2.1443895715, 3.5891510898
H, 0, -0.5222690644, 1.0796354268, 4.0506504123

Eelec= -1035.4684856

Eelec+ZPE= -1035.075905

H= -1035.055414

G= -1035.124111

E. Cartesian coordinates and total energies of the reported key transition states and intermediates involved in the first C-C bond forming and dehydration steps for the simplified model of chiral phosphoric acid-catalyzed diarylation reaction between 2,2-difluoroacetophenone and indole at BH and HLYP/6-31G(d) level.

(1) IN1c

C, 0, 1.9689214454, 5.3738748208, -0.5632031727
C, 0, 1.9596507312, 4.2421369103, -1.25344661
C, 0, 1.0561869677, 5.6735793729, 0.5297796067
C, 0, 0.6023978573, 4.7749519333, 1.3922533644
O, 0, 1.0094263359, 3.2679171627, -1.0852805705
O, 0, 1.0322827661, 3.4725507877, 1.4180308624
P, 0, 0.7979582923, 2.4145137836, 0.2485577663
O, 0, -0.5033645102, 1.7461615313, 0.2170734336
O, 0, 2.0570822421, 1.5130282316, 0.4389198014
H, 0, 2.6963919053, 6.1185885317, -0.8429565046
H, 0, 2.6438259179, 4.022903569, -2.0537593993
H, 0, 0.7305916427, 6.6927262008, 0.6618443218
H, 0, -0.0767953984, 5.0030691041, 2.1941244437
H, 0, 1.9126285946, 0.5623410433, 0.2469279697
C, 0, 1.4585945067, -2.0745294275, 0.0586983911
O, 0, 1.806564985, -1.0294018686, -0.4454074675
C, 0, 1.4583432244, -3.3410536751, -0.6875484743
C, 0, 1.0072817307, -2.0701550885, 1.520302792
F, 0, 1.1517293349, -0.8335162014, 2.0176804031
F, 0, 1.8180087952, -2.9011035646, 2.2189110463
C, 0, 1.863696804, -3.3110348239, -2.022280105
C, 0, 1.8725075731, -4.4692867309, -2.7715234958
C, 0, 1.472024326, -5.6678371394, -2.1952611023
C, 0, 1.0656184111, -5.7056536053, -0.8712379846
C, 0, 1.0592547131, -4.547395262, -0.114776065
H, 0, -0.0195199517, -2.3854445632, 1.6515752888
H, 0, 2.1651123941, -2.3705745145, -2.4497672048
H, 0, 2.1873410306, -4.4427623013, -3.8016129593
H, 0, 1.476612521, -6.5729444312, -2.780884059

H, 0, 0.754694897, -6.6361910353, -0.4265607879
H, 0, 0.7541956712, -4.5932596432, 0.915212001
C, 0, -2.6920096036, -3.8854817925, -1.3628156896
C, 0, -2.2009437632, -2.7468794166, -2.0208990387
C, 0, -1.9013024688, -1.594817414, -1.3284225619
C, 0, -2.1039193457, -1.6021340433, 0.0506216562
C, 0, -2.5940604388, -2.7361629324, 0.7335846166
C, 0, -2.8905396618, -3.890120528, -0.0004710677
N, 0, -1.8877964295, -0.6180397165, 0.9750339335
C, 0, -2.2263367279, -1.0902918799, 2.2101875356
C, 0, -2.6600146576, -2.3785965197, 2.1180647744
H, 0, -2.9183109742, -4.768482127, -1.9385746665
H, 0, -2.0575893706, -2.775784743, -3.0889764769
H, 0, -1.5265998061, -0.7150766748, -1.8259015679
H, 0, -3.2728912431, -4.7690772843, 0.4946381725
H, 0, -1.4900623482, 0.2891483293, 0.7732793869
H, 0, -2.1261459401, -0.4617025888, 3.0742891472
H, 0, -3.0008729769, -2.9916277759, 2.9306193164

Eelec= -1744.1499908

Eelec+ZPE= -1743.783010

H= -1743.755789

G= -1743.846992

(2) TS1c

C, 0, -2.8101607856, 5.1716254335, -2.0907561307
C, 0, -2.3715001646, 4.4308728027, -1.0804673297
C, 0, -2.024786209, 5.4807921086, -3.2759499408
C, 0, -1.1610890884, 4.6411288585, -3.8330125354
O, 0, -1.091351883, 3.9707688099, -0.9815464915
O, 0, -1.0014182799, 3.3490118479, -3.4236221498
P, 0, -0.4035974562, 2.9131272452, -1.9898603369
O, 0, 1.0659123035, 3.1041067956, -1.9027636876
O, 0, -0.9550817478, 1.5301938859, -1.7575439582
H, 0, -3.8087037951, 5.5719197519, -2.0156727634
H, 0, -2.9705881546, 4.2014276028, -0.2156680743
H, 0, -2.1511946715, 6.4455618407, -3.7408528763
H, 0, -0.5747758043, 4.8863974765, -4.7020033713
H, 0, -0.6969296539, 0.607495209, -0.6727526899
C, 0, -0.3585377403, -1.3195531468, -0.511257521
O, 0, -0.5392916897, -0.1534581214, 0.0127466157
C, 0, -0.4148578749, -2.4560882075, 0.4293265954
C, 0, -0.9572255535, -1.4979460212, -1.9099584859
F, 0, -2.1947913644, -2.0050648997, -1.7528583579
F, 0, -0.2571192775, -2.3805584585, -2.6607283116
C, 0, -0.4660968804, -2.191195362, 1.7959793712
C, 0, -0.5465799111, -3.2330843259, 2.7035111729
C, 0, -0.5699799639, -4.5444002353, 2.2575590343
C, 0, -0.5168408566, -4.8140282235, 0.8969105293
C, 0, -0.4394763963, -3.7789669146, -0.0146572613

H, 0, -1.0241243877, -0.554642052, -2.4329501946
H, 0, -0.4529538995, -1.1706283169, 2.1332611727
H, 0, -0.5921224929, -3.0186457681, 3.7585180351
H, 0, -0.6334400901, -5.3549658206, 2.9652700638
H, 0, -0.5420326634, -5.8323439998, 0.5456016762
H, 0, -0.4083438023, -3.9979048633, -1.0666323005
C, 0, 3.2375374433, -0.8582470351, 2.4700276308
C, 0, 3.3353465926, 0.5313026087, 2.3558722908
C, 0, 2.9634550242, 1.1835025834, 1.195649706
C, 0, 2.4958147494, 0.3957348391, 0.1574434067
C, 0, 2.3772014349, -0.995581884, 0.2522734997
C, 0, 2.7544076008, -1.6312995, 1.4305293898
N, 0, 2.0910038743, 0.7730511539, -1.1164593848
C, 0, 1.7411368776, -0.2978332018, -1.8044330155
C, 0, 1.7820135247, -1.4413924899, -0.9891607024
H, 0, 3.5449647283, -1.3335520413, 3.3871361634
H, 0, 3.7110627752, 1.1045675446, 3.1873865525
H, 0, 3.0334794741, 2.25378685, 1.0977473417
H, 0, 2.6763005736, -2.7011088082, 1.5306895045
H, 0, 1.8881061997, 1.7407069151, -1.4296362736
H, 0, 1.4026540853, -0.2093382973, -2.819089997
H, 0, 1.7945852769, -2.4438101693, -1.3682696109

Eelec= -1744.1177045

Eelec+ZPE= -1743.750402

H= -1743.725435

G= -1743.806783

(3) IN2c

C, 0, -5.493948, -0.970367, 1.762887
C, 0, -4.306943, -0.465685, 2.076069
C, 0, -6.155958, -0.761155, 0.484152
C, 0, -5.5177, -0.674256, -0.676214
O, 0, -3.624624, 0.404845, 1.277055
O, 0, -4.177269, -0.890144, -0.813513
P, 0, -3.026589, 0.047011, -0.179716
O, 0, -2.918058, 1.342962, -0.923561
O, 0, -1.798947, -0.799983, -0.07974
H, 0, -5.994592, -1.563692, 2.511375
H, 0, -3.823079, -0.639656, 3.022057
H, 0, -7.231054, -0.678498, 0.467744
H, 0, -6.018044, -0.505162, -1.614404
C, 0, 1.509706, -0.856928, -0.153378
O, 0, 0.703763, -0.592835, 0.939736
C, 0, 2.945473, -1.017937, 0.315234
C, 0, 0.998907, -2.137572, -0.83806
F, 0, 1.459086, -3.223419, -0.201906
F, 0, 1.446622, -2.196887, -2.126335
C, 0, 3.263894, -0.811334, 1.649989
C, 0, 4.57707, -0.925127, 2.080671

C, 0, 5. 582647, -1. 248167, 1. 185188
C, 0, 5. 267434, -1. 4662, -0. 147481
C, 0, 3. 957473, -1. 351745, -0. 580089
H, 0, -0. 243261, -0. 658352, 0. 700736
H, 0, -0. 08352, -2. 175458, -0. 853517
H, 0, 2. 47902, -0. 562835, 2. 340456
H, 0, 4. 811323, -0. 761562, 3. 120229
H, 0, 6. 602921, -1. 33629, 1. 521942
H, 0, 6. 039943, -1. 731149, -0. 851078
H, 0, 3. 72491, -1. 547524, -1. 613635
C, 0, 2. 751219, 3. 532882, 0. 528328
C, 0, 1. 558168, 4. 242888, 0. 483375
C, 0, 0. 423682, 3. 693612, -0. 098129
C, 0, 0. 551659, 2. 422916, -0. 61121
C, 0, 1. 728398, 1. 686211, -0. 566982
C, 0, 2. 850842, 2. 247069, 0. 006841
N, 0, -0. 425986, 1. 656291, -1. 284117
C, 0, 0. 055068, 0. 530285, -1. 655005
C, 0, 1. 456883, 0. 34429, -1. 192607
H, 0, 3. 61819, 3. 985967, 0. 979925
H, 0, 1. 511886, 5. 234724, 0. 90107
H, 0, -0. 508512, 4. 230292, -0. 146077
H, 0, 3. 779554, 1. 706343, 0. 057979
H, 0, -1. 491095, 1. 774103, -1. 249809
H, 0, -0. 56149, -0. 190744, -2. 155909
H, 0, 2. 11349, 0. 102213, -2. 021652

Eelec= -1744. 1357339

Eelec+ZPE= -1743. 766183

H= -1743. 741087

G= -1743. 822858

(4) IN3c

C, 0, -1. 2587593776, -0. 5706936983, -2. 3432306574
C, 0, -2. 4140738469, -1. 274454323, -2. 7079522775
C, 0, -2. 6864514861, -2. 5192463558, -2. 1839346035
C, 0, -1. 7727812572, -3. 046927782, -1. 278060076
C, 0, -0. 6106633744, -2. 3558115415, -0. 8914796045
C, 0, -0. 3573878047, -1. 097582748, -1. 4449116525
N, 0, -1. 7771264521, -4. 2452414847, -0. 6124006124
C, 0, -0. 6618054415, -4. 3287667386, 0. 1756244539
C, 0, 0. 0824259092, -3. 1974904046, 0. 0482328369
C, 0, 1. 367409642, -2. 8532319502, 0. 741395429
C, 0, 1. 6325632785, -3. 8125121515, 1. 9019764897
C, 0, 2. 5586440487, -2. 8305159016, -0. 2152589174
C, 0, 2. 7359251758, -3. 8741050459, -1. 1181095011
C, 0, 3. 8258263851, -3. 8935870208, -1. 9697636842
C, 0, 4. 7559971054, -2. 8663677211, -1. 9347350501
C, 0, 4. 5861558375, -1. 824811364, -1. 0399358894
C, 0, 3. 496408501, -1. 8060168151, -0. 1819180008

F, 0, 2. 7533828381, -3. 4230913153, 2. 5447182787
F, 0, 1. 8275984861, -5. 0794499603, 1. 47241392
O, 0, 1. 164289287, -1. 5984903446, 1. 3694134993
H, 0, -1. 0737991459, 0. 399166205, -2. 7749125722
H, 0, -3. 1010383801, -0. 8349851603, -3. 4128372245
H, 0, -3. 5733301145, -3. 0635565478, -2. 4667384304
H, 0, 0. 5311566102, -0. 5508237569, -1. 1790843995
H, 0, -2. 4704174877, -4. 9580298832, -0. 702290615
H, 0, -0. 476544428, -5. 2086442159, 0. 7591093319
H, 0, 0. 8126372464, -3. 8071659736, 2. 6106100816
H, 0, 2. 0127143882, -4. 670175959, -1. 1583062101
H, 0, 3. 9449818122, -4. 7093189265, -2. 6645560465
H, 0, 5. 6032558095, -2. 877860329, -2. 6013321647
H, 0, 5. 3016434175, -1. 0192436935, -1. 0035906975
H, 0, 3. 3919848114, -0. 9815903685, 0. 5023381213
H, 0, 1. 9492280437, -1. 3061662416, 1. 8555574797
C, 0, 0. 6764591622, 4. 3834451035, 3. 3855428735
C, 0, 0. 2087383356, 3. 1744142833, 3. 6619808464
C, 0, 1. 9905124578, 4. 6448823267, 2. 817466067
C, 0, 2. 5930426289, 3. 8593064948, 1. 9362468577
O, 0, 0. 9601755971, 2. 0321273092, 3. 5457336994
O, 0, 1. 9904422638, 2. 7596414707, 1. 3766385705
P, 0, 1. 5589187131, 1. 4553066226, 2. 1846452821
O, 0, 2. 5988697075, 0. 456467254, 2. 4452572005
O, 0, 0. 3529653182, 0. 9575404149, 1. 3144124454
H, 0, 0. 038356751, 5. 2230321317, 3. 6089579724
H, 0, -0. 7673018127, 2. 9878722898, 4. 0729066476
H, 0, 2. 5110591677, 5. 5395534155, 3. 1185194455
H, 0, 3. 5670720693, 4. 0529322631, 1. 5241317339
H, 0, 0. 3922936039, -0. 0110948621, 1. 1748433234

Eelec== -1744. 1490673

Eelec+ZPE= -1743. 779327

H= -1743. 753433

G= -1743. 838335

(5) TS3c

C, 0, 1. 8525816077, -2. 4806268014, 2. 1694388911
C, 0, 2. 141840128, -1. 2735843648, 2. 8060636726
C, 0, 2. 2308600433, -0. 0994176129, 2. 0842398289
C, 0, 2. 0149673958, -0. 1765480389, 0. 7198702459
C, 0, 1. 7148274407, -1. 3751394931, 0. 054568091
C, 0, 1. 6402677769, -2. 5468767999, 0. 8045859941
N, 0, 2. 0488705215, 0. 8423519848, -0. 2229838728
C, 0, 1. 7823855479, 0. 3579195816, -1. 419264445
C, 0, 1. 5646287596, -1. 0247656558, -1. 3569694657
C, 0, 0. 9708368109, -1. 7566004688, -2. 3984464895
C, 0, 1. 2791158089, -1. 4085517798, -3. 8442001726
C, 0, 0. 7861426144, -3. 2344336071, -2. 22170078
C, 0, 1. 91588561, -4. 0327103398, -2. 3880498938

C, 0, 1. 833434511, -5. 4050840007, -2. 2281109367
C, 0, 0. 6237977431, -5. 9931965514, -1. 8947198914
C, 0, -0. 4983389781, -5. 2002107815, -1. 7217136806
C, 0, -0. 4232791325, -3. 8257564064, -1. 8851045476
F, 0, 1. 2446543494, -0. 0907446866, -4. 0873139284
F, 0, 0. 365321717, -1. 9831251779, -4. 6576436869
H, 0, 1. 790777521, -3. 3835413402, 2. 754759909
H, 0, 2. 29861722, -1. 2567896483, 3. 871922634
H, 0, 2. 4544722677, 0. 8411053143, 2. 5594508088
H, 0, 1. 4155170094, -3. 49144687, 0. 3437019932
H, 0, 1. 8826768992, 1. 8361640013, -0. 0674262899
H, 0, 1. 66805445, 1. 0215776861, -2. 2474977364
H, 0, 2. 2579987006, -1. 788395856, -4. 1164607151
H, 0, 2. 8690971153, -3. 5834011289, -2. 6172165094
H, 0, 2. 7156305034, -6. 0101872176, -2. 357377229
H, 0, 0. 5582253389, -7. 061236402, -1. 7670280569
H, 0, -1. 4410874639, -5. 649177702, -1. 4551818762
H, 0, -1. 2906744848, -3. 2105671215, -1. 7375183774
O, 0, -0. 8166325533, -1. 1298902527, -2. 4639054771
H, 0, -0. 8230034722, -0. 137107973, -2. 2162294826
H, 0, -1. 1814998117, -1. 1906678812, -3. 3526135615
C, 0, -3. 6340805521, 3. 9715671374, -0. 5252918897
C, 0, -3. 0755057748, 2. 8403356252, -0. 1087570702
C, 0, -2. 8897338817, 5. 0939448854, -1. 0754869403
C, 0, -1. 8024863529, 4. 9598933715, -1. 8258007182
O, 0, -1. 7340940918, 2. 6363479487, -0. 0310059276
O, 0, -1. 342305191, 3. 7533994094, -2. 2585680594
P, 0, -0. 6960582716, 2. 63253063, -1. 2829719801
O, 0, 0. 6251972025, 3. 050335111, -0. 7555279493
O, 0, -0. 8155524754, 1. 3487857644, -2. 0447116444
H, 0, -4. 705943802, 4. 0562838063, -0. 4387948499
H, 0, -3. 6515701291, 2. 0187382192, 0. 2842581282
H, 0, -3. 2378761234, 6. 0944173637, -0. 8725613194
H, 0, -1. 2466490718, 5. 79705112, -2. 2137567453

Eelec= -1744. 0982583

Eelec+ZPE= -1743. 731104

H= -1743. 705657

G= -1743. 789167

(6) IN4c

C, 0, -3. 0972065709, -3. 0454971049, 2. 9331817002
C, 0, -3. 4587376459, -1. 7820138856, 3. 386979081
C, 0, -2. 8520511863, -0. 6445733297, 2. 8753409082
C, 0, -1. 8973101144, -0. 8360883909, 1. 9017549971
C, 0, -1. 53217029, -2. 0897436775, 1. 4056623443
C, 0, -2. 1366398318, -3. 2152452486, 1. 9451195854
N, 0, -1. 1194085002, 0. 1474785144, 1. 2738628591
C, 0, -0. 293740265, -0. 3894786436, 0. 4437305643
C, 0, -0. 4686343112, -1. 837233586, 0. 415681956

C, 0, 0.2579199453, -2.6624683958, -0.3706809022
 C, 0, 1.4500764147, -2.1223998314, -1.13574539
 C, 0, -0.0139371781, -4.0983601947, -0.5399364596
 C, 0, 1.0138078052, -5.0380125214, -0.4443471845
 C, 0, 0.7458952101, -6.3816888964, -0.6293497698
 C, 0, -0.5374007561, -6.8019218595, -0.9449602001
 C, 0, -1.5574737086, -5.8719651447, -1.073036302
 C, 0, -1.2992994206, -4.5284450768, -0.8669815383
 F, 0, 1.5319520189, -2.7416587425, -2.327229941
 F, 0, 2.5683292488, -2.450152663, -0.432128005
 H, 0, -3.5729015561, -3.9150206979, 3.3556275191
 H, 0, -4.2123453343, -1.6848254937, 4.1505330926
 H, 0, -3.1005540772, 0.3450328872, 3.2196003437
 H, 0, -1.8765623272, -4.2037297745, 1.6137591308
 H, 0, -1.2127536589, 1.2286946451, 1.4370269717
 H, 0, 0.3917889736, 0.2157016999, -0.1296292301
 H, 0, 1.4525720729, -1.0543136677, -1.3017478261
 H, 0, 2.0137699457, -4.7129762361, -0.2191987644
 H, 0, 1.5430306106, -7.1006561881, -0.536807498
 H, 0, -0.7393150243, -7.8490559634, -1.1007878892
 H, 0, -2.5522198623, -6.1903578624, -1.3380585352
 H, 0, -2.0899275987, -3.8051775712, -0.9773776862
 O, 0, 1.6681547823, 1.0802825856, -1.4451234709
 H, 0, 0.9943765623, 1.7799949004, -1.3350239398
 H, 0, 2.4729352117, 1.473043521, -1.1071936008
 C, 0, -1.3496562744, 6.6950940861, -0.0639946801
 C, 0, -1.9252362545, 5.6249767251, -0.5990851413
 C, 0, -0.6897857834, 6.6956587759, 1.2326639408
 C, 0, -0.0014627368, 5.6676422728, 1.7149954565
 O, 0, -2.0638240068, 4.4412533298, 0.0612879838
 O, 0, 0.2705363962, 4.5399759161, 1.0014548685
 P, 0, -0.8344417267, 3.4760919288, 0.4764740752
 O, 0, -1.3418366975, 2.6466865288, 1.6214704856
 O, 0, -0.2525318981, 2.7733828054, -0.6910402067
 H, 0, -1.3853406797, 7.6147167543, -0.6263119681
 H, 0, -2.397684352, 5.6314252696, -1.5668976676
 H, 0, -0.7536254706, 7.5819816293, 1.8439172816
 H, 0, 0.4668049, 5.6792998722, 2.6849466518

Eelec= -1744.1279146

Eelec+ZPE= -1743.762218

H= -1743.735006

G= -1743.824153

F. Cartesian coordinates and total energies of the reported key transition states and intermediates involved in the first C-C bond forming and dehydration steps for the simplified model of chiral phosphoric acid-catalyzed diarylation reaction between 2-fluoroacetophenone and indole at BH and HLYP/6-31G(d) level.

(1) IN1d

C, 0, -5.7742647875, -0.6475869999, -1.2823308341
 C, 0, -4.8284914682, 0.0909350878, -1.8458602007
 C, 0, -5.5410757451, -1.5898333357, -0.1981115573
 C, 0, -4.6540676217, -1.4074071151, 0.770164472
 O, 0, -3.4966562011, -0.0354295683, -1.5446259575
 O, 0, -3.930932484, -0.2508719005, 0.9158954073
 P, 0, -2.8361708269, 0.2671559409, -0.123719846
 O, 0, -1.511057761, -0.3514420307, -0.0308535499
 O, 0, -2.9117139604, 1.8098160581, 0.0814988442
 H, 0, -6.7769448766, -0.5427193161, -1.6640253185
 H, 0, -5.0096709385, 0.7939670697, -2.6392293549
 H, 0, -6.1318779865, -2.4909242016, -0.1643931501
 H, 0, -4.4829443599, -2.1091119591, 1.5670095993
 H, 0, -2.0492655491, 2.2297492638, 0.297281689
 C, 0, 0.4686023574, 2.1750016436, 0.7766112816
 O, 0, -0.4202566231, 2.8012533372, 0.2373373825
 C, 0, 1.8541505271, 2.2104233437, 0.2741450272
 C, 0, 0.1663489903, 1.3539933544, 2.0089848972
 F, 0, -1.1426231081, 1.5239750397, 2.358762548
 C, 0, 2.1865240096, 3.1677744741, -0.6834442761
 C, 0, 3.469226287, 3.2234916855, -1.1905017379
 C, 0, 4.4234113025, 2.3105406925, -0.7603141548
 C, 0, 4.0972513002, 1.3472178323, 0.1806519545
 C, 0, 2.8176578321, 1.3009600407, 0.7058592983
 H, 0, 0.348747201, 0.3040521948, 1.8136207119
 H, 0, 0.7943569746, 1.6824750042, 2.8339904245
 H, 0, 1.4268997434, 3.8554493513, -1.0132275822
 H, 0, 3.726475142, 3.9690065077, -1.9248629303
 H, 0, 5.4211960899, 2.3456444421, -1.166930251
 H, 0, 4.8265705109, 0.6180572637, 0.4897361554
 H, 0, 2.5777533238, 0.5331942565, 1.4224524203
 C, 0, 4.6125491043, -2.4062847087, -1.1653146901
 C, 0, 3.6298972388, -1.9006995499, -2.0304481156
 C, 0, 2.3364043417, -1.6990593695, -1.603148458
 C, 0, 2.037107478, -2.014561129, -0.2800633353
 C, 0, 3.0098910959, -2.521701794, 0.6075675279
 C, 0, 4.3146087887, -2.7172369045, 0.1429403202
 N, 0, 0.85839593, -1.914812547, 0.4066331489
 C, 0, 1.0596845234, -2.3390157951, 1.6924046676
 C, 0, 2.3544889885, -2.7181169811, 1.8642772795
 H, 0, 5.6135402685, -2.557720083, -1.5365454878
 H, 0, 3.893207837, -1.6677351974, -3.0496335349
 H, 0, 1.5806651072, -1.3094844938, -2.2657507504
 H, 0, 5.0744467092, -3.1114658126, 0.7996077422
 H, 0, -0.0021593988, -1.512806296, 0.0674388697
 H, 0, 0.2434185615, -2.3469230642, 2.3898822022
 H, 0, 2.7866761321, -3.1073507314, 2.7664602021

Eelec= -1644.943464

Eelec+ZPE= -1644.568748

H= -1644. 542270

G= -1644. 631386

(2) TS1d

C, 0, -5. 8571366347, -0. 1019812684, 1. 3172319874
C, 0, -4. 7932546701, 0. 6717084565, 1. 4936900029
C, 0, -5. 8041440495, -1. 4285059383, 0. 721849502
C, 0, -4. 9769527601, -1. 7736232704, -0. 2575943795
O, 0, -3. 5188121107, 0. 2558123549, 1. 2409424753
O, 0, -4. 1610918947, -0. 8965837841, -0. 9069958839
P, 0, -2. 9470817737, -0. 069291242, -0. 2364800514
O, 0, -2. 7435697456, 1. 1606653641, -1. 0435937081
O, 0, -1. 7731106039, -0. 9850629398, -0. 0218931006
H, 0, -6. 8115077408, 0. 279154463, 1. 6441348991
H, 0, -4. 8439962506, 1. 658422681, 1. 9217638038
H, 0, -6. 4812670006, -2. 1842320766, 1. 0872410749
H, 0, -4. 9459951466, -2. 7655547446, -0. 6757997626
H, 0, -0. 421883773, -0. 6581932529, 0. 483005874
C, 0, 1. 4155912237, -1. 1252462899, -0. 0019510533
O, 0, 0. 5572780888, -0. 521188932, 0. 7599939535
C, 0, 2. 7945797387, -1. 1647565249, 0. 5353320473
C, 0, 0. 8830696101, -2. 353329396, -0. 7225303409
F, 0, 1. 5483915128, -2. 5984450527, -1. 9020928214
C, 0, 3. 105690008, -0. 4068717637, 1. 6620628547
C, 0, 4. 3750889473, -0. 4657460864, 2. 2106933734
C, 0, 5. 3454111886, -1. 2731856282, 1. 6391734
C, 0, 5. 0421072598, -2. 0276473488, 0. 5147666513
C, 0, 3. 7754417964, -1. 9755092996, -0. 0367715512
H, 0, 1. 0305638214, -3. 2099651701, -0. 068653871
H, 0, -0. 1717258664, -2. 2341578787, -0. 9274322286
H, 0, 2. 3456084986, 0. 2114602446, 2. 1042120022
H, 0, 4. 6044786482, 0. 1187760908, 3. 0864976763
H, 0, 6. 3332206242, -1. 3178373077, 2. 0683515983
H, 0, 5. 7920160578, -2. 6600964693, 0. 0686982146
H, 0, 3. 5475917871, -2. 5627122133, -0. 9086128301
C, 0, 3. 0434441781, 3. 2944093529, 0. 1407965228
C, 0, 1. 7931927363, 3. 9068653079, 0. 2575450906
C, 0, 0. 6562648148, 3. 3190297732, -0. 2646360753
C, 0, 0. 8183442775, 2. 1034910217, -0. 9065276684
C, 0, 2. 0573906902, 1. 4635301048, -1. 0233834439
C, 0, 3. 1880531368, 2. 0720390355, -0. 4901007656
N, 0, -0. 1307798461, 1. 3172684278, -1. 5491961188
C, 0, 0. 45147071, 0. 2479105997, -2. 0551714868
C, 0, 1. 8043474245, 0. 1947693806, -1. 67686345
H, 0, 3. 9103932426, 3. 7858056527, 0. 5513584303
H, 0, 1. 714543646, 4. 8569341134, 0. 7599783119
H, 0, -0. 3124826414, 3. 78230948, -0. 1815037097
H, 0, 4. 1558419258, 1. 6052019103, -0. 5681594059
H, 0, -1. 1603927497, 1. 4205376767, -1. 4719245273

H, 0, -0.1207354491, -0.4851497456, -2.5905704381
H, 0, 2.5343841132, -0.4090418679, -2.1783410743

Eelec= -1644.9106618
Eelec+ZPE= -1644.534960
H= -1644.510727
G= -1644.590427

(3) IN2d

C, 0, 3.7115373281, 4.6187078957, 0.5868972396
C, 0, 2.9960829501, 3.8736040431, -0.2468732892
C, 0, 3.2660396625, 5.00876468, 1.9159717989
C, 0, 2.5315579811, 4.2371200863, 2.7077326025
O, 0, 1.7121264271, 3.4872152728, 0.0012749336
O, 0, 2.2133185586, 2.9444754389, 2.410770294
P, 0, 1.2587078479, 2.4900497888, 1.1898638303
O, 0, -0.1753031263, 2.8088510401, 1.4835757508
O, 0, 1.6094972529, 1.0709079413, 0.8844140535
H, 0, 4.6769931848, 4.9579073917, 0.2465121055
H, 0, 3.3448663204, 3.5820152671, -1.2230379955
H, 0, 3.5510451429, 5.9787114741, 2.29144606
H, 0, 2.1953364831, 4.5436005998, 3.683646651
H, 0, 1.233422736, -0.0846264503, -0.3699656832
C, 0, 0.4462377296, -1.8743248453, -0.1985479107
O, 0, 0.9401819171, -0.8184994537, -0.9475065124
C, 0, 0.248477586, -3.0692399411, -1.1156711015
C, 0, 1.4480908795, -2.1841678625, 0.9210226731
F, 0, 0.8503805299, -2.9423876178, 1.9154005944
C, 0, 0.4146147305, -2.9296599883, -2.4875136381
C, 0, 0.223193992, -4.0143115511, -3.3299797825
C, 0, -0.1366395954, -5.2481081682, -2.8136431096
C, 0, -0.2964142955, -5.3951091168, -1.4442149485
C, 0, -0.1045921729, -4.3139550534, -0.600195083
H, 0, 2.286244466, -2.7417404315, 0.5194804247
H, 0, 1.8039195989, -1.2632190601, 1.3687436504
H, 0, 0.6943985371, -1.9702513239, -2.8826612097
H, 0, 0.3567890891, -3.8917605874, -4.3928327037
H, 0, -0.2859167878, -6.0899171129, -3.4703708417
H, 0, -0.5658004075, -6.3532533471, -1.0298620564
H, 0, -0.2108263068, -4.4470354906, 0.4632549428
C, 0, -3.5243601581, -0.8381669593, -2.3453799353
C, 0, -3.7201674298, 0.5096894971, -2.0725208782
C, 0, -3.0565824636, 1.1270785327, -1.0211712265
C, 0, -2.2034971047, 0.3365225128, -0.2851198367
C, 0, -1.9776479378, -1.009426485, -0.5457338393
C, 0, -2.6510873169, -1.6124999551, -1.5884272568
N, 0, -1.4458588994, 0.700653016, 0.8503624299
C, 0, -0.7919063104, -0.3031917943, 1.3004817395
C, 0, -0.9613666016, -1.5067012293, 0.4461610286
H, 0, -4.0578003342, -1.2939289778, -3.1631216092

H, 0, -4.3990660342, 1.0838374706, -2.680692605
H, 0, -3.1994952209, 2.1691463501, -0.7908820265
H, 0, -2.5036322815, -2.65312207, -1.8186688832
H, 0, -1.1589180468, 1.6851430265, 1.1604719418
H, 0, -0.1353898479, -0.1970579023, 2.1421939986
H, 0, -1.2883172515, -2.3606185506, 1.030726219

Eelec= -1644.9269117
Eelec+ZPE= -1644.549195
H= -1644.524832
G= -1644.604894

(4) IN3d

C, 0, -3.0704229339, -0.2406538206, -2.343214605
C, 0, -4.4096777489, -0.6457799556, -2.4108994179
C, 0, -4.9119415117, -1.5954675394, -1.5477460346
C, 0, -4.0395545487, -2.1336966104, -0.6083408865
C, 0, -2.6919341926, -1.7396052813, -0.5189608389
C, 0, -2.2105140755, -0.77629723, -1.4096095092
N, 0, -4.2538374276, -3.0809975668, 0.359181395
C, 0, -3.090940877, -3.2933936319, 1.0489080577
C, 0, -2.1065416955, -2.494729518, 0.5579535764
C, 0, -0.6874946963, -2.3982982001, 1.0341677397
C, 0, -0.484731355, -3.1297134867, 2.3629662134
C, 0, 0.3005579255, -2.9051948443, -0.0148875144
C, 0, 0.123656075, -4.173176704, -0.5630221452
C, 0, 1.0244159981, -4.6770273665, -1.483281967
C, 0, 2.1180585146, -3.9206011701, -1.8775833136
C, 0, 2.2996453002, -2.6592074399, -1.3407174618
C, 0, 1.3987374681, -2.1530759076, -0.413679098
F, 0, -0.7428041378, -4.477884881, 2.2522089277
O, 0, -0.4650481812, -1.030454004, 1.3532956288
H, 0, -2.7089183913, 0.5029171455, -3.0344718222
H, 0, -5.058632917, -0.2075116105, -3.1517282821
H, 0, -5.9423296661, -1.9094111017, -1.6000107624
H, 0, -1.1814427333, -0.4616076078, -1.3716205133
H, 0, -5.1127959896, -3.5637253413, 0.519890795
H, 0, -3.0473581794, -4.0210943736, 1.8343420589
H, 0, 0.5445848989, -3.0104539491, 2.6896222894
H, 0, -1.1557190771, -2.7115037535, 3.1056873782
H, 0, -0.7258535442, -4.7636470704, -0.2675451447
H, 0, 0.8691270035, -5.6605392721, -1.8969766416
H, 0, 2.8178091776, -4.3112444291, -2.5987377432
H, 0, 3.1428918308, -2.0581295003, -1.6408113434
H, 0, 1.5675277906, -1.1654953322, -0.0192533007
H, 0, 0.4538992051, -0.8475001732, 1.594424341
C, 0, 0.6779607941, 5.1161264918, 2.0805293671
C, 0, 0.0416968951, 4.1069428968, 2.6579748972
C, 0, 1.8917862326, 4.9755460483, 1.2901452802
C, 0, 2.1590568876, 3.9395467891, 0.5078027229

O, 0, 0. 5232923721, 2. 8216800722, 2. 6660512868
O, 0, 1. 2634544855, 2. 9263119032, 0. 2702298973
P, 0, 0. 728076798, 1. 9092726421, 1. 3736632687
O, 0, 1. 5731331046, 0. 750317587, 1. 6782777835
O, 0, -0. 6904566668, 1. 5744024942, 0. 7984980653
H, 0, 0. 2679268948, 6. 1033718223, 2. 2190655476
H, 0, -0. 8606831809, 4. 2154276855, 3. 2326288721
H, 0, 2. 6230651273, 5. 7666553154, 1. 3279015298
H, 0, 3. 0605998927, 3. 8383853073, -0. 0692739708
H, 0, -0. 8936099451, 0. 618611472, 0. 8819383968

Eelec=-1644. 9362726

Eelec+ZPE= -1644. 558546

H= -1644. 533383

G= -1644. 616551

(5) TS3d

C, 0, 3. 0539991897, 3. 506713358, 0. 3738561003
C, 0, 2. 014291657, 4. 4001654759, 0. 108647844
C, 0, 0. 8258980297, 3. 9568707224, -0. 4346891087
C, 0, 0. 7074097655, 2. 5997581969, -0. 6856751699
C, 0, 1. 7263560912, 1. 6727616675, -0. 4006951428
C, 0, 2. 9263764893, 2. 1547229764, 0. 1213948109
N, 0, -0. 3480316778, 1. 9091620497, -1. 2572683504
C, 0, -0. 0465859907, 0. 6229155158, -1. 3481891887
C, 0, 1. 2168616498, 0. 3727488535, -0. 824254082
C, 0, 1. 6773259377, -0. 9540794206, -0. 6179358056
C, 0, 1. 2749955927, -1. 9671212378, -1. 6573218634
C, 0, 2. 9755591503, -1. 198611042, 0. 0688702464
C, 0, 4. 0330450036, -1. 7831487856, -0. 6208326783
C, 0, 5. 2581203785, -1. 9644887329, -0. 000000763
C, 0, 5. 4302510172, -1. 5877172349, 1. 32096484
C, 0, 4. 3730036009, -1. 0237675096, 2. 0204498224
C, 0, 3. 1542643593, -0. 8245919322, 1. 3985774569
F, 0, 1. 5231432918, -3. 2397501785, -1. 2013576023
H, 0, 3. 9785149532, 3. 8802994051, 0. 7828822186
H, 0, 2. 1450391152, 5. 4485524803, 0. 3202329716
H, 0, 0. 0216566782, 4. 6367355931, -0. 6625496766
H, 0, 3. 7460739993, 1. 4914672503, 0. 3295372119
H, 0, -1. 3133487688, 2. 1934810623, -1. 3348297715
H, 0, -0. 7920282486, -0. 0653433005, -1. 6812255546
H, 0, 0. 2213598025, -1. 8918286914, -1. 8890812058
H, 0, 1. 8600674873, -1. 8058435598, -2. 5583235932
H, 0, 3. 9124513739, -2. 0989447491, -1. 642776778
H, 0, 6. 0715883911, -2. 4102750679, -0. 5481420548
H, 0, 6. 3803475361, -1. 7393566629, 1. 8066843774
H, 0, 4. 4970666883, -0. 7386978308, 3. 0522127371
H, 0, 2. 3295417479, -0. 3953651246, 1. 9390765488
O, 0, 0. 521528357, -1. 652076549, 0. 7390882397
H, 0, -0. 4443792211, -1. 5091207338, 0. 4471512485

H, 0, 0.652123829, -2.6060465937, 0.75818746
C, 0, -5.4306083849, 0.602687824, 1.4952279278
C, 0, -4.1971627849, 0.4677623731, 1.9751608067
C, 0, -6.0278676104, 0.065731705, 0.2798019936
C, 0, -5.5043804447, -0.7754735698, -0.6042193639
O, 0, -3.1541358704, -0.2218680007, 1.4463553808
O, 0, -4.2675134269, -1.3430874133, -0.5445704065
P, 0, -2.9499910155, -0.4815299059, -0.1494850992
O, 0, -2.9118239233, 0.8002181245, -0.890537106
O, 0, -1.8037635964, -1.44578715, -0.2421451567
H, 0, -6.0847462508, 1.2014850707, 2.108161333
H, 0, -3.9225260397, 0.9147364142, 2.9152455465
H, 0, -7.0342251928, 0.3891792972, 0.0688521839
H, 0, -6.0594647153, -1.1121454388, -1.4627377852

Eelec= -1644.8958464
Eelec+ZPE= -1644.519837
H= -1644.495033
G= -1644.576614

(6) IN4d

C, 0, 2.8709098865, -2.4937986248, 1.7111586311
C, 0, 3.1613666739, -1.1653262455, 2.0015648062
C, 0, 2.280765884, -0.1541135031, 1.6481813405
C, 0, 1.118144972, -0.5366968338, 1.0167447245
C, 0, 0.7834507459, -1.8641230205, 0.7379419775
C, 0, 1.689233105, -2.8575427383, 1.0799427305
N, 0, 0.1080097159, 0.3006231687, 0.5229176119
C, 0, -0.813813666, -0.3922252626, -0.0534365683
C, 0, -0.5116134134, -1.8141566454, 0.0334423358
C, 0, -1.3233594548, -2.7747947987, -0.4679184556
C, 0, -2.5000580329, -2.4144909875, -1.3487768004
C, 0, -1.1313654458, -4.2152195571, -0.2306447439
C, 0, -1.2385041025, -5.1267950747, -1.2834485867
C, 0, -1.1054681551, -6.4831145843, -1.0471241376
C, 0, -0.8999505796, -6.9515957214, 0.2416880454
C, 0, -0.8243448645, -6.0563986149, 1.2977199937
C, 0, -0.9333980838, -4.6970917318, 1.0635823221
F, 0, -2.1126411944, -2.6280147416, -2.6625885665
H, 0, 3.5775753069, -3.2608022699, 1.9818309376
H, 0, 4.0845546357, -0.917158282, 2.4981462167
H, 0, 2.4871943879, 0.8843400836, 1.8447452063
H, 0, 1.4928153974, -3.8920332159, 0.8655085604
H, 0, 0.0798103043, 1.3844789434, 0.6369737259
H, 0, -1.6778289607, 0.0835343033, -0.4935669164
H, 0, -3.3331608162, -3.0758199129, -1.1381487931
H, 0, -2.8239603947, -1.3871545987, -1.253402542
H, 0, -1.4136186013, -4.764932778, -2.2810671741
H, 0, -1.1705315397, -7.1755269781, -1.870221868
H, 0, -0.8091578617, -8.0099736902, 0.4237430279

H, 0, -0.685637355, -6.4154440088, 2.3042726051
H, 0, -0.8856384882, -4.0044770085, 1.8871971756
O, 0, -3.4659613609, 0.7386168615, -1.1381685159
H, 0, -3.2853313211, 1.4157035209, -0.4556730091
H, 0, -3.4789401616, 1.2312896888, -1.9586981783
C, 0, -2.2635377057, 6.4505582996, 1.7490609401
C, 0, -2.3429202929, 5.2909379553, 2.3910213078
C, 0, -1.3247651423, 6.714793229, 0.6694276379
C, 0, -0.9505174006, 5.8080593955, -0.2257642579
O, 0, -1.4730185888, 4.262666824, 2.189168457
O, 0, -1.4946434622, 4.5631406929, -0.3116499493
P, 0, -1.3672117022, 3.4068056401, 0.8197762311
O, 0, 0.0166686348, 2.8257838588, 0.8129703054
O, 0, -2.5179246728, 2.4899333411, 0.643129925
H, 0, -2.9319183076, 7.2387762993, 2.0576829916
H, 0, -3.0530184945, 5.101181988, 3.1783541019
H, 0, -0.9062875458, 7.7048278539, 0.5796572237
H, 0, -0.2405534807, 6.0166204813, -1.0086520335

Eelec= -1644.9176955

Eelec+ZPE= -1644.543489

H= -1644.517015

G= -1644.604717

G. Cartesian coordinates and total energies of the different conformers (A-F) of the chiral phosphoric acid which is determined by the conformation of the isopropyl groups on the 2,4,6-triisopropylphenyl substituent (BH and HLYP/6-31G(d) level).

(1) Conformer A

C, 0, -0.6964378137, 3.0993060272, -5.0200854913
C, 0, 0.5337306308, 3.324890534, -4.3743832449
C, 0, 0.7655971628, 2.8300922727, -3.123539985
C, 0, -0.2193668328, 2.0747324367, -2.4439187951
C, 0, -1.4385875716, 1.8113896892, -3.1161823567
C, 0, -1.6567539928, 2.3549803061, -4.4028506352
C, 0, -0.0259598955, 1.5395402045, -1.1307098585
C, 0, -0.972016491, 0.6740580383, -0.6443951027
C, 0, -2.1847797073, 0.3679213552, -1.3085937577
C, 0, -2.4043402512, 0.9804770182, -2.5091937265
C, 0, 1.174879559, 1.8705695522, -0.318898629
C, 0, 1.5426893767, 3.2225405135, -0.0283468018
C, 0, 2.7686740398, 3.4695058548, 0.6377328382
C, 0, 3.5767535234, 2.3834971702, 1.037067304
C, 0, 3.1877918603, 1.0859209761, 0.8633441851
C, 0, 1.9603518812, 0.8692820593, 0.1936234729
C, 0, 0.7181149216, 4.3295571889, -0.3400129368
C, 0, 1.1081610211, 5.6028935683, -0.0410539491
C, 0, 2.3465573559, 5.8472952361, 0.5818686215

C, 0, 3. 1538093202, 4. 8011697559, 0. 9154142754
O, 0, -0. 7830250798, 0. 1061006632, 0. 6000558466
O, 0, 1. 5725435665, -0. 4479765539, 0. 0038289031
P, 0, 0. 3399224587, -1. 0010092762, 0. 8495912112
O, 0, 0. 5008980371, -1. 2846324081, 2. 2679266367
O, 0, -0. 0209506697, -2. 2519626262, -0. 0585186649
C, 0, -4. 8140438161, -1. 1454009899, 0. 9427746494
C, 0, -5. 0459517534, -2. 3798829007, 0. 3611662488
C, 0, -4. 3260773752, -2. 7004906192, -0. 7803707216
C, 0, -3. 3923405143, -1. 8368362454, -1. 3382124489
C, 0, -3. 1709995419, -0. 5892703915, -0. 724127323
C, 0, -3. 8947711819, -0. 2405823102, 0. 4258652334
C, 0, -3. 7546750547, 1. 1114013254, 1. 1043120572
C, 0, -3. 3663936237, 0. 9846496808, 2. 5781235294
C, 0, -5. 0337647926, 1. 9366601842, 0. 941133755
C, 0, -2. 6806503706, -2. 2735914233, -2. 6107885699
C, 0, -3. 636594788, -2. 2357164891, -3. 8070401276
C, 0, -2. 0401249958, -3. 6576944444, -2. 4967428308
C, 0, -6. 0570028027, -3. 3381295786, 0. 9538573827
C, 0, -5. 3999982984, -4. 6358615335, 1. 4262333145
C, 0, -7. 2035751878, -3. 6274341184, -0. 0159442688
C, 0, 4. 9675074651, -1. 3606557704, 3. 1221853276
C, 0, 4. 1340353414, -0. 3254626079, 2. 7118715637
C, 0, 4. 030619971, -0. 0511869138, 1. 3402378786
C, 0, 4. 7476719775, -0. 8254239682, 0. 4128796989
C, 0, 5. 5582199961, -1. 8507028048, 0. 8766441576
C, 0, 5. 6856774588, -2. 1356070757, 2. 2287526164
C, 0, 6. 5755752638, -3. 2579067153, 2. 7190203183
C, 0, 8. 0409580628, -3. 0276578397, 2. 3473446528
C, 0, 6. 0926020798, -4. 6210334429, 2. 2215168114
C, 0, 4. 6942061065, -0. 5646570631, -1. 0831331137
C, 0, 4. 169525543, -1. 7760684054, -1. 8558180939
C, 0, 6. 0567651136, -0. 1182764855, -1. 6181843654
C, 0, 3. 3890410425, 0. 4690075456, 3. 7725030801
C, 0, 4. 3464378295, 1. 3788205529, 4. 5471790483
C, 0, 2. 600591911, -0. 4247753136, 4. 7312106099
H, 0, -0. 8684885321, 3. 5032190966, -6. 0043446459
H, 0, 1. 3027406666, 3. 8903682987, -4. 8749992399
H, 0, 1. 7141617935, 3. 0061534767, -2. 6495377022
H, 0, -2. 5961419598, 2. 1544129875, -4. 893475599
H, 0, -3. 3289469736, 0. 7979922037, -3. 0322382936
H, 0, 4. 5175052506, 2. 5896195583, 1. 5213734243
H, 0, -0. 2351858649, 4. 1608127563, -0. 8075666553
H, 0, 0. 4589373983, 6. 429557956, -0. 2795877716
H, 0, 2. 6449523175, 6. 8585301818, 0. 8052281239
H, 0, 4. 0960047757, 4. 9710611973, 1. 4120926236
H, 0, -0. 4105667237, -2. 9535673921, 0. 4691643585
H, 0, -5. 3732388395, -0. 8752011614, 1. 8250002084
H, 0, -4. 4986136494, -3. 6526701246, -1. 2559248533

H, 0, -2. 9611743059, 1. 6619236522, 0. 6107618803
H, 0, -3. 2139900989, 1. 971329888, 3. 0108629554
H, 0, -2. 4469122776, 0. 419331313, 2. 6935752994
H, 0, -4. 1447126813, 0. 4917310887, 3. 1568003715
H, 0, -4. 9079259843, 2. 9236100302, 1. 3820024397
H, 0, -5. 8795790485, 1. 4595735474, 1. 4316867462
H, 0, -5. 2884266674, 2. 0648410847, -0. 1082358172
H, 0, -1. 8772748466, -1. 5730626372, -2. 8091772038
H, 0, -3. 1128103949, -2. 497044859, -4. 7244305946
H, 0, -4. 0764565387, -1. 2505877796, -3. 9392790208
H, 0, -4. 4534305729, -2. 9426454653, -3. 675862833
H, 0, -1. 507795905, -3. 8953012267, -3. 4152527726
H, 0, -2. 7784792874, -4. 440143021, -2. 3382960473
H, 0, -1. 3238432207, -3. 6923696759, -1. 6826495994
H, 0, -6. 4841166672, -2. 8504334803, 1. 8295733982
H, 0, -6. 1318888612, -5. 2851882767, 1. 9023140968
H, 0, -4. 6073487451, -4. 4363282555, 2. 1428504412
H, 0, -4. 9653911828, -5. 1837573146, 0. 5925581473
H, 0, -7. 9481452476, -4. 2687002932, 0. 4513760006
H, 0, -6. 8459576045, -4. 1341676079, -0. 9099129028
H, 0, -7. 6944832847, -2. 709499711, -0. 3289083331
H, 0, 5. 0551437573, -1. 5731996287, 4. 1759686825
H, 0, 6. 1093294609, -2. 4401577705, 0. 1607733837
H, 0, 6. 5108748175, -3. 2650363762, 3. 8067030932
H, 0, 8. 6697042504, -3. 8141913425, 2. 7600258432
H, 0, 8. 397426388, -2. 0737251938, 2. 7276499771
H, 0, 8. 1786633086, -3. 0269505773, 1. 2680852651
H, 0, 6. 7090850641, -5. 4194385199, 2. 6299820445
H, 0, 6. 1441988973, -4. 68469634, 1. 1365359781
H, 0, 5. 0620781705, -4. 8024752379, 2. 5154886499
H, 0, 4. 0034157688, 0. 2523526493, -1. 2634803122
H, 0, 4. 0884642651, -1. 5420981178, -2. 9156726956
H, 0, 3. 187629967, -2. 0702125143, -1. 4972764794
H, 0, 4. 8359922226, -2. 6304124965, -1. 7582670853
H, 0, 5. 9910549905, 0. 1180909992, -2. 6785185692
H, 0, 6. 8058748789, -0. 897898321, -1. 4985141557
H, 0, 6. 4133708083, 0. 7662981528, -1. 0959449257
H, 0, 2. 6660956268, 1. 1046653677, 3. 2720371651
H, 0, 3. 8006564487, 1. 9742556655, 5. 2765074293
H, 0, 4. 8781354028, 2. 0600198597, 3. 8868973747
H, 0, 5. 0914036041, 0. 7951980941, 5. 0846367745
H, 0, 2. 0340201416, 0. 1930896524, 5. 4254810303
H, 0, 3. 2553399091, -1. 0597893461, 5. 3244538187
H, 0, 1. 9024011401, -1. 051246088, 4. 1873636537

Eelec= -2580. 69747095

Eelec+ZPE= -2579. 707705

H= -2579. 653842

G= -2579. 795893

(2) Conformer B

C, 0, -2.805064605, 6.6449791699, -1.8176419647
C, 0, -1.4378498269, 6.4295085003, -1.5617159766
C, 0, -1.0145581072, 5.2822292031, -0.9552817518
C, 0, -1.9347943995, 4.2777813164, -0.5721437988
C, 0, -3.3047387141, 4.4786938667, -0.8731082045
C, 0, -3.7143150092, 5.6865594594, -1.4829965011
C, 0, -1.5406380145, 3.0608739332, 0.0695182712
C, 0, -2.4885581387, 2.082933987, 0.2293964307
C, 0, -3.858893227, 2.2456422213, -0.0891022892
C, 0, -4.2373737786, 3.4572151232, -0.5930023896
C, 0, -0.1435457267, 2.8320072057, 0.5234025266
C, 0, 0.5210673281, 3.7361205512, 1.4111353516
C, 0, 1.8923846328, 3.5265102615, 1.6996718904
C, 0, 2.5601759071, 2.4144202608, 1.1435925613
C, 0, 1.9123590778, 1.4837056615, 0.3824435245
C, 0, 0.5441034132, 1.7193536145, 0.109746743
C, 0, -0.1384421243, 4.8123398876, 2.050894156
C, 0, 0.5349724371, 5.6476428005, 2.8945175023
C, 0, 1.9075744505, 5.4616963204, 3.1452608173
C, 0, 2.5667348473, 4.4212986317, 2.5618334445
O, 0, -2.1199018374, 0.8799097574, 0.7985079481
O, 0, -0.1112245038, 0.7829454439, -0.6746294861
P, 0, -1.1914585155, -0.1605125678, 0.0206881425
O, 0, -0.7575850728, -1.2414678869, 0.8932032878
O, 0, -1.9775272581, -0.6114191489, -1.2825482499
C, 0, -6.1242721617, -0.280158472, 1.57200681
C, 0, -6.7138001636, -0.9216148848, 0.4964145871
C, 0, -6.3522639237, -0.5092685839, -0.777739722
C, 0, -5.4290919048, 0.5047835888, -0.9975468893
C, 0, -4.8408747376, 1.1386101708, 0.1134445845
C, 0, -5.1965331005, 0.7418261129, 1.4111560747
C, 0, -4.6458143157, 1.4174152913, 2.6553747189
C, 0, -3.9518659748, 0.4284435692, 3.5931350503
C, 0, -5.7458282246, 2.1907619428, 3.3871933963
C, 0, -5.1268317063, 0.9024537221, -2.4352521668
C, 0, -6.3066023905, 1.6630422482, -3.0480159286
C, 0, -4.7547331756, -0.2866494722, -3.3223383122
C, 0, -7.7190091951, -2.032736311, 0.712838457
C, 0, -7.2103947321, -3.3691925301, 0.1700848214
C, 0, -9.0871013233, -1.6882448518, 0.1229237544
C, 0, 3.6958547672, -1.8393658772, 0.1845291077
C, 0, 2.9917228626, -0.7628750877, 0.7072116411
C, 0, 2.6228554141, 0.2845306875, -0.1544159278
C, 0, 2.9533280646, 0.2218893093, -1.5153024683
C, 0, 3.6527075278, -0.8822459931, -1.9863318668
C, 0, 4.0364190973, -1.9225299518, -1.1572608097
C, 0, 4.8009582352, -3.1080765365, -1.7065425401

C, 0, 4. 0102137027, -4. 4091581044, -1. 5626350789
C, 0, 6. 1854249336, -3. 2366821375, -1. 0697169146
C, 0, 2. 6040783012, 1. 3289843706, -2. 494945615
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C, 0, 3. 8638755397, 1. 9997936826, -3. 0470730921
C, 0, 2. 6696801094, -0. 7593576024, 2. 1932938381
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C, 0, 1. 9759757015, -2. 0442718163, 2. 6484638088
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H, 0, -4. 7629477208, 5. 8272387467, -1. 6927367814
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H, 0, 3. 6133758711, 4. 2533056842, 2. 7608301974
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H, 0, -6. 8063279515, -0. 9889695815, -1. 6299650928
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H, 0, -6. 5263769644, 1. 5244701916, 3. 7483427866
H, 0, -6. 2122873096, 2. 924711853, 2. 7342937007
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H, 0, -9. 0358745387, -1. 5841724551, -0. 9588757359
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H, 0, 4. 9461965734, -2. 9293397132, -2. 771724351
H, 0, 4. 5494256776, -5. 238047916, -2. 0171771496
H, 0, 3. 0377470409, -4. 3320493469, -2. 0419116172
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H, 0, 6. 7399843018, -4. 0578601505, -1. 5196197872

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H, 0, 1. 4246142472, 1. 6504983399, -4. 2799729235
H, 0, 0. 7983349298, 0. 3798472349, -3. 2332601052
H, 0, 2. 2132756644, 0. 0821429141, -4. 2375331049
H, 0, 3. 5987738966, 2. 8270005978, -3. 7028185428
H, 0, 4. 4671282308, 1. 301206461, -3. 6228539299
H, 0, 4. 484917464, 2. 3901068877, -2. 2443765528
H, 0, 1. 9785625655, 0. 054281418, 2. 3868484614
H, 0, 3. 6866737467, -0. 4613137025, 4. 0841006508
H, 0, 4. 4094215, 0. 4338669796, 2. 7514573467
H, 0, 4. 6597049075, -1. 2981687659, 2. 8814082327
H, 0, 1. 7090446773, -1. 9635669128, 3. 7006099148
H, 0, 2. 6236100491, -2. 9125809681, 2. 5455373074
H, 0, 1. 0682222029, -2. 2140759358, 2. 0803210643

Eelec= -2580. 69746007
Eelec+ZPE= -2579. 707581
H= -2579. 653761
G= -2579. 795680

(3) Conformer C

C, 0, -1. 6153961937, 5. 408878099, -1. 6627600137
C, 0, -0. 2989060909, 5. 3229497144, -1. 1716549433
C, 0, 0. 1580833836, 4. 1713014006, -0. 5991476096
C, 0, -0. 6741293572, 3. 0317343162, -0. 4902957999
C, 0, -1. 9842002551, 3. 1102598573, -1. 0214859314
C, 0, -2. 4359031131, 4. 3232109922, -1. 5898628194
C, 0, -0. 2380804802, 1. 8023415083, 0. 097848047
C, 0, -1. 0524686964, 0. 7033516043, -0. 026176048
C, 0, -2. 3751552727, 0. 7598711153, -0. 5318898652
C, 0, -2. 8132434336, 1. 9689669453, -0. 991406954
C, 0, 1. 0582333531, 1. 7105343088, 0. 8202995525
C, 0, 1. 3758035854, 2. 5809201282, 1. 9114714355
C, 0, 2. 6744738025, 2. 5208083928, 2. 4755399655
C, 0, 3. 6081077887, 1. 58409187, 1. 9820212707
C, 0, 3. 2852777371, 0. 6774117952, 1. 0132314618
C, 0, 1. 9823517519, 0. 7622951475, 0. 4683296376
C, 0, 0. 4413038214, 3. 4762159734, 2. 4837347405
C, 0, 0. 7896692438, 4. 2842203667, 3. 5273122577
C, 0, 2. 0928388235, 4. 2510712042, 4. 0577774999
C, 0, 3. 0103586091, 3. 3848511173, 3. 5427893715
O, 0, -0. 6201398565, -0. 5173631105, 0. 4510163869
O, 0, 1. 6515597003, -0. 142067507, -0. 5264525257
P, 0, 0. 6209246587, -1. 3052227318, -0. 1711215824
O, 0, 1. 0453598475, -2. 4034590298, 0. 6842010499
O, 0, 0. 2235542507, -1. 7193615012, -1. 6505531169
C, 0, -4. 8424924405, -1. 9471836776, 0. 4422964546

C, 0, -4. 9547150563, -2. 6895876308, -0. 7197482245
 C, 0, -4. 2149771617, -2. 2777971828, -1. 8160961863
 C, 0, -3. 372838518, -1. 1747251483, -1. 7668111589
 C, 0, -3. 2650204016, -0. 4442342043, -0. 567953087
 C, 0, -4. 0240909834, -0. 8263121668, 0. 5521247335
 C, 0, -4. 1018649976, -0. 0884277656, 1. 887522242
 C, 0, -4. 8454962335, 1. 2458835311, 1. 7796817804
 C, 0, -2. 7890583561, 0. 0752219408, 2. 6547248739
 C, 0, -2. 6357319156, -0. 7673323672, -3. 0346090801
 C, 0, -3. 5180685394, 0. 1156758746, -3. 9230953189
 C, 0, -2. 1326048263, -1. 9567464002, -3. 8549139615
 C, 0, -5. 8588902178, -3. 9018233225, -0. 7814984054
 C, 0, -5. 0675366289, -5. 1850167402, -1. 0391352258
 C, 0, -6. 973045351, -3. 7300882126, -1. 8147623278
 C, 0, 5. 5711640077, -2. 3268102988, 0. 9035971275
 C, 0, 4. 6149943873, -1. 4278454168, 1. 3567665877
 C, 0, 4. 2694646305, -0. 339891058, 0. 5364871332
 C, 0, 4. 8758607582, -0. 18781031, -0. 7182832648
 C, 0, 5. 8213932396, -1. 1210688655, -1. 1247882463
 C, 0, 6. 1868677531, -2. 195711756, -0. 3321753865
 C, 0, 7. 2230680054, -3. 1915279427, -0. 8082768654
 C, 0, 6. 6278495427, -4. 5901433212, -0. 9775611539
 C, 0, 8. 4457015423, -3. 2248002827, 0. 1095426554
 C, 0, 4. 563754498, 0. 9759847684, -1. 6433862981
 C, 0, 4. 0020818357, 0. 5037440937, -2. 9855481911
 C, 0, 5. 7889267772, 1. 8710512591, -1. 8430200847
 C, 0, 4. 0002198735, -1. 6520377561, 2. 7293262082
 C, 0, 5. 0053320265, -1. 3278322492, 3. 8380084815
 C, 0, 3. 4453779121, -3. 0667885104, 2. 9026843049
 H, 0, -1. 9646823185, 6. 3275186688, -2. 1050003566
 H, 0, 0. 3567684038, 6. 1745595542, -1. 2529731349
 H, 0, 1. 1690065312, 4. 1213419491, -0. 2367773671
 H, 0, -3. 4412272366, 4. 3670348397, -1. 978239726
 H, 0, -3. 8219635984, 2. 0549342328, -1. 3610430029
 H, 0, 4. 598665797, 1. 5688129489, 2. 4069792202
 H, 0, -0. 5612582989, 3. 5100269913, 2. 0972415113
 H, 0, 0. 0575132996, 4. 9510377369, 3. 9527995169
 H, 0, 2. 355941381, 4. 8999720027, 4. 8770563763
 H, 0, 4. 006969234, 3. 333205114, 3. 9519289399
 H, 0, 0. 1249122298, -2. 6715219967, -1. 7214440585
 H, 0, -5. 4220134233, -2. 2455927885, 1. 3026767674
 H, 0, -4. 2949127721, -2. 8301353135, -2. 7377776374
 H, 0, -4. 725100196, -0. 7261516564, 2. 5116070221
 H, 0, -5. 0319096919, 1. 6484703305, 2. 7737152821
 H, 0, -5. 8046169154, 1. 1214085466, 1. 2824839106
 H, 0, -4. 2712687133, 1. 983343072, 1. 2276943904
 H, 0, -3. 0100198723, 0. 3524749782, 3. 683714953
 H, 0, -2. 1621278673, 0. 8569251866, 2. 2403852681
 H, 0, -2. 2143054908, -0. 8454419445, 2. 6682080245

H, 0, -1.7649203719, -0.1876714819, -2.7474749446
H, 0, -2.9825263034, 0.4047794407, -4.8254541493
H, 0, -3.82595544, 1.0227581198, -3.4131671521
H, 0, -4.4171942397, -0.4194230584, -4.2227036187
H, 0, -1.4307238939, -1.61340616, -4.6107327754
H, 0, -2.9425756938, -2.4640907139, -4.3741220988
H, 0, -1.6280475765, -2.6913101081, -3.2352264655
H, 0, -6.3306755153, -3.9989383642, 0.1958590275
H, 0, -5.7251457124, -6.0517740119, -1.0200109013
H, 0, -4.2955134095, -5.3278773679, -0.2874712291
H, 0, -4.5828898254, -5.1592429999, -2.0130675082
H, 0, -7.645264768, -4.5855901694, -1.7992395496
H, 0, -6.5683123167, -3.6469763489, -2.8213154639
H, 0, -7.5576838958, -2.8352310201, -1.6171974233
H, 0, 5.8382888586, -3.1581979052, 1.5356442466
H, 0, 6.2927852597, -1.0032845051, -2.0884177913
H, 0, 7.5599402331, -2.8580827849, -1.789614724
H, 0, 7.3710177722, -5.2782622924, -1.3758416695
H, 0, 5.7793934849, -4.5754755963, -1.656781304
H, 0, 6.2828180807, -4.9889405856, -0.0260064199
H, 0, 9.202330545, -3.9009116897, -0.2836987413
H, 0, 8.1809765744, -3.5697969904, 1.1068116666
H, 0, 8.8902913652, -2.2376367632, 0.2072619365
H, 0, 3.8004853209, 1.5893077786, -1.1757507704
H, 0, 3.734048717, 1.3578535519, -3.6046567478
H, 0, 3.1132572396, -0.1034644119, -2.8423253986
H, 0, 4.7307865808, -0.0861468028, -3.5374623705
H, 0, 5.5362857759, 2.7302021152, -2.4615403787
H, 0, 6.5978037992, 1.3353990341, -2.3352014554
H, 0, 6.1660156298, 2.2385237241, -0.8916409068
H, 0, 3.1614008903, -0.9726354161, 2.8381566024
H, 0, 4.5455877837, -1.4483829709, 4.8169938667
H, 0, 5.3741372354, -0.3075505254, 3.7628053934
H, 0, 5.8664672675, -1.9916736031, 3.7908185414
H, 0, 2.9603324623, -3.1534524641, 3.8732145695
H, 0, 4.2316028394, -3.8181504369, 2.8666970047
H, 0, 2.7115839949, -3.2887975268, 2.1360786198

Eelec= -2580.68967051
Eelec+ZPE= -2579.699723
H= -2579.645965
G= -2579.787862

(4) Conformer D

C, 0, -1.9510310306, 5.1063256699, -2.2217280871
C, 0, -0.5511983432, 5.0109146829, -2.1079402725
C, 0, 0.0262803094, 3.9504215802, -1.4717061808
C, 0, -0.7634533255, 2.9148255113, -0.9178379754

C, 0, -2. 1688724466, 2. 9952482472, -1. 0700325835
 C, 0, -2. 7389162567, 4. 1168142391, -1. 7145638114
 C, 0, -0. 2028810735, 1. 7792264539, -0. 2505468249
 C, 0, -1. 0420968612, 0. 7373565344, 0. 059744118
 C, 0, -2. 453774446, 0. 8091353268, -0. 0425312698
 C, 0, -2. 9792218114, 1. 9473157619, -0. 5842867939
 C, 0, 1. 2397555923, 1. 7304945129, 0. 1073049895
 C, 0, 1. 8502182912, 2. 7766110852, 0. 8734150847
 C, 0, 3. 2566698061, 2. 7669283036, 1. 0421031555
 C, 0, 4. 0147570866, 1. 6988562278, 0. 514603739
 C, 0, 3. 4307184899, 0. 6238261952, -0. 0886375508
 C, 0, 2. 0263400874, 0. 6759415777, -0. 2741096395
 C, 0, 1. 1128814348, 3. 8130207935, 1. 4929727689
 C, 0, 1. 740552125, 4. 7964543387, 2. 2021301334
 C, 0, 3. 1418753722, 4. 808474977, 2. 3281472507
 C, 0, 3. 8794781837, 3. 8118312754, 1. 7618884162
 O, 0, -0. 5107923416, -0. 4246111048, 0. 5837465164
 O, 0, 1. 4495701039, -0. 3661428432, -0. 9738905468
 P, 0, 0. 4291805122, -1. 378685425, -0. 2883501395
 O, 0, 0. 9345093436, -2. 4990655204, 0. 4904241223
 O, 0, -0. 3818393026, -1. 7828359982, -1. 5920572319
 C, 0, -4. 575815651, -1. 4381980572, 2. 1503819988
 C, 0, -5. 0846686416, -2. 3558970804, 1. 2482931345
 C, 0, -4. 71949017, -2. 2152632476, -0. 0798475316
 C, 0, -3. 8627303536, -1. 2093637426, -0. 507683661
 C, 0, -3. 3471504394, -0. 2962364722, 0. 4309410538
 C, 0, -3. 7218603054, -0. 4022461738, 1. 7827900058
 C, 0, -3. 3334978469, 0. 5539801346, 2. 9094046965
 C, 0, -3. 965444115, 1. 9408262267, 2. 7615101284
 C, 0, -1. 8397808312, 0. 6602011971, 3. 2213837081
 C, 0, -3. 5509303316, -1. 1112625345, -1. 9936151318
 C, 0, -4. 6540752921, -0. 3554958984, -2. 7409515805
 C, 0, -3. 3403974599, -2. 4757194615, -2. 6554265566
 C, 0, -6. 0057097218, -3. 4658108498, 1. 7069116472
 C, 0, -5. 3780043056, -4. 8440183047, 1. 4924131616
 C, 0, -7. 3793682557, -3. 3810908977, 1. 0405166591
 C, 0, 5. 5335006161, -2. 5213866213, -0. 2341536828
 C, 0, 4. 7882765073, -1. 4769660405, 0. 3031817605
 C, 0, 4. 2344441112, -0. 5334176697, -0. 5835424912
 C, 0, 4. 4492425406, -0. 6625593562, -1. 964931465
 C, 0, 5. 2080671893, -1. 7248279912, -2. 4394097851
 C, 0, 5. 7587738732, -2. 6699460451, -1. 5936458742
 C, 0, 6. 5718105434, -3. 8237371744, -2. 140474539
 C, 0, 5. 9097135881, -5. 1713119805, -1. 8494569788
 C, 0, 8. 0121500236, -3. 7997381705, -1. 627333039
 C, 0, 3. 9159343051, 0. 3404810022, -2. 9750769296
 C, 0, 3. 0018115991, -0. 3152034427, -4. 0115829288
 C, 0, 5. 0595356618, 1. 0997226293, -3. 6523265447
 C, 0, 4. 6985339173, -1. 4725081989, 1. 8304044409

C, 0, 3. 3388220971, -1. 1755102943, 2. 4602713703
C, 0, 5. 7989741144, -0. 6156662181, 2. 4662735723
H, 0, -2. 3928837877, 5. 9539960266, -2. 7194252557
H, 0, 0. 0716087878, 5. 7816257799, -2. 5320471931
H, 0, 1. 0973335896, 3. 8904506511, -1. 4016998857
H, 0, -3. 8122565434, 4. 1659041561, -1. 8091431326
H, 0, -4. 0498977409, 2. 0476539053, -0. 6564257002
H, 0, 5. 0862011748, 1. 7237372502, 0. 6222370086
H, 0, 0. 0408564114, 3. 8178986646, 1. 4133031101
H, 0, 1. 1558869697, 5. 5693935868, 2. 6737866354
H, 0, 3. 6248324556, 5. 5958152676, 2. 8834406347
H, 0, 4. 9527072003, 3. 7946611227, 1. 8682412413
H, 0, -0. 6435265544, -2. 7056937265, -1. 5601925234
H, 0, -4. 8600809724, -1. 5245328904, 3. 1880684467
H, 0, -5. 1109868339, -2. 9074865084, -0. 8069044146
H, 0, -3. 7846149886, 0. 1176363345, 3. 7984710387
H, 0, -3. 812260394, 2. 5161063628, 3. 6728390757
H, 0, -5. 0365191835, 1. 8676417131, 2. 5876838597
H, 0, -3. 5273050025, 2. 5001839661, 1. 9411035219
H, 0, -1. 710977804, 1. 1245010635, 4. 1973118301
H, 0, -1. 3090417462, 1. 2744437693, 2. 5027497075
H, 0, -1. 3648071333, -0. 3155713348, 3. 2450816801
H, 0, -2. 6279177729, -0. 5545502617, -2. 109452866
H, 0, -4. 4221451824, -0. 292172444, -3. 8024947645
H, 0, -4. 774903006, 0. 6556781377, -2. 3652750172
H, 0, -5. 60941809, -0. 86596909, -2. 6352727288
H, 0, -2. 8812525026, -2. 3486586964, -3. 6326683295
H, 0, -4. 278925269, -3. 0040924139, -2. 80651094
H, 0, -2. 7029490946, -3. 1236169436, -2. 0589546347
H, 0, -6. 1530996558, -3. 336330306, 2. 7786938752
H, 0, -6. 0268221084, -5. 6259080282, 1. 8820126702
H, 0, -4. 4161338168, -4. 9197781834, 1. 9927663474
H, 0, -5. 2186817264, -5. 0427738589, 0. 4345065878
H, 0, -8. 0420142505, -4. 1511529962, 1. 4301628538
H, 0, -7. 305653369, -3. 5235977662, -0. 035650473
H, 0, -7. 8428482539, -2. 4136723178, 1. 2163660321
H, 0, 5. 9487522301, -3. 2484745642, 0. 4466091309
H, 0, 5. 3747871768, -1. 817212002, -3. 5015214519
H, 0, 6. 6081691003, -3. 7038526818, -3. 2230939625
H, 0, 6. 476226069, -5. 9827141684, -2. 3023401565
H, 0, 4. 8964422822, -5. 2032053619, -2. 2412588969
H, 0, 5. 8564129153, -5. 360934301, -0. 7795942909
H, 0, 8. 5935356035, -4. 6011122247, -2. 079014653
H, 0, 8. 0483614399, -3. 9333127931, -0. 5482250256
H, 0, 8. 4969248707, -2. 8552412469, -1. 8612180156
H, 0, 3. 3209291282, 1. 0779502493, -2. 4475828818
H, 0, 2. 5915818357, 0. 4381095234, -4. 6815439901
H, 0, 2. 1739044558, -0. 8276515698, -3. 531161781
H, 0, 3. 5407614996, -1. 0369404523, -4. 6215106069

H, 0, 4. 6665958076, 1. 8514223565, -4. 3343352482
H, 0, 5. 6957975183, 0. 4305445585, -4. 227466015
H, 0, 5. 6855256909, 1. 6026493248, -2. 9190831626
H, 0, 4. 9256451726, -2. 4994817597, 2. 1111832383
H, 0, 3. 3824201413, -1. 4266738986, 3. 5188744363
H, 0, 2. 5530720325, -1. 7706523508, 2. 0075565876
H, 0, 3. 0654524172, -0. 1277108885, 2. 3933975552
H, 0, 5. 8409397463, -0. 7997134169, 3. 5382554763
H, 0, 5. 613524928, 0. 4449856422, 2. 3260800418
H, 0, 6. 7746316656, -0. 8473736344, 2. 0455903696

Eelec= -2580. 68169646
Eelec+ZPE= -2579. 691160
H= -2579. 637659
G= -2579. 778348

(5) Conformer E

C, 0, 1. 0080826166, 4. 862882255, 3. 1653767822
C, 0, -0. 3527243074, 4. 5500586261, 2. 9872582185
C, 0, -0. 7328221128, 3. 5404480309, 2. 1510418166
C, 0, 0. 2284356712, 2. 774868143, 1. 448934837
C, 0, 1. 5973192897, 3. 067745416, 1. 6617335256
C, 0, 1. 9592046592, 4. 1338476007, 2. 5165093168
C, 0, -0. 1209499862, 1. 6995593272, 0. 5706737119
C, 0, 0. 8894602874, 0. 8933512474, 0. 1083473783
C, 0, 2. 2661625414, 1. 1898148863, 0. 2678832294
C, 0, 2. 5809837634, 2. 283309793, 1. 0230638907
C, 0, -1. 5320514564, 1. 4699664132, 0. 1607586145
C, 0, -2. 3073873784, 2. 5207353865, -0. 4294946898
C, 0, -3. 691760497, 2. 311598053, -0. 6433358497
C, 0, -4. 2622390753, 1. 059232748, -0. 3288463175
C, 0, -3. 5111578806, 0. 008128331, 0. 1085251956
C, 0, -2. 1308323124, 0. 247980739, 0. 325808819
C, 0, -1. 7514684367, 3. 7567413045, -0. 8369255079
C, 0, -2. 5315953381, 4. 7315040343, -1. 3890983633
C, 0, -3. 9144750635, 4. 5350036736, -1. 5600893392
C, 0, -4. 4774343831, 3. 3481274113, -1. 1968697349
O, 0, 0. 5695133486, -0. 2319754121, -0. 6257219089
O, 0, -1. 3893715034, -0. 7986439478, 0. 8338078355
P, 0, -0. 1745481087, -1. 4717332761, 0. 0566838693
O, 0, -0. 4307772769, -2. 5407461124, -0. 8966477871
O, 0, 0. 6851612501, -1. 8993419488, 1. 320959404
C, 0, 4. 753923889, -0. 2056506929, -2. 2274959727
C, 0, 5. 4281990099, -1. 1613441894, -1. 4878765117
C, 0, 5. 0492888998, -1. 3301617163, -0. 167056215
C, 0, 4. 0228912704, -0. 5912785075, 0. 407077284
C, 0, 3. 3430360091, 0. 3656858277, -0. 3689314239
C, 0, 3. 7251463573, 0. 57413984, -1. 7069978183

C, 0, 3. 1628148463, 1. 630264677, -2. 6572318304
C, 0, 3. 5224577165, 3. 0601554049, -2. 2441844452
C, 0, 1. 6756570871, 1. 5119821591, -2. 9950062127
C, 0, 3. 7055737055, -0. 8220195474, 1. 8769788423
C, 0, 4. 6665424468, -0. 0417229391, 2. 7791774414
C, 0, 3. 73412413, -2. 3013904036, 2. 2713459954
C, 0, 6. 5403929613, -1. 979956014, -2. 1072397393
C, 0, 6. 1994453492, -3. 4705496575, -2. 1328834743
C, 0, 7. 8807092163, -1. 7365457621, -1. 4123180975
C, 0, -4. 7601712027, -3. 5059172069, -0. 4899342234
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Eelec= -2580. 67323077

Eelec+ZPE= -2579. 682588

H= -2579. 629110

G= -2579. 770983

(6) Conformer F

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C, 0, 1. 4426610013, 4. 7163568143, 2. 0631328305
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C, 0, 2. 2932329671, 1. 9584866389, -0. 2670067256

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P, 0, 0. 4186194627, -1. 0966260985, -0. 9265299074
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Eelec= -2580.66305021
Eelec+ZPE= -2579.672318
H= -2579.618856
G= -2579.759874

H. Cartesian coordinates and total energies of the reported transition states for the C-C bond-formation step of the chiral phosphoric acid-catalyzed Friedel-Crafts reaction (real system) between indole and 2,2,2-trifluoroacetophenone using ONIOM(BH and HLYP/6-31G(d) : HF/3-21G) method.

(1) TS1-*re-exo* (Conformer A)

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H, 0, 4. 6043305519, -5. 8327905703, -0. 6691606395
H, 0, 3. 7569348105, -4. 4210998511, -0. 049720798
H, 0, 3. 5745866804, -4. 8930803485, -1. 739831043
H, 0, 3. 3041735558, -7. 9866626378, -1. 1516921853
H, 0, 2. 3200815264, -7. 1033813631, -2. 3041134862
H, 0, 1. 5498629362, -8. 0066674148, -1. 0079401978
H, 0, -2. 0990628276, -3. 2414676656, 1. 9570691477
H, 0, -0. 8204383128, -2. 8640308036, 3. 9861131526
H, 0, 0. 1209889171, -2. 3100214517, 2. 6048991983
H, 0, 0. 5153553815, -3. 8338082653, 3. 3928266753
H, 0, -2. 3268165185, -4. 9517912639, 3. 7206659205
H, 0, -1. 0260234922, -5. 8898311531, 3. 0017120812
H, 0, -2. 5374807158, -5. 6754145029, 2. 1298671738
H, 0, -1. 972147636, -3. 1431738378, -2. 8277230958
H, 0, -2. 0381823054, -4. 7604705973, -4. 6863472772
H, 0, -2. 2972291592, -5. 5986479116, -3. 160687268
H, 0, -0. 7358328145, -5. 6884814982, -3. 957386092
H, 0, -0. 5496950669, -2. 7150000507, -4. 7907503519
H, 0, 0. 7968693076, -3. 5381858823, -4. 0249951686
H, 0, 0. 1410689736, -2. 0521088741, -3. 3154456609
C, 0, 3. 7581073774, -0. 2060827027, 0. 8723385268
O, 0, 2. 8689942987, 0. 7065687768, 0. 6710966845
C, 0, 5. 0426315062, 0. 2778764142, 1. 5191027293
C, 0, 3. 178571685, -1. 4472327027, 1. 5817368934
F, 0, 3. 0554095595, -1. 2243234419, 2. 8804873304
F, 0, 1. 9676129755, -1. 7429561086, 1. 1105626903
F, 0, 3. 9262756022, -2. 5557803047, 1. 4365468427
C, 0, 5. 1714025144, 1. 6423262674, 1. 7445379785
C, 0, 6. 3215610796, 2. 1521793307, 2. 324600156
C, 0, 7. 3571638956, 1. 3055017707, 2. 6838321846
C, 0, 7. 234593051, -0. 057797984, 2. 4625365605
C, 0, 6. 0860498648, -0. 5697119826, 1. 8828917409
H, 0, 4. 3597264455, 2. 2874998243, 1. 4614589371
H, 0, 6. 4063205243, 3. 2130747639, 2. 4965720393
H, 0, 8. 2519273265, 1. 7021509564, 3. 1359106549
H, 0, 8. 0319336968, -0. 7263317188, 2. 7444749799
H, 0, 6. 0086577283, -1. 6318910141, 1. 7284463621

C, 0, 5. 9573634041, 2. 2579944265, -2. 2723630474
C, 0, 4. 8401805687, 2. 6632325084, -2. 9996137174
C, 0, 3. 6751841824, 1. 913793475, -2. 9968152445
C, 0, 3. 6886769054, 0. 7567920614, -2. 2450614345
C, 0, 4. 7870253011, 0. 3352727933, -1. 5015324114
C, 0, 5. 9408217352, 1. 1002023647, -1. 5093632474
N, 0, 2. 6900021791, -0. 216837429, -2. 1049814161
C, 0, 3. 1065405842, -1. 2037869565, -1. 3671515519
C, 0, 4. 3665526467, -0. 8702824768, -0. 7649774784
H, 0, 6. 8505959689, 2. 8600790065, -2. 3001921169
H, 0, 4. 8826730619, 3. 5719732059, -3. 5768708801
H, 0, 2. 8051927935, 2. 2181558647, -3. 5539783041
H, 0, 6. 8037788318, 0. 8080158381, -0. 935426952
H, 0, 1. 7015119421, -0. 1302985938, -2. 3492140191
H, 0, 2. 4628170808, -2. 0399368839, -1. 1675992889
H, 0, 5. 0632322634, -1. 6510281666, -0. 5158630129

ONIOM: extrapolated energy = -3604. 103554242496
E+ZPE= -3602. 823020
H= -3602. 754947
G= -3602. 928059

(2) TS1-re-exo (Conformer B)

C, 0, -6. 0887330109, 4. 7448829136, -0. 3603120867
C, 0, -5. 2747036153, 4. 7531348497, -1. 5139725227
C, 0, -4. 0138189602, 4. 2511271202, -1. 4750190309
C, 0, -3. 4871880979, 3. 7033783763, -0. 2762386864
C, 0, -4. 3135679009, 3. 6621817815, 0. 8619020966
C, 0, -5. 6194275075, 4. 2105241172, 0. 794457719
C, 0, -2. 1636447188, 3. 1625510644, -0. 1855059023
C, 0, -1. 8031178371, 2. 5050565247, 0. 948750109
C, 0, -2. 6273756525, 2. 4404299203, 2. 0984741751
C, 0, -3. 8372888536, 3. 0500105368, 2. 0474652355
C, 0, -1. 1985188253, 3. 2958545573, -1. 317104693
C, 0, -0. 8505471863, 4. 5796205145, -1. 848960588
C, 0, -0. 0549237665, 4. 6406759857, -3. 0083198957
C, 0, 0. 4112382217, 3. 4393284008, -3. 5969576362
C, 0, 0. 1718580301, 2. 2307729369, -3. 0306501497
C, 0, -0. 6305215692, 2. 1876091685, -1. 8639444847
C, 0, -1. 248328043, 5. 7963673234, -1. 2361808308
C, 0, -0. 8938865556, 6. 9921268787, -1. 7725755735
C, 0, -0. 1254923551, 7. 0507955642, -2. 9558964477
C, 0, 0. 283812824, 5. 9047122092, -3. 5544140353
O, 0, -0. 5583890417, 1. 895546921, 1. 016144405
O, 0, -0. 8728917581, 0. 9444619224, -1. 2930383623
P, 0, -0. 232056356, 0. 5783347033, 0. 1472767762
O, 0, 1. 2319721136, 0. 3784418367, 0. 1382565174
O, 0, -1. 1237702492, -0. 5554042709, 0. 6474643373
C, 0, -0. 779810846, 1. 7267724623, 5. 3085843473

C, 0, -1. 296897467, 0. 5045267516, 5. 6915452239
C, 0, -2. 2506578874, -0. 0881241611, 4. 8816676965
C, 0, -2. 6857033227, 0. 5035097336, 3. 7070363175
C, 0, -2. 1505346886, 1. 7471033031, 3. 3391181033
C, 0, -1. 1923309251, 2. 3633024494, 4. 1467662535
C, 0, -0. 583769872, 3. 719594021, 3. 7928786073
C, 0, 0. 9297515228, 3. 5880854807, 3. 5200281934
C, 0, -0. 8599995796, 4. 7587864189, 4. 9007312387
C, 0, -3. 759697553, -0. 2005411391, 2. 8738896769
C, 0, -5. 1436471002, -0. 0080763648, 3. 5363377519
C, 0, -3. 4857517271, -1. 7071424346, 2. 6842441932
C, 0, -0. 826176024, -0. 1640532487, 6. 9769022027
C, 0, -0. 2097424644, -1. 5510506452, 6. 6959042436
C, 0, -1. 9805665893, -0. 2791585561, 7. 9954930052
C, 0, 2. 5294117628, -0. 5173850869, -4. 122271713
C, 0, 2. 0722433389, 0. 6648193256, -3. 5555980919
C, 0, 0. 7053520847, 0. 9639182861, -3. 6255586355
C, 0, -0. 1696003345, 0. 0895753591, -4. 2782333508
C, 0, 0. 334677726, -1. 0715313457, -4. 8422209892
C, 0, 1. 677355382, -1. 3950736736, -4. 7710866687
C, 0, 2. 1840167849, -2. 6956447021, -5. 3830806462
C, 0, 2. 5521860382, -3. 7034257915, -4. 272193187
C, 0, 3. 3789212603, -2. 4680818579, -6. 3313625982
C, 0, -1. 660974942, 0. 3916790832, -4. 4157214818
C, 0, -2. 5272009996, -0. 7506862093, -3. 8469217941
C, 0, -2. 0154065192, 0. 6757678659, -5. 8914123535
C, 0, 3. 0905094085, 1. 6088128826, -2. 9108132396
C, 0, 4. 0476371406, 2. 1750556349, -3. 9834155726
C, 0, 3. 8807496696, 0. 9188935657, -1. 7800351256
H, 0, -7. 0791220944, 5. 151467138, -0. 4078349209
H, 0, -5. 6613431056, 5. 1557021966, -2. 4288803978
H, 0, -3. 4047452907, 4. 2561921904, -2. 3527661424
H, 0, -6. 2329510485, 4. 1818169024, 1. 6738353528
H, 0, -4. 4661945278, 3. 0488480936, 2. 9142833128
H, 0, 0. 9918797677, 3. 4959698072, -4. 496188246
H, 0, -1. 8268438584, 5. 7575881708, -0. 3387067388
H, 0, -1. 1944120721, 7. 9026106255, -1. 2938111928
H, 0, 0. 1388245612, 8. 0036656171, -3. 3689501566
H, 0, 0. 8806295393, 5. 9348392413, -4. 4451996567
H, 0, -0. 0413720708, 2. 1962250635, 5. 9284534206
H, 0, -2. 6618251298, -1. 0343957436, 5. 1664278038
H, 0, -1. 0508566481, 4. 0753093083, 2. 8876916967
H, 0, 1. 3436166438, 4. 5516115451, 3. 2390784829
H, 0, 1. 0962194084, 2. 8902228464, 2. 7114056191
H, 0, 1. 4525570542, 3. 2406032891, 4. 4040029265
H, 0, -0. 4745711298, 5. 7291231069, 4. 6044916526
H, 0, -0. 3791601816, 4. 4753983474, 5. 8295026711
H, 0, -1. 9245697668, 4. 853000403, 5. 0823523605
H, 0, -3. 7740209669, 0. 249469741, 1. 8933289566

H, 0, -5.9174011335, -0.4714195624, 2.9326831059
H, 0, -5.385746464, 1.0405639219, 3.6547404199
H, 0, -5.1538261181, -0.4689695647, 4.517993389
H, 0, -4.2437385811, -2.1249292467, 2.0287540284
H, 0, -3.5405937607, -2.2407561299, 3.6267236935
H, 0, -2.5211143296, -1.8738129727, 2.2331016019
H, 0, -0.0560718844, 0.4642665528, 7.4117428357
H, 0, 0.1814624484, -1.98189967, 7.6122486969
H, 0, 0.5961609864, -1.4749058823, 5.975671826
H, 0, -0.9554395583, -2.2274733081, 6.2955294208
H, 0, -1.6249149341, -0.7131684591, 8.9245839679
H, 0, -2.7696696739, -0.9115323486, 7.6054876841
H, 0, -2.4005943067, 0.6967188033, 8.2088388146
H, 0, 3.5751759905, -0.7437505488, -4.0687751397
H, 0, -0.3333059229, -1.7385778415, -5.3502859015
H, 0, 1.3729393954, -3.1209518502, -5.9639962715
H, 0, 2.8826680726, -4.6426656414, -4.7043261268
H, 0, 1.6952660631, -3.8983232831, -3.6407634188
H, 0, 3.3582845527, -3.3096886676, -3.6617863369
H, 0, 3.6606121796, -3.4016608668, -6.8071139092
H, 0, 4.2401142201, -2.09645053, -5.7887801715
H, 0, 3.1253917011, -1.7510405375, -7.1030983212
H, 0, -1.881023168, 1.2805776549, -3.847358226
H, 0, -3.5726957579, -0.4608263294, -3.8577169744
H, 0, -2.2349943198, -0.9678156892, -2.83086608
H, 0, -2.4248629248, -1.6517335757, -4.4415765239
H, 0, -3.0673318634, 0.9268177016, -5.9819468863
H, 0, -1.8199840156, -0.1941903796, -6.5077592627
H, 0, -1.4303903137, 1.5041944196, -6.2747033409
H, 0, 2.555265871, 2.4344314989, -2.4692060249
H, 0, 4.7306435624, 2.8890180102, -3.5348001985
H, 0, 3.497040863, 2.6758205198, -4.7717402595
H, 0, 4.633267886, 1.3815741835, -4.4330982296
H, 0, 4.5912224021, 1.6183471335, -1.3504301827
H, 0, 4.4370526468, 0.0649124085, -2.1505947809
H, 0, 3.1949315432, 0.6059729786, -1.0074615883
H, 0, -0.8357867935, -1.6060561093, 0.6794120245
C, 0, -0.367496129, -3.8577475637, 0.1362404361
O, 0, -0.6475499537, -2.8938613777, 0.9461656495
C, 0, -0.7986307616, -5.2364309911, 0.6012339759
C, 0, -0.8181302315, -3.5618535312, -1.308996274
F, 0, -2.1181531329, -3.7717408987, -1.4420241748
F, 0, -0.5843445453, -2.2893893492, -1.6293839278
F, 0, -0.1963937889, -4.3102460288, -2.2372565019
C, 0, -1.3666435322, -5.336612665, 1.8647184111
C, 0, -1.7760685117, -6.5660086286, 2.3548076922
C, 0, -1.6203349574, -7.7099141281, 1.5896172366
C, 0, -1.0547687236, -7.6169009291, 0.3270669609
C, 0, -0.6449645033, -6.3892205966, -0.1650199078

H, 0, -1.4816884289, -4.4408354836, 2.4474150122
H, 0, -2.2181165583, -6.6280730702, 3.3361254349
H, 0, -1.9393433321, -8.6666798869, 1.9705950793
H, 0, -0.93490659, -8.5001839816, -0.2792646153
H, 0, -0.2163518497, -6.3396139055, -1.1509517137
C, 0, 2.3900242377, -5.0036128563, 3.5818952422
C, 0, 2.6880194404, -3.71290932, 4.0136473657
C, 0, 2.6188466045, -2.635302522, 3.1461255302
C, 0, 2.2463053629, -2.9130760286, 1.8468992697
C, 0, 1.9338730889, -4.1910049982, 1.3928768169
C, 0, 2.0005927023, -5.2556299769, 2.2751038357
N, 0, 2.1509979384, -2.0447169843, 0.7506204581
C, 0, 1.8400216151, -2.6973654052, -0.3308106165
C, 0, 1.4861438276, -4.0499807137, -0.0043988206
H, 0, 2.4590030424, -5.8214470978, 4.2801228231
H, 0, 2.9800680159, -3.5496141524, 5.0377737094
H, 0, 2.8460380969, -1.6330938288, 3.4685439407
H, 0, 1.7533285747, -6.2545692326, 1.9582268548
H, 0, 2.1188009741, -1.0236770842, 0.7702597737
H, 0, 1.7354264503, -2.1785328027, -1.2652953149
H, 0, 1.6388153079, -4.8315769269, -0.7274408514

ONIOM: extrapolated energy = -3604.103364621992

E+ZPE= -3602.822848

H= -3602.754728

G= -3602.928426

(3) TS1-*re-exo* (Conformer C)

C, 0, -5.7423174635, 2.0907145735, 4.0299843314
C, 0, -5.849521553, 0.7578040805, 3.5766498493
C, 0, -5.113962381, 0.3245022617, 2.5209298502
C, 0, -4.2184364402, 1.1992526979, 1.8520914562
C, 0, -4.0855048707, 2.5161926428, 2.3295899826
C, 0, -4.8805447527, 2.9440084521, 3.4229375872
C, 0, -3.4221597509, 0.7889040242, 0.7340365414
C, 0, -2.4686631643, 1.6374594949, 0.2648591397
C, 0, -2.3096024568, 2.9605371519, 0.7442319475
C, 0, -3.1405840703, 3.3837843339, 1.728276685
C, 0, -3.6135919513, -0.5506202418, 0.1024232792
C, 0, -4.8894117915, -0.958103716, -0.4060359818
C, 0, -5.0486180521, -2.281813429, -0.8572656628
C, 0, -3.9397424659, -3.1635934127, -0.8356026357
C, 0, -2.7070627209, -2.745244951, -0.4565653972
C, 0, -2.5656228949, -1.4110009105, -0.0016339447
C, 0, -5.9936560738, -0.0720834616, -0.5044439047
C, 0, -7.185277245, -0.499557575, -0.9949211113
C, 0, -7.3530055793, -1.8377358707, -1.4133883706
C, 0, -6.3106547571, -2.7029159744, -1.3477827556
O, 0, -1.6277328343, 1.2204354343, -0.7570030805

O, 0, -1.2996348927, -0.993828218, 0.3901318732
P, 0, -0.5013446288, 0.0969281626, -0.5001212057
O, 0, -0.0359606165, -0.4006255884, -1.8115348842
O, 0, 0.5255334633, 0.6591924932, 0.4783880479
C, 0, -0.5333882721, 5.2788790875, -1.6429521692
C, 0, 0.619306726, 5.6002966894, -0.9531482789
C, 0, 0.8117554322, 5.0439839394, 0.2999752775
C, 0, -0.1071842135, 4.1756045619, 0.8660141342
C, 0, -1.2726378415, 3.8650060298, 0.1493356837
C, 0, -1.48772104, 4.4225476806, -1.1127555598
C, 0, -2.7433179776, 4.1207354873, -1.9297188915
C, 0, -2.3850362749, 3.3744383354, -3.2324680057
C, 0, -3.5347709947, 5.4120281458, -2.2293104142
C, 0, 0.1628180451, 3.6163271386, 2.2651593302
C, 0, -0.1444427562, 4.6972225541, 3.3274775322
C, 0, 1.6108308148, 3.1151300996, 2.4465304796
C, 0, 1.6458480487, 6.5459319806, -1.5635975594
C, 0, 3.0204225641, 5.8599050749, -1.7149639897
C, 0, 1.7729470215, 7.8389285042, -0.7297612289
C, 0, 0.1683762426, -4.8692900707, -1.6835127545
C, 0, -0.9463887966, -4.0404590448, -1.703173415
C, 0, -1.5184072989, -3.6557521386, -0.4852787291
C, 0, -0.9868612512, -4.1315482874, 0.7193596023
C, 0, 0.1155470446, -4.9694241689, 0.689387166
C, 0, 0.7133403009, -5.3417716099, -0.5022980726
C, 0, 1.9017749795, -6.2957180789, -0.5479607253
C, 0, 1.3914054772, -7.7548130023, -0.5538716739
C, 0, 2.8954257106, -6.0869334889, 0.6130885422
C, 0, -1.6079987347, -3.7759634009, 2.0696114119
C, 0, -0.5774358817, -3.1322691838, 3.019481493
C, 0, -2.2475913732, -5.0272531813, 2.7095151019
C, 0, -1.5221593087, -3.6177668833, -3.0569342723
C, 0, -2.104608084, -4.8460775859, -3.7916725418
C, 0, -0.4763349776, -2.9004533979, -3.9344771704
H, 0, -6.3355973373, 2.4171450988, 4.8605880315
H, 0, -6.5152252888, 0.08301112, 4.0767554801
H, 0, -5.1963000533, -0.6866688028, 2.1859698891
H, 0, -4.7759435148, 3.9542938794, 3.7677894156
H, 0, -3.067530608, 4.3911196851, 2.0843932158
H, 0, -4.0790253588, -4.1766630631, -1.1569061335
H, 0, -5.8710324159, 0.9424655801, -0.1925330276
H, 0, -8.0076745922, 0.1833567763, -1.0710668466
H, 0, -8.3029068211, -2.1593589647, -1.791125963
H, 0, -6.4198909159, -3.7180461604, -1.6766942082
H, 0, 1.5995721236, 0.455082147, 0.4527188497
H, 0, -0.6942561157, 5.7048357666, -2.6138204299
H, 0, 1.6992680785, 5.2854608015, 0.8472995408
H, 0, -3.3808037585, 3.4749437297, -1.3460434083
H, 0, -3.2876018184, 3.1376744384, -3.7873907804

H, 0, -1. 8712545449, 2. 4530471066, -2. 9966058996
H, 0, -1. 7500244704, 3. 984710368, -3. 8647623307
H, 0, -4. 452601057, 5. 1716029246, -2. 7562465576
H, 0, -2. 9578629427, 6. 087412745, -2. 8499346654
H, 0, -3. 7910860698, 5. 9274420098, -1. 3107063692
H, 0, -0. 4916569527, 2. 7730603213, 2. 4227871386
H, 0, 0. 0077972593, 4. 2982232777, 4. 3251835775
H, 0, -1. 1655697827, 5. 0493757347, 3. 2532037358
H, 0, 0. 5155337745, 5. 547511588, 3. 1947735985
H, 0, 1. 7093122512, 2. 6654871414, 3. 429815301
H, 0, 2. 321946221, 3. 9319175118, 2. 3900059451
H, 0, 1. 8610542459, 2. 3705532887, 1. 7084737118
H, 0, 1. 2950272534, 6. 8179055294, -2. 5534893586
H, 0, 3. 7200706707, 6. 5241241136, -2. 2126368294
H, 0, 2. 9339387965, 4. 9484855009, -2. 2945368018
H, 0, 3. 4289720682, 5. 6038056787, -0. 744657657
H, 0, 2. 4709132951, 8. 5254229164, -1. 1984077329
H, 0, 2. 1350719945, 7. 6144540161, 0. 2668117192
H, 0, 0. 8119823232, 8. 3316132447, -0. 6397498635
H, 0, 0. 6126658006, -5. 1678145675, -2. 6132947326
H, 0, 0. 5117279509, -5. 3334697573, 1. 6144074721
H, 0, 2. 428913682, -6. 1174966173, -1. 4798264126
H, 0, 2. 2217679899, -8. 4506877446, -0. 6198749724
H, 0, 0. 7280146455, -7. 9267667437, -1. 3931545496
H, 0, 0. 8436930786, -7. 9564562282, 0. 3596886429
H, 0, 3. 7910895098, -6. 6739856734, 0. 4388780689
H, 0, 2. 4663558115, -6. 4168998533, 1. 5522331999
H, 0, 3. 1751475276, -5. 0474208456, 0. 7170450074
H, 0, -2. 3917343551, -3. 0550043166, 1. 9031118465
H, 0, -1. 0715476097, -2. 7940700447, 3. 9243257582
H, 0, -0. 1079936231, -2. 2868462607, 2. 5401128639
H, 0, 0. 1892333224, -3. 8442959307, 3. 3044695932
H, 0, -2. 7229364935, -4. 7653862622, 3. 649312625
H, 0, -1. 4968312895, -5. 7834033007, 2. 9084393266
H, 0, -2. 9970081891, -5. 4546466183, 2. 0528973508
H, 0, -2. 3251118915, -2. 9196595762, -2. 8807439498
H, 0, -2. 5659393354, -4. 5391977481, -4. 7246824891
H, 0, -2. 8535116657, -5. 3437811624, -3. 1860169318
H, 0, -1. 3237346992, -5. 5627760499, -4. 0185638617
H, 0, -0. 9255704746, -2. 6185965294, -4. 8817094672
H, 0, 0. 3708282653, -3. 5433300307, -4. 1463884031
H, 0, -0. 1438172001, -2. 0060678468, -3. 4303557601
C, 0, 3. 7300219997, -0. 5104675369, 0. 7453966434
O, 0, 2. 9204275403, 0. 4669192072, 0. 5130625829
C, 0, 5. 0694677675, -0. 109980347, 1. 3344425047
C, 0, 3. 0635843522, -1. 6565035845, 1. 5334403231
F, 0, 3. 004868253, -1. 3631290161, 2. 8224561423
F, 0, 1. 8164947807, -1. 8620552173, 1. 1116568923
F, 0, 3. 7047329432, -2. 8332979244, 1. 4201849304

C, 0, 5. 3265940191, 1. 2478516939, 1. 4736555211
C, 0, 6. 5327472033, 1. 683668577, 1. 9973888092
C, 0, 7. 4971867753, 0. 7683591721, 2. 3852228243
C, 0, 7. 2468242355, -0. 5886171422, 2. 2492829025
C, 0, 6. 041977349, -1. 0267607426, 1. 7261544661
H, 0, 4. 5691916189, 1. 9467951224, 1. 1686010497
H, 0, 6. 7171906129, 2. 7406221792, 2. 1025348788
H, 0, 8. 4357259038, 1. 1072981117, 2. 793353759
H, 0, 7. 9882008324, -1. 3094969968, 2. 5540302699
H, 0, 5. 8662627374, -2. 0848096578, 1. 6374432013
C, 0, 6. 0721081648, 1. 564628317, -2. 5694057151
C, 0, 4. 9784371911, 2. 0397118014, -3. 29023759
C, 0, 3. 7482534166, 1. 4068808032, -3. 2223569301
C, 0, 3. 6727698847, 0. 2918064722, -2. 4129736882
C, 0, 4. 7464559543, -0. 1965118889, -1. 6746080294
C, 0, 5. 9670148174, 0. 4525058863, -1. 7478859674
N, 0, 2. 5902322347, -0. 5728013867, -2. 2004042046
C, 0, 2. 9312413519, -1. 5579515646, -1. 4222890066
C, 0, 4. 2328761761, -1. 3165919988, -0. 8662242389
H, 0, 7. 0172023356, 2. 0761737404, -2. 6484771763
H, 0, 5. 0913201076, 2. 911313844, -3. 9134465674
H, 0, 2. 8954881444, 1. 7651129177, -3. 7740777994
H, 0, 6. 8138471573, 0. 1070696777, -1. 1795489989
H, 0, 1. 6075700853, -0. 396369323, -2. 4236233401
H, 0, 2. 2178943314, -2. 3192809483, -1. 1657827616
H, 0, 4. 8584316424, -2. 1457638282, -0. 5869251375

ONIOM: extrapolated energy = -3604. 102749228115
E+ZPE= -3602. 822452
H= -3602. 754288
G= -3602. 928498

(4) TS1-*re*-exo (Conformer D)

C, 0, -5. 82910783, 1. 549256101, 4. 133369365
C, 0, -5. 833673251, 0. 2193102491, 3. 6592789706
C, 0, -5. 0770421266, -0. 136757516, 2. 589625452
C, 0, -4. 2619409426, 0. 8175988556, 1. 9270261591
C, 0, -4. 2298401355, 2. 1333222518, 2. 4249483467
C, 0, -5. 0451154446, 2. 4785750384, 3. 5324669923
C, 0, -3. 4473863921, 0. 4903370002, 0. 7946431944
C, 0, -2. 569086155, 1. 4198007773, 0. 3328129153
C, 0, -2. 5099217204, 2. 7433818659, 0. 8330546103
C, 0, -3. 3630464339, 3. 0834232822, 1. 8302806995
C, 0, -3. 5417500472, -0. 8469922606, 0. 1369096451
C, 0, -4. 7902312131, -1. 3406205209, -0. 3636609716
C, 0, -4. 8545263829, -2. 6628499109, -0. 8414810332
C, 0, -3. 6803470805, -3. 4551886939, -0. 8577419949
C, 0, -2. 4768681599, -2. 9504589618, -0. 4892570205
C, 0, -2. 4316425909, -1. 6205244723, -0. 0028904326

C, 0, -5.960661844, -0.5404615363, -0.4281931013
 C, 0, -7.1233845937, -1.0484478356, -0.9111562695
 C, 0, -7.1946080859, -2.3869023883, -1.3555078863
 C, 0, -6.0879692891, -3.1701689839, -1.3231386524
 O, 0, -1.7068883433, 1.0869979896, -0.702541213
 O, 0, -1.1959825126, -1.1204221678, 0.3879178087
 P, 0, -0.4892901585, 0.0600459448, -0.4626564262
 O, 0, 0.0363553301, -0.3561004695, -1.7793143772
 O, 0, 0.4719540933, 0.689502656, 0.5437137266
 C, 0, -0.91481409, 5.2029115736, -1.5419071219
 C, 0, 0.2080184361, 5.612843075, -0.8429205772
 C, 0, 0.4350547364, 5.0722470057, 0.4074262735
 C, 0, -0.4172120972, 4.1315218566, 0.9707743316
 C, 0, -1.5470044192, 3.7322579793, 0.2485250218
 C, 0, -1.7985330817, 4.2757358752, -1.0176072088
 C, 0, -3.0262709636, 3.8805906441, -1.8380005986
 C, 0, -2.6128678453, 3.18884121, -3.1542802783
 C, 0, -3.9242235669, 5.1060631864, -2.1131921387
 C, 0, -0.1079362082, 3.5971754411, 2.3711448328
 C, 0, -0.4890667611, 4.6578777111, 3.4299628355
 C, 0, 1.3718178481, 3.1991252161, 2.5520532041
 C, 0, 1.18677553, 6.6189678996, -1.4347949666
 C, 0, 0.4908027016, 7.9469522765, -1.7994956795
 C, 0, 1.9025773771, 6.0218742014, -2.6660626278
 C, 0, 0.4802735337, -4.8654873289, -1.8543784253
 C, 0, -0.6734917244, -4.0934787971, -1.8177575654
 C, 0, -1.2243025707, -3.7671732839, -0.5731982252
 C, 0, -0.62079366, -4.2293823802, 0.6023082166
 C, 0, 0.5292846303, -4.9972773028, 0.5169070705
 C, 0, 1.0960612372, -5.3242368125, -0.7033930951
 C, 0, 2.3805441, -6.1399872152, -0.8162145422
 C, 0, 2.5469045469, -7.1832233636, 0.305919689
 C, 0, 3.5974920602, -5.1862412922, -0.8395558786
 C, 0, -1.2366598216, -3.9583463559, 1.9748454387
 C, 0, -0.2026076183, -3.449408206, 2.9987186199
 C, 0, -1.9364266956, -5.2360802735, 2.4879111567
 C, 0, -1.3041908446, -3.6585154362, -3.1427956217
 C, 0, -1.800975544, -4.8886068475, -3.9342017391
 C, 0, -0.3255137092, -2.8182719029, -3.989303468
 H, 0, -6.437825745, 1.8138630377, 4.9747286448
 H, 0, -6.4375237396, -0.5146586803, 4.1545096126
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 H, 0, -5.0182814622, 3.4884313857, 3.893030383
 H, 0, -3.366411362, 4.0871436596, 2.2035622602
 H, 0, -3.7451600561, -4.4678268612, -1.2033340234
 H, 0, -5.9116976284, 0.4740645497, -0.0967912828
 H, 0, -7.9966933673, -0.4293332797, -0.9615627886
 H, 0, -8.1228128464, -2.7730518061, -1.7266655707
 H, 0, -6.1238151078, -4.1837479836, -1.6723840525

H, 0, 1. 5488085966, 0. 5583819288, 0. 5384824696
H, 0, -1. 1086928921, 5. 6122849653, -2. 5129609787
H, 0, 1. 3006194054, 5. 3853181253, 0. 9552468146
H, 0, -3. 6052296276, 3. 1739564589, -1. 2641880184
H, 0, -3. 4952969048, 2. 8846266832, -3. 7086709533
H, 0, -2. 0210278607, 2. 3110390804, -2. 936116741
H, 0, -2. 0365563645, 3. 8608793867, -3. 7801279612
H, 0, -4. 8196247991, 4. 7996925657, -2. 6445085104
H, 0, -3. 4064861523, 5. 8390005896, -2. 7206580347
H, 0, -4. 2210758601, 5. 58091659, -1. 1849980303
H, 0, -0. 7019742511, 2. 7110681523, 2. 5324928473
H, 0, -0. 3098823188, 4. 2733810491, 4. 428888873
H, 0, -1. 5320840479, 4. 9387378754, 3. 3544248998
H, 0, 0. 1106681071, 5. 5512892938, 3. 2949407898
H, 0, 1. 5032511213, 2. 7632750847, 3. 5377341997
H, 0, 2. 0239520048, 4. 0632185623, 2. 4885836012
H, 0, 1. 6720065267, 2. 4694489856, 1. 8177462938
H, 0, 1. 9372089968, 6. 8300307373, -0. 6806385826
H, 0, 1. 2182521703, 8. 6661627093, -2. 1619365477
H, 0, -0. 0082469284, 8. 3674705433, -0. 9344298228
H, 0, -0. 247460444, 7. 7935904012, -2. 5778241708
H, 0, 2. 6317663497, 6. 7238612579, -3. 058528156
H, 0, 1. 1866066071, 5. 8010848342, -3. 4495821227
H, 0, 2. 4131564237, 5. 1036024581, -2. 3997110726
H, 0, 0. 901345658, -5. 1280581297, -2. 8055717303
H, 0, 0. 9798278666, -5. 3514120437, 1. 4198326998
H, 0, 2. 3475098221, -6. 670892822, -1. 7617088215
H, 0, 3. 4054569127, -7. 8120142465, 0. 096210878
H, 0, 1. 6697646413, -7. 8147688074, 0. 3829725524
H, 0, 2. 7147917288, -6. 7049739837, 1. 2636882053
H, 0, 4. 5239258203, -5. 7485041365, -0. 9013721349
H, 0, 3. 6174292057, -4. 5802039212, 0. 0572451036
H, 0, 3. 5447046239, -4. 528083584, -1. 7006461818
H, 0, -1. 9842640651, -3. 1906068627, 1. 865127285
H, 0, -0. 7089638906, -3. 1520474636, 3. 9108540011
H, 0, 0. 329050682, -2. 5978585768, 2. 6028926143
H, 0, 0. 512905783, -4. 2225681726, 3. 2558838032
H, 0, -2. 4049281959, -5. 0495862574, 3. 4490017294
H, 0, -1. 2180474342, -6. 0392697721, 2. 6074988707
H, 0, -2. 7002724972, -5. 5618644093, 1. 7910416436
H, 0, -2. 15630829, -3. 0347328946, -2. 9243760732
H, 0, -2. 2988427664, -4. 569916072, -4. 8441570769
H, 0, -2. 5004755863, -5. 4731776252, -3. 3472362796
H, 0, -0. 9721379626, -5. 5306218749, -4. 2089181137
H, 0, -0. 8050193635, -2. 5208610816, -4. 9168288726
H, 0, 0. 5639771577, -3. 385627653, -4. 2405399399
H, 0, -0. 0511357835, -1. 929470347, -3. 4409372184
C, 0, 3. 7511450761, -0. 2712803971, 0. 8357882724
O, 0, 2. 8794828538, 0. 6579996971, 0. 6343371903

C, 0, 5. 0486301744, 0. 1889893368, 1. 4752590832
C, 0, 3. 1480564555, -1. 493595231, 1. 5578176188
F, 0, 3. 0115672301, -1. 2486575977, 2. 8513291453
F, 0, 1. 9361986746, -1. 7779174049, 1. 0781919012
F, 0, 3. 8778270631, -2. 6160729186, 1. 4389379522
C, 0, 5. 20294768, 1. 5509438637, 1. 6998651713
C, 0, 6. 3653868761, 2. 0406006079, 2. 2727113699
C, 0, 7. 3883509816, 1. 1759463504, 2. 6253598626
C, 0, 7. 2406282126, -0. 1848860633, 2. 4045478087
C, 0, 6. 0795724699, -0. 6766306164, 1. 8321740871
H, 0, 4. 401059102, 2. 2101617321, 1. 4213043795
H, 0, 6. 4697964369, 3. 0998572002, 2. 4440286066
H, 0, 8. 2927740447, 1. 5568426711, 3. 0717474996
H, 0, 8. 0280798627, -0. 8672821392, 2. 6810748075
H, 0, 5. 9832057673, -1. 7371960232, 1. 6777826673
C, 0, 6. 0122712547, 2. 1174896514, -2. 317583523
C, 0, 4. 9060679045, 2. 5541423199, -3. 043293837
C, 0, 3. 719565178, 1. 8392771749, -3. 0364344736
C, 0, 3. 700620483, 0. 6841077022, -2. 2820913469
C, 0, 4. 7874336293, 0. 2317838307, -1. 5396881833
C, 0, 5. 9631670884, 0. 9623394799, -1. 5518315698
N, 0, 2. 6736678136, -0. 2591526989, -2. 1379962953
C, 0, 3. 0614660252, -1. 2556410702, -1. 3981642593
C, 0, 4. 3321632333, -0. 958417821, -0. 7975700382
H, 0, 6. 9228499723, 2. 6928537839, -2. 3484222479
H, 0, 4. 9741205513, 3. 4601145266, -3. 6224561988
H, 0, 2. 8576145985, 2. 1676915247, -3. 5924490932
H, 0, 6. 8182338606, 0. 6464746891, -0. 9786549813
H, 0, 1. 6881097816, -0. 1447707089, -2. 3833810475
H, 0, 2. 3933501587, -2. 0713219891, -1. 1952639045
H, 0, 5. 0048651787, -1. 7607078921, -0. 550050603

ONIOM: extrapolated energy = -3604. 102542290252

E+ZPE= -3602. 821819

H= -3602. 753768

G= -3602. 927909

(5) TS1-si-exo (Conformer A')

C, 0, 2. 9629421137, -5. 5287243115, 3. 8176298193
C, 0, 3. 9213607428, -4. 539509448, 3. 5052492962
C, 0, 3. 6806999396, -3. 626473136, 2. 5298585393
C, 0, 2. 4594371814, -3. 6424400733, 1. 8066077666
C, 0, 1. 491640803, -4. 6050299674, 2. 144853329
C, 0, 1. 7797440224, -5. 5571061851, 3. 1556442648
C, 0, 2. 1603313845, -2. 7019975141, 0. 7692703118
C, 0, 0. 901917439, -2. 6730388649, 0. 2520542026
C, 0, -0. 0886545393, -3. 6273430363, 0. 5893120655
C, 0, 0. 2383110145, -4. 5908781245, 1. 4864027219
C, 0, 3. 2039039275, -1. 7698698812, 0. 252240345

C, 0, 4. 4411423598, -2. 2645266813, -0. 2724201236
 C, 0, 5. 4386359387, -1. 3416145206, -0. 6379896177
 C, 0, 5. 1715322918, 0. 0446576802, -0. 5401141447
 C, 0, 3. 9576265878, 0. 5117064855, -0. 1533612552
 C, 0, 2. 97906269, -0. 4284333614, 0. 2488158353
 C, 0, 4. 6955020182, -3. 6474988645, -0. 4689832254
 C, 0, 5. 8860170776, -4. 0706338734, -0. 9649760926
 C, 0, 6. 9004483344, -3. 1440735259, -1. 2930737971
 C, 0, 6. 6791597737, -1. 8157020345, -1. 1363922639
 O, 0, 0. 5693613503, -1. 6954671139, -0. 6803921285
 O, 0, 1. 7520883124, 0. 0549733108, 0. 6840929063
 P, 0, 0. 4310395643, -0. 152751218, -0. 2311116001
 O, 0, 0. 3839588619, 0. 7136295421, -1. 422390099
 O, 0, -0. 6885095502, -0. 026428324, 0. 8063882213
 C, 0, -2. 8469024281, -4. 0407712941, -1. 9507008134
 C, 0, -3. 9758581788, -3. 6917360678, -1. 2297592614
 C, 0, -3. 8163524557, -3. 2891232869, 0. 0821615514
 C, 0, -2. 5699765265, -3. 2308030412, 0. 6901684612
 C, 0, -1. 4427202303, -3. 6008230111, -0. 052819121
 C, 0, -1. 5835472423, -4. 0069928424, -1. 3854559272
 C, 0, -0. 3844519533, -4. 4265945754, -2. 2355903126
 C, 0, -0. 1958030352, -3. 4703254094, -3. 4321521707
 C, 0, -0. 5264345758, -5. 8888755373, -2. 710228024
 C, 0, -2. 4815944378, -2. 7989128344, 2. 1564598747
 C, 0, -2. 9528478359, -3. 9518311307, 3. 0732504883
 C, 0, -3. 312370314, -1. 5348317466, 2. 4630573302
 C, 0, -5. 3632600852, -3. 7146300261, -1. 8597729748
 C, 0, -5. 6770697542, -5. 0691879472, -2. 5276797929
 C, 0, -5. 5109445161, -2. 5569967732, -2. 8712565896
 C, 0, 3. 3796419469, 4. 0308133314, -1. 3964545888
 C, 0, 3. 5645859797, 2. 6551723743, -1. 3984617434
 C, 0, 3. 6678159183, 1. 9816954245, -0. 1717335308
 C, 0, 3. 5705452018, 2. 695877164, 1. 0265692656
 C, 0, 3. 3921579309, 4. 0715632473, 0. 9781748178
 C, 0, 3. 3038165802, 4. 7580410679, -0. 2215193048
 C, 0, 3. 2047141691, 6. 2799153489, -0. 2247934168
 C, 0, 2. 1626633899, 6. 8198401484, -1. 225496365
 C, 0, 4. 5958205918, 6. 8846817105, -0. 5223522292
 C, 0, 3. 6807413989, 2. 010798468, 2. 3879879249
 C, 0, 2. 3690175489, 2. 1556804061, 3. 1884842846
 C, 0, 4. 8831178031, 2. 559443502, 3. 186202695
 C, 0, 3. 6759251805, 1. 9398903144, -2. 7486819345
 C, 0, 4. 9279470375, 2. 4210496874, -3. 5153558937
 C, 0, 2. 403783541, 2. 1320045391, -3. 6020045879
 H, 0, 3. 1730069851, -6. 2456514299, 4. 5859666664
 H, 0, 4. 8442510961, -4. 5097018238, 4. 0493276362
 H, 0, 4. 4078160906, -2. 8776446599, 2. 300954286
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 H, 0, -0. 478294254, -5. 34854938, 1. 7286291091

H, 0, 5. 9382534451, 0. 7389778357, -0. 8209090293
H, 0, 3. 9312118326, -4. 3531650778, -0. 2264062025
H, 0, 6. 0601450058, -5. 1173277366, -1. 1152151682
H, 0, 7. 8367760983, -3. 4976059921, -1. 6760945757
H, 0, 7. 4336310499, -1. 0996185818, -1. 3982810241
H, 0, -1. 5306570474, 0. 6135811193, 0. 6685791586
H, 0, -2. 949099906, -4. 3488934516, -2. 9715883278
H, 0, -4. 6834323127, -3. 0044077325, 0. 6418852227
H, 0, 0. 5031844381, -4. 366727552, -1. 6256509611
H, 0, 0. 6774938478, -3. 7611549632, -4. 0079963382
H, 0, -0. 054694533, -2. 4600948905, -3. 074384115
H, 0, -1. 0579263435, -3. 4974217041, -4. 0887589363
H, 0, 0. 3588590236, -6. 1888785132, -3. 2618692722
H, 0, -1. 3844061853, -6. 0048479983, -3. 3617919371
H, 0, -0. 647419159, -6. 5568850968, -1. 8650258352
H, 0, -1. 4507965775, -2. 5705989553, 2. 3799068012
H, 0, -2. 8571864733, -3. 6658662159, 4. 1158596287
H, 0, -2. 3739369818, -4. 8523646926, 2. 9123248874
H, 0, -3. 9941756545, -4. 1813112742, 2. 8761918114
H, 0, -3. 1416984205, -1. 2427869977, 3. 494766125
H, 0, -4. 3735757167, -1. 7205462504, 2. 3460845179
H, 0, -3. 0304591432, -0. 7093200154, 1. 8311448494
H, 0, -6. 0851846176, -3. 5585629155, -1. 0655411639
H, 0, -6. 6974217727, -5. 075515455, -2. 8971304305
H, 0, -5. 5614907248, -5. 8826784075, -1. 8209849502
H, 0, -5. 0167543753, -5. 2496427672, -3. 3677543101
H, 0, -6. 508146592, -2. 5511454758, -3. 3004523666
H, 0, -4. 7926384205, -2. 6659376124, -3. 6761639142
H, 0, -5. 3391332993, -1. 6100036533, -2. 3802959371
H, 0, 3. 3159034925, 4. 5416582368, -2. 3351295621
H, 0, 3. 3432636642, 4. 623993095, 1. 8966413706
H, 0, 2. 9070318189, 6. 5930909631, 0. 7706082713
H, 0, 2. 089088237, 7. 8982133608, -1. 1333967965
H, 0, 1. 1842739935, 6. 394948304, -1. 0389368489
H, 0, 2. 4493048584, 6. 5945286939, -2. 2457431526
H, 0, 4. 5567326288, 7. 9684889127, -0. 4831432074
H, 0, 4. 9263782602, 6. 5876741041, -1. 5110993856
H, 0, 5. 3263475852, 6. 5382608513, 0. 1989560064
H, 0, 3. 8486482443, 0. 9583004667, 2. 2240022024
H, 0, 2. 4601682013, 1. 64960417, 4. 144087998
H, 0, 1. 5510214735, 1. 7069892797, 2. 6425590734
H, 0, 2. 1439676534, 3. 1988942259, 3. 3810702774
H, 0, 4. 9854823896, 2. 0168980225, 4. 1202022219
H, 0, 4. 7503209501, 3. 6091330648, 3. 4206427468
H, 0, 5. 8023961197, 2. 4484064976, 2. 6225433027
H, 0, 3. 7824301573, 0. 882922812, -2. 565418874
H, 0, 5. 0340675393, 1. 8631446831, -4. 4397665419
H, 0, 5. 8261924054, 2. 279694852, -2. 9251429553
H, 0, 4. 8486416153, 3. 4731695694, -3. 7631577218

H, 0, 2. 5235249932, 1. 6236952864, -4. 553761482
H, 0, 2. 2219770943, 3. 1817376354, -3. 8056362825
H, 0, 1. 5554939429, 1. 7042372511, -3. 0880112851
C, 0, -3. 5542715218, 1. 7822511524, -0. 0165331299
O, 0, -2. 6140118032, 1. 4531705034, 0. 8067677196
C, 0, -4. 8201029819, 2. 309284809, 0. 6430289466
C, 0, -3. 8643424477, 0. 6567336728, -1. 026930781
C, 0, -4. 8024414752, 2. 4627678271, 2. 0229348216
C, 0, -5. 9161467505, 2. 9473019344, 2. 6896426127
C, 0, -7. 0592692453, 3. 2863273375, 1. 984501011
C, 0, -7. 0841118615, 3. 1335783526, 0. 6064814463
C, 0, -5. 971827004, 2. 6492097882, -0. 0615727654
F, 0, -4. 6293551348, -0. 2699743591, -0. 4631127184
F, 0, -2. 7477853169, 0. 0658433112, -1. 442599153
F, 0, -4. 507355349, 1. 0733964842, -2. 1306639186
H, 0, -3. 90631038, 2. 1939863164, 2. 5525467899
H, 0, -5. 8893955962, 3. 0585715964, 3. 7617258324
H, 0, -7. 9262803264, 3. 6632331617, 2. 5028532624
H, 0, -7. 9713736799, 3. 3877619486, 0. 0492313882
H, 0, -6. 0161989657, 2. 5280386234, -1. 1304221224
C, 0, -2. 500152277, 5. 9192090941, 1. 560518598
C, 0, -1. 1254095203, 5. 7426070749, 1. 6940089003
C, 0, -0. 4453194829, 4. 8094035141, 0. 9276339129
C, 0, -1. 2030033267, 4. 0841544537, 0. 0323913742
C, 0, -2. 580142742, 4. 2244056984, -0. 1068403665
C, 0, -3. 2433081272, 5. 1563990967, 0. 6713396966
N, 0, -0. 7881788999, 3. 1186662441, -0. 8994632841
C, 0, -1. 7921798957, 2. 6819637057, -1. 5971804411
C, 0, -3. 0279681114, 3. 185864031, -1. 0575930316
H, 0, -2. 9981744697, 6. 656955966, 2. 1678520208
H, 0, -0. 5800943318, 6. 3404419304, 2. 4054121791
H, 0, 0. 615137593, 4. 6523248625, 1. 0216802986
H, 0, -4. 3096855676, 5. 2837186022, 0. 5956776829
H, 0, 0. 1311932997, 2. 7023882377, -0. 9847347857
H, 0, -1. 6384946073, 1. 9302977963, -2. 34554319
H, 0, -3. 8480139024, 3. 3664340338, -1. 7311163879

ONIOM: extrapolated energy = -3604. 100941758964

E+ZPE= -3602. 819457

H= -3602. 751419

G= -3602. 924481

(6) TS1-si-exo (Conformer B')

C, 0, 2. 6003074692, -5. 6302027393, 3. 9007501816
C, 0, 3. 6029254191, -4. 6780828883, 3. 6127448645
C, 0, 3. 4284016316, -3. 7684573528, 2. 6202147097
C, 0, 2. 2332802007, -3. 7508545259, 1. 8548603839
C, 0, 1. 2219676193, -4. 676976623, 2. 1664853636
C, 0, 1. 4411880359, -5. 62646214, 3. 1967358206

C, 0, 2. 0031003033, -2. 8114296652, 0. 7996790198
 C, 0, 0. 7664120676, -2. 7460997083, 0. 2366778063
 C, 0, -0. 2643183304, -3. 6690947067, 0. 5392230764
 C, 0, -0. 0033815277, -4. 6321570927, 1. 4579740056
 C, 0, 3. 0955262289, -1. 9254629526, 0. 3039687691
 C, 0, 4. 3233799735, -2. 4765780368, -0. 1852442657
 C, 0, 5. 3636861431, -1. 5996743335, -0. 5439915758
 C, 0, 5. 1491483153, -0. 2030789747, -0. 4716822338
 C, 0, 3. 9476821447, 0. 3172993593, -0. 1153555646
 C, 0, 2. 9229020292, -0. 5764419829, 0. 2777942553
 C, 0, 4. 5274252475, -3. 8715683578, -0. 3546499253
 C, 0, 5. 7103687352, -4. 3486793081, -0. 8186552694
 C, 0, 6. 7668142261, -3. 4678283247, -1. 1401051215
 C, 0, 6. 5945748416, -2. 1295127024, -1. 0089832916
 O, 0, 0. 5005758514, -1. 7597406745, -0. 7091231758
 O, 0, 1. 7056156612, -0. 0397815137, 0. 678395663
 P, 0, 0. 3913581191, -0. 2163141409, -0. 2557343172
 O, 0, 0. 3807812298, 0. 6632295689, -1. 4377259946
 O, 0, -0. 7467163046, -0. 0802482694, 0. 7616593606
 C, 0, -2. 8851878042, -4. 0480839583, -2. 1411078266
 C, 0, -4. 0356164603, -3. 6129092419, -1. 509801531
 C, 0, -3. 9397983246, -3. 1751074232, -0. 2004680112
 C, 0, -2. 7339663012, -3. 1722688083, 0. 4853565539
 C, 0, -1. 5798101238, -3. 6132087801, -0. 1767341787
 C, 0, -1. 6564765062, -4. 0542204602, -1. 5011398249
 C, 0, -0. 4300686195, -4. 5534012724, -2. 2643404413
 C, 0, -0. 1144487223, -3. 6272414818, -3. 4581142929
 C, 0, -0. 6188704978, -6. 0135157238, -2. 728996391
 C, 0, -2. 7141184041, -2. 7476248121, 1. 9569697133
 C, 0, -3. 2668628495, -3. 8983567585, 2. 8312511696
 C, 0, -3. 5240317761, -1. 4662685336, 2. 241405061
 C, 0, -5. 353212458, -3. 5901013401, -2. 2766362886
 C, 0, -5. 6082223442, -2. 1694865115, -2. 8283188993
 C, 0, -6. 5516873581, -4. 0612481677, -1. 4285908249
 C, 0, 3. 5406503401, 3. 8450834527, -1. 4000687088
 C, 0, 3. 6542026192, 2. 4618240293, -1. 3865476642
 C, 0, 3. 726320918, 1. 7987170323, -0. 1521913109
 C, 0, 3. 6737817333, 2. 5305941382, 1. 0378724174
 C, 0, 3. 5686652055, 3. 9132951789, 0. 9741040423
 C, 0, 3. 5089597053, 4. 5889755125, -0. 2334394122
 C, 0, 3. 4851629398, 6. 1135907509, -0. 2567025766
 C, 0, 2. 4398535024, 6. 6878140012, -1. 2348052364
 C, 0, 4. 8939088929, 6. 6465706903, -0. 6036466972
 C, 0, 3. 7526171346, 1. 8540718124, 2. 4056648814
 C, 0, 2. 4423791225, 2. 0554150441, 3. 1962999174
 C, 0, 4. 9701705842, 2. 3621581211, 3. 2074635686
 C, 0, 3. 7318387427, 1. 7248289974, -2. 7273172175
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 C, 0, 2. 4813529103, 1. 9811226796, -3. 5955814363

H, 0, 2. 7581272036, -6. 3449237254, 4. 6835136775
H, 0, 4. 5066336676, -4. 6739981246, 4. 1888728862
H, 0, 4. 1885168003, -3. 0475272375, 2. 4090593032
H, 0, 0. 6648655418, -6. 3335213617, 3. 4154914382
H, 0, -0. 7502396211, -5. 3674801813, 1. 6762229824
H, 0, 5. 9481749065, 0. 4567171138, -0. 7455009529
H, 0, 3. 73149952, -4. 5431034565, -0. 1173505512
H, 0, 5. 8464058925, -5. 4037030826, -0. 9485675689
H, 0, 7. 6961115141, -3. 8637953911, -1. 4978858034
H, 0, 7. 3815906225, -1. 4475826956, -1. 2661863684
H, 0, -1. 5286371244, 0. 6299815721, 0. 6490090024
H, 0, -2. 949190026, -4. 3918677474, -3. 1550429473
H, 0, -4. 8171963419, -2. 8257820112, 0. 3002896075
H, 0, 0. 4181005321, -4. 5308697535, -1. 5980245998
H, 0, 0. 7776758896, -3. 971351904, -3. 9724823691
H, 0, 0. 054716402, -2. 6196693406, -3. 1047444106
H, 0, -0. 9335350336, -3. 6208549404, -4. 1681756456
H, 0, 0. 2845895948, -6. 368719115, -3. 2143850818
H, 0, -1. 434869305, -6. 094698147, -3. 4371432638
H, 0, -0. 8330443698, -6. 6604157683, -1. 8858596764
H, 0, -1. 6908962869, -2. 5512269638, 2. 2379478459
H, 0, -3. 2132673526, -3. 6315416854, 3. 8819198531
H, 0, -2. 7114952065, -4. 8156239959, 2. 6833242205
H, 0, -4. 3041145188, -4. 0891760722, 2. 5790692338
H, 0, -3. 419056537, -1. 2118172761, 3. 291680649
H, 0, -4. 5794736667, -1. 60941505, 2. 0432930198
H, 0, -3. 1691737674, -0. 6322004169, 1. 6609544835
H, 0, -5. 2534837421, -4. 2690227621, -3. 1170419631
H, 0, -6. 5424123032, -2. 1346660061, -3. 3803573844
H, 0, -4. 8044003116, -1. 8719163811, -3. 4924557021
H, 0, -5. 6538005688, -1. 458853473, -2. 0154635932
H, 0, -7. 4387130396, -4. 129221249, -2. 0497203738
H, 0, -6. 7613268514, -3. 3621680031, -0. 6279366053
H, 0, -6. 3599559134, -5. 0356475535, -0. 9945345325
H, 0, 3. 5001995981, 4. 3480112484, -2. 3443699985
H, 0, 3. 5550404832, 4. 4784873416, 1. 8860474819
H, 0, 3. 2323174765, 6. 4546902279, 0. 7418647808
H, 0, 2. 4229031137, 7. 7700220022, -1. 1616241907
H, 0, 1. 4483359872, 6. 3158047989, -1. 0090061856
H, 0, 2. 681962837, 6. 4295418542, -2. 2588024504
H, 0, 4. 9076012412, 7. 7313950581, -0. 5786470443
H, 0, 5. 1805654103, 6. 3219146159, -1. 597379789
H, 0, 5. 6283972315, 6. 2748035456, 0. 1008519062
H, 0, 3. 8812050029, 0. 7945141065, 2. 2506276215
H, 0, 2. 5074363452, 1. 5549706943, 4. 1569522301
H, 0, 1. 6115913484, 1. 6334826672, 2. 648103841
H, 0, 2. 2558849042, 3. 1082531237, 3. 3775877376
H, 0, 5. 0471096231, 1. 8210378544, 4. 1446927467
H, 0, 4. 875525585, 3. 4171503533, 3. 4363852269

H, 0, 5. 8877007276, 2. 2139643044, 2. 6495805362
H, 0, 3. 77458936, 0. 6655988177, -2. 5303999187
H, 0, 5. 0971240077, 1. 5498571781, -4. 4055469407
H, 0, 5. 9000268593, 1. 9345459381, -2. 8882997433
H, 0, 5. 0014730718, 3. 1751161134, -3. 7462883758
H, 0, 2. 5814478007, 1. 4567772818, -4. 540856147
H, 0, 2. 3623166504, 3. 0372179222, -3. 8120181136
H, 0, 1. 6046050376, 1. 6076058772, -3. 0872807903
C, 0, -3. 4748059544, 1. 979757553, 0. 0216917335
O, 0, -2. 5500035161, 1. 5546938306, 0. 8172691636
C, 0, -4. 6823356627, 2. 5893366759, 0. 7195754807
C, 0, -3. 8961907841, 0. 9118158538, -1. 0104633998
C, 0, -4. 6288933828, 2. 6985552353, 2. 1027567059
C, 0, -5. 6865549517, 3. 2535602203, 2. 8047306375
C, 0, -6. 8089945735, 3. 7080675942, 2. 1320868012
C, 0, -6. 8698362903, 3. 5998231152, 0. 7510063749
C, 0, -5. 8135104285, 3. 0449267815, 0. 0477083215
F, 0, -4. 7188753823, 0. 0329337068, -0. 4453716413
F, 0, -2. 8415680582, 0. 2446189185, -1. 469106699
F, 0, -4. 52975061, 1. 4103952968, -2. 083565743
H, 0, -3. 7493025742, 2. 3403338046, 2. 606569275
H, 0, -5. 6324029024, 3. 3295272349, 3. 878868503
H, 0, -7. 63243157, 4. 1399955883, 2. 6778483567
H, 0, -7. 7419863991, 3. 9437956491, 0. 2186125267
H, 0, -5. 8862030963, 2. 9608298011, -1. 0230592609
C, 0, -2. 1407414656, 6. 0135290567, 1. 6583071625
C, 0, -0. 7803360206, 5. 7445743703, 1. 7840621262
C, 0, -0. 1653419553, 4. 780153797, 1. 001571893
C, 0, -0. 9716416245, 4. 1189649099, 0. 0990977752
C, 0, -2. 3366312457, 4. 352233016, -0. 0329755415
C, 0, -2. 9347350019, 5. 314890222, 0. 7606773399
N, 0, -0. 6245410417, 3. 1416239013, -0. 848402116
C, 0, -1. 6573678247, 2. 7828919431, -1. 5487060723
C, 0, -2. 855269486, 3. 3609592265, -0. 9978443698
H, 0, -2. 5874540082, 6. 7734256561, 2. 2781248702
H, 0, -0. 1948106915, 6. 2946838382, 2. 5020127429
H, 0, 0. 8829845469, 4. 5541472852, 1. 0872558174
H, 0, -3. 9905603322, 5. 5132766411, 0. 6904616018
H, 0, 0. 2671807577, 2. 6720410551, -0. 9464905211
H, 0, -1. 5558256611, 2. 0326788226, -2. 3074914509
H, 0, -3. 661763279, 3. 608086326, -1. 6665530365

ONIOM: extrapolated energy = -3604. 100485411717
E+ZPE= -3602. 818770
H= -3602. 750760
G= -3602. 923425

(7) TS1-*si*-exo (Conformer C')

C, 0, 2. 3877583013, -5. 5007314735, 4. 0718331438

C, 0, 3. 4194389695, -4. 5923004832, 3. 7474514417
 C, 0, 3. 2765369655, -3. 723570171, 2. 7140690173
 C, 0, 2. 0858376935, -3. 7051926917, 1. 9419998399
 C, 0, 1. 0463954083, -4. 5867702234, 2. 2882024999
 C, 0, 1. 2326415076, -5. 4950167002, 3. 361289909
 C, 0, 1. 8882967704, -2. 8078412789, 0. 8445080557
 C, 0, 0. 6566252783, -2. 7302898084, 0. 2732071801
 C, 0, -0. 4016589483, -3. 6096620186, 0. 6083431289
 C, 0, -0. 1730502307, -4. 5387213686, 1. 5699797883
 C, 0, 3. 0113794081, -1. 9857901512, 0. 3094627579
 C, 0, 4. 2161615763, -2. 609412281, -0. 1491306938
 C, 0, 5. 2914927999, -1. 7941140112, -0. 5460332091
 C, 0, 5. 1334330719, -0. 388892794, -0. 538424352
 C, 0, 3. 9536184769, 0. 1977027005, -0. 2121136532
 C, 0, 2. 890888944, -0. 6334400975, 0. 2161608418
 C, 0, 4. 3635687633, -4. 0182134545, -0. 2515752818
 C, 0, 5. 5265090991, -4. 5643027439, -0. 6891417693
 C, 0, 6. 6184202231, -3. 7433739082, -1. 048879641
 C, 0, 6. 5005634562, -2. 3945738432, -0. 9817484682
 O, 0, 0. 4257813064, -1. 7777139683, -0. 7156067552
 O, 0, 1. 6944274269, -0. 0299992087, 0. 5840114898
 P, 0, 0. 3658647079, -0. 2140922004, -0. 3279884767
 O, 0, 0. 3714657568, 0. 6073523968, -1. 5537906568
 O, 0, -0. 7578732943, 0. 0042001133, 0. 6871821856
 C, 0, -3. 0226307052, -3. 9856503572, -2. 0732879994
 C, 0, -4. 1684597787, -3. 5300906236, -1. 4481969788
 C, 0, -4. 0685438664, -3. 0791992056, -0. 1436648765
 C, 0, -2. 8635802463, -3. 0834734174, 0. 5435966065
 C, 0, -1. 7135089638, -3. 5446919517, -0. 1124069973
 C, 0, -1. 7945919805, -3. 9996823822, -1. 4320655377
 C, 0, -0. 576723077, -4. 5321210019, -2. 1866136673
 C, 0, -0. 2613923862, -3. 6532204794, -3. 4153712472
 C, 0, -0. 7820997789, -6. 006487544, -2. 5965494668
 C, 0, -2. 8453556812, -2. 6443933505, 2. 0111066431
 C, 0, -3. 4798456371, -3. 7506419671, 2. 8871862276
 C, 0, -3. 5784528625, -1. 3113002852, 2. 2626033572
 C, 0, -5. 4875293972, -3. 5053772324, -2. 2121206112
 C, 0, -5. 7713904998, -2. 0750489042, -2. 7217959269
 C, 0, -6. 6727985773, -4. 024560966, -1. 3731807845
 C, 0, 3. 8308461284, 3. 6836395491, -1. 6486657399
 C, 0, 3. 8046162138, 2. 2965412841, -1. 5757986609
 C, 0, 3. 8175994003, 1. 6871861563, -0. 3151114778
 C, 0, 3. 8269012124, 2. 4759575046, 0. 8423264317
 C, 0, 3. 8618444667, 3. 8572179735, 0. 7198285992
 C, 0, 3. 8860110822, 4. 4792489095, -0. 5195816451
 C, 0, 4. 072965913, 5. 9865932433, -0. 6623931619
 C, 0, 5. 5378970518, 6. 3535956242, -0. 3317066872
 C, 0, 3. 1064470994, 6. 812722059, 0. 208523599
 C, 0, 3. 8317821793, 1. 8530736201, 2. 2381388923

C, 0, 2. 5273183787, 2. 1888429533, 2. 9917084789
C, 0, 5. 070710023, 2. 2949563604, 3. 046152897
C, 0, 3. 8029894561, 1. 497773133, -2. 8826512659
C, 0, 5. 0964076044, 1. 7629968, -3. 6849691414
C, 0, 2. 5558040494, 1. 8098825351, -3. 737463239
H, 0, 2. 5207776662, -6. 18380904, 4. 8867998419
H, 0, 4. 3201936209, -4. 5888934132, 4. 3281802631
H, 0, 4. 0586579458, -3. 0356497172, 2. 4748929382
H, 0, 0. 4349203272, -6. 1687374639, 3. 6066677026
H, 0, -0. 9428043725, -5. 2408714281, 1. 8166904167
H, 0, 5. 9596331547, 0. 2249792469, -0. 8370890303
H, 0, 3. 5410495552, -4. 6451893656, 0. 0148018585
H, 0, 5. 619550566, -5. 6289635429, -0. 7686284345
H, 0, 7. 5311731531, -4. 1933540035, -1. 3847328088
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H, 0, -7. 5644493315, -4. 082125763, -1. 9887957284
H, 0, -6. 8842248721, -3. 3590499845, -0. 5448712907
H, 0, -6. 4633269948, -5. 0114607652, -0. 9773367853
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H, 0, 3. 9066174909, 4. 4533132869, 1. 6090570387
H, 0, 3. 8878484138, 6. 2427329605, -1. 6999846595
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H, 0, 5. 7596134825, 6. 1138732711, 0. 7019802922
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H, 0, 3. 259789657, 6. 6076914041, 1. 261962895
H, 0, 2. 0756520257, 6. 5970015595, -0. 0411914747
H, 0, 3. 8782477202, 0. 7812592618, 2. 12842526

H, 0, 2. 5369696828, 1. 7310835054, 3. 9755359437
H, 0, 1. 6765102683, 1. 8044228375, 2. 4463533309
H, 0, 2. 4182537765, 3. 2603357896, 3. 1191957555
H, 0, 5. 0891663779, 1. 7829244385, 4. 0025121561
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H, 0, 2. 4981634332, 2. 8660972764, -3. 9767021457
H, 0, 1. 6662367516, 1. 5025143938, -3. 2075039962
C, 0, -3. 5125341693, 2. 0372937725, -0. 0313221866
O, 0, -2. 5528897478, 1. 6264264847, 0. 7324910268
C, 0, -4. 6687391966, 2. 6969047507, 0. 706419158
C, 0, -4. 0075347369, 0. 9369696001, -0. 9946802074
C, 0, -4. 5361227933, 2. 8656316275, 2. 0781456088
C, 0, -5. 5455894755, 3. 4673772905, 2. 8120332911
C, 0, -6. 6980518083, 3. 9089490157, 2. 1830156753
C, 0, -6. 8376091501, 3. 7413076857, 0. 8135837007
C, 0, -5. 8295205609, 3. 1402190315, 0. 0784373086
F, 0, -4. 8363266139, 0. 1115515301, -0. 3628710563
F, 0, -2. 9920591599, 0. 2162238571, -1. 4612811017
F, 0, -4. 6646809658, 1. 4095283226, -2. 0660437709
H, 0, -3. 6351264532, 2. 5151738948, 2. 548417264
H, 0, -5. 4303398729, 3. 5894752975, 3. 8770474222
H, 0, -7. 4840377122, 4. 3768159428, 2. 7537720435
H, 0, -7. 7337512441, 4. 0748230973, 0. 3155305382
H, 0, -5. 9629027835, 3. 0097260442, -0. 9819546881
C, 0, -1. 911413984, 6. 0292037966, 1. 4120551279
C, 0, -0. 56014874, 5. 6950394801, 1. 4544247523
C, 0, -0. 0443992447, 4. 6898954757, 0. 6513326248
C, 0, -0. 9401006837, 4. 0555357668, -0. 1823152449
C, 0, -2. 2980817813, 4. 3528153989, -0. 2296542987
C, 0, -2. 7961014985, 5. 3564771155, 0. 5819183814
N, 0, -0. 7018961349, 3. 0449195009, -1. 1275993025
C, 0, -1. 7941323546, 2. 7212955041, -1. 7482345529
C, 0, -2. 9256377409, 3. 3644046334, -1. 1308724646
H, 0, -2. 2784890263, 6. 8203543117, 2. 04493401
H, 0, 0. 0978748451, 6. 2271593078, 2. 1211794636
H, 0, 0. 9966843563, 4. 417287256, 0. 6752741957
H, 0, -3. 8436180476, 5. 6049981799, 0. 5772267252
H, 0, 0. 1481473562, 2. 5029126467, -1. 2526420981
H, 0, -1. 7809714884, 1. 9500589283, -2. 4929494564
H, 0, -3. 7688279691, 3. 6290314252, -1. 7452748007

ONIOM: extrapolated energy = -3604.099051444950

E+ZPE= -3602.817741

H= -3602.749717

G= -3602.922821

(8) TS1-si-exo (Conformer D')

C, 0, 4.7115538439, -4.3656550576, 3.5478731361
C, 0, 5.3161743083, -3.1477520865, 3.1663711253
C, 0, 4.7481244182, -2.3602045625, 2.2176523152
C, 0, 3.5319454888, -2.7401680567, 1.5917641024
C, 0, 2.9127461072, -3.9349385629, 2.0004723657
C, 0, 3.5398759842, -4.7454806444, 2.9806702685
C, 0, 2.89426095, -1.9433015094, 0.5866111637
C, 0, 1.6457350228, -2.2874925015, 0.169958427
C, 0, 1.0042532133, -3.4820429242, 0.5785431822
C, 0, 1.6618323025, -4.2938529768, 1.4435637805
C, 0, 3.5805260978, -0.7509841969, 0.0103973924
C, 0, 4.8715406302, -0.864604131, -0.5987903272
C, 0, 5.5408263171, 0.3093078297, -0.990894209
C, 0, 4.9042875934, 1.5618878692, -0.8189144653
C, 0, 3.6348244575, 1.6586663612, -0.3496758443
C, 0, 2.981950559, 0.4691962011, 0.0543037534
C, 0, 5.4937883725, -2.1150971747, -0.8520791528
C, 0, 6.7198823492, -2.1751610485, -1.4314870792
C, 0, 7.4059486754, -0.9936633348, -1.7898701037
C, 0, 6.8290115654, 0.2147591783, -1.5768346295
O, 0, 0.9737717695, -1.4690269022, -0.730552956
O, 0, 1.6886780301, 0.5734799335, 0.5525841211
P, 0, 0.4472770474, -0.0042314643, -0.3083454738
O, 0, 0.1366594835, 0.7590800966, -1.5335859074
O, 0, -0.6390408985, -0.1321429378, 0.7614620319
C, 0, -1.7131640855, -4.7107196698, -1.7299379206
C, 0, -2.8323460773, -4.6903623012, -0.9143424314
C, 0, -2.6871501532, -4.2481515894, 0.3856489376
C, 0, -1.464569691, -3.8228798753, 0.888307496
C, 0, -0.345693711, -3.858205462, 0.0497173524
C, 0, -0.4718927662, -4.3063696837, -1.2716295514
C, 0, 0.7242450081, -4.3756949974, -2.2209259996
C, 0, 0.5313466387, -3.4266629407, -3.422528809
C, 0, 0.973017885, -5.8246716915, -2.692502273
C, 0, -1.3860693518, -3.3637790899, 2.3470408625
C, 0, -1.5133569571, -4.5829605262, 3.2896328978
C, 0, -2.4624025572, -2.316916109, 2.7054617134
C, 0, -4.1943619083, -5.142971941, -1.4263902766
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C, 0, 1. 8618107269, 2. 5862419013, 3. 1704030767
C, 0, 4. 1686939509, 3. 6616852914, 3. 0891413324
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H, 0, 4. 9782204307, -3. 0121261263, -0. 5858314673
H, 0, 7. 1733804366, -3. 1267341068, -1. 624625399
H, 0, 8. 3765336303, -1. 0606779613, -2. 2391889325
H, 0, 7. 3316550848, 1. 1194672662, -1. 8586619587
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H, 0, -0. 4227525553, -2. 9045328096, 2. 506277228
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H, 0, 3. 7723447021, 4. 618797036, 3. 4073310786
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H, 0, 3. 4191230746, 5. 0140537849, -3. 7573765232
H, 0, 1. 7357243295, 2. 6244440428, -4. 6129113054
H, 0, 0. 993509564, 3. 91704601, -3. 686218733
H, 0, 0. 8954102349, 2. 2403386108, -3. 119322347
C, 0, -3. 9941321901, 0. 5376917119, 0. 1069572906
O, 0, -2. 9189760558, 0. 6972878521, 0. 8065917834
C, 0, -5. 2882474909, 0. 7967093274, 0. 8616838678
C, 0, -4. 0216921838, -0. 8254159882, -0. 6199028908
C, 0, -5. 1839391232, 1. 2511418257, 2. 1693248179
C, 0, -6. 3227517551, 1. 5162507036, 2. 9125122368
C, 0, -7. 5779968324, 1. 3317891749, 2. 3563718971
C, 0, -7. 6888033219, 0. 8748923936, 1. 0517756516
C, 0, -6. 5515585976, 0. 6091411096, 0. 3074751495
F, 0, -4. 4112761189, -1. 7816786473, 0. 2100127244
F, 0, -2. 8160372952, -1. 1409271228, -1. 0828615055
F, 0, -4. 8539494949, -0. 8696401309, -1. 6783957314
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H, 0, -6. 2276049566, 1. 8663071073, 3. 9278085934
H, 0, -8. 4644153105, 1. 5378375324, 2. 9345227594
H, 0, -8. 6612936137, 0. 7205726216, 0. 6126634751
H, 0, -6. 6593039231, 0. 2441174758, -0. 6997609547
C, 0, -4. 3430631222, 5. 0771601064, 0. 6258637039
C, 0, -2. 9862418707, 5. 3893768424, 0. 58635895
C, 0, -2. 0777619807, 4. 5593752172, -0. 0504635087
C, 0, -2. 5956494005, 3. 424758581, -0. 6385346748
C, 0, -3. 9438158362, 3. 0828430006, -0. 6059068995
C, 0, -4. 8353977354, 3. 9194985334, 0. 0419594907
N, 0, -1. 9358165052, 2. 4429883214, -1. 3931135007
C, 0, -2. 7750198095, 1. 5619234426, -1. 8448816588
C, 0, -4. 0710364402, 1. 7623039942, -1. 2543001438
H, 0, -5. 0230479811, 5. 7468779822, 1. 1262074688
H, 0, -2. 636967526, 6. 2931933631, 1. 0567903287
H, 0, -1. 0245599836, 4. 7811648684, -0. 0844927446
H, 0, -5. 8831509125, 3. 6777876153, 0. 0972287559

H, 0, -0.9333773583, 2.2909725936, -1.4740136163
H, 0, -2.4228079299, 0.7362705242, -2.4313555275
H, 0, -4.9490574005, 1.5062008635, -1.8212720259

ONIOM: extrapolated energy = -3604.099599250958
E+ZPE= -3602.818328
H= -3602.750367
G= -3602.923220

(9) TS1-*re-endo*

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C, 0, -0.5771097449, 5.3855440582, -1.9423460068
C, 0, -1.198489459, 4.2626888491, -1.3345564526
C, 0, -2.5470333974, 3.9995564008, -1.6340281951
C, 0, -3.2582557962, 4.8842165399, -2.4844154863
C, 0, -0.5046491766, 3.3723830887, -0.4544668597
C, 0, -1.1246968055, 2.2314207163, -0.0451019493
C, 0, -2.4721273894, 1.9348167516, -0.3653633414
C, 0, -3.1610904449, 2.8392417107, -1.1060535161
C, 0, 0.8906987652, 3.6671619225, -0.0161347392
C, 0, 1.2251237056, 4.8838434647, 0.6585030118
C, 0, 2.5799667594, 5.1621629784, 0.9199859211
C, 0, 3.5688480361, 4.2165240705, 0.554296126
C, 0, 3.2405685715, 3.0170551082, 0.0115799267
C, 0, 1.8758831645, 2.7634552686, -0.2618335895
C, 0, 0.2445519254, 5.8090544403, 1.1022984523
C, 0, 0.6075725788, 6.9516725652, 1.7387670624
C, 0, 1.9698506329, 7.2461881972, 1.9687978204
C, 0, 2.928133903, 6.3728110069, 1.5718633407
O, 0, -0.423690837, 1.3244121305, 0.747943402
O, 0, 1.5384392736, 1.5339056377, -0.8219841788
P, 0, 0.7892019809, 0.4592077196, 0.1275285337
O, 0, 1.6206262281, -0.1100893787, 1.1971127355
O, 0, 0.2379818253, -0.5180405968, -0.9267102278
C, 0, -4.3188428917, -0.4812014037, 1.8709259098
C, 0, -4.5617355048, -1.5495925763, 1.0255075367
C, 0, -4.0748889897, -1.4840617914, -0.268380972
C, 0, -3.3643786811, -0.3909775614, -0.7387803601
C, 0, -3.1462503369, 0.6889553369, 0.1290788121
C, 0, -3.6291755491, 0.6435872443, 1.4403019437
C, 0, -3.4281520547, 1.8114377599, 2.4067057651
C, 0, -2.4642940654, 1.4215425062, 3.5465511767
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C, 0, -2.8812693022, -0.385240107, -2.1924527112
C, 0, -4.0248549687, 0.0701521337, -3.1287152325
C, 0, -2.3733552765, -1.7662678944, -2.6648772683
C, 0, -5.3195635758, -2.7965905148, 1.4703307529
C, 0, -6.4843670514, -2.4868005929, 2.431568671

C, 0, -4. 3469419424, -3. 810209769, 2. 11382365
C, 0, 5. 9421894747, 0. 4048685683, 0. 4150377259
C, 0, 4. 9415671173, 1. 3148220206, 0. 7379997033
C, 0, 4. 2873080941, 1. 9908047645, -0. 299304587
C, 0, 4. 6487887631, 1. 7467329198, -1. 6315671088
C, 0, 5. 659548279, 0. 8378945849, -1. 903289155
C, 0, 6. 3232902032, 0. 1612209615, -0. 8913375135
C, 0, 7. 5001558549, -0. 7639546316, -1. 1807713605
C, 0, 8. 739099766, 0. 0777290607, -1. 5619933762
C, 0, 7. 1985342912, -1. 8018047858, -2. 28007917
C, 0, 3. 9810322982, 2. 4813842631, -2. 79428604
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ONIOM: extrapolated energy = -3604.089807

E + ZPE= -3602.807784

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Experimental details

1. General information:

All reactions were performed under an Ar atmosphere in oven-dried glassware with magnetic stirring. Reactions were monitored through thin-layer chromatography (TLC). Chromatograms were visualized by fluorescence quenching under UV light at 254 nm. ^1H and ^{13}C NMR were recorded on Varian Mercury Plus 400 instruments at 400 MHz (^1H NMR) and 100 (^{13}C NMR). Chemical shifts were reported in ppm down field from internal Me_4Si . Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), br (broad). Coupling constants were reported in Hertz (Hz). HRMS were recorded on an IonSpec FT-ICR mass spectrometer with EI resource.

2. Materials:

Unless otherwise stated, all solvents and reagents were purchased from commercial suppliers and used without further purification. Dichloromethane and chloroform employed in the reactions was freshly distilled from CaH_2 . Analytical thin layer chromatography was performed on 0.20 mm Qingdao Haiyang

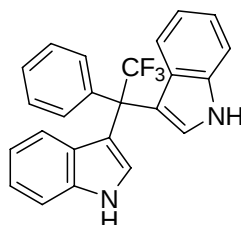
silica gel plates. Silica gel (200-300 mesh) (from Qingdao Haiyang Chem. Company, Ltd.) was used for flash chromatography.

3. Experimental procedures and characterization data

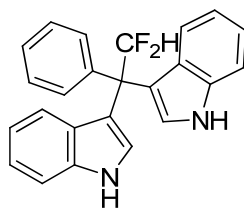
3.1 General procedures and supplementary information in the experimental section

3.1.1 General procedures for diarylation reaction

To a flame-dried Schlenk tube was added indole (0.14 mmol), 2,2,2-trifluoro-1-(1*H*-indole-3-yl)-1-phenylethanol or 2,2-difluoro-1-(1*H*-indole-3-yl)-1-phenylethanol (0.14 mmol), racemic phosphoric acid **1**, and solvent (toluene, 1 mL). After the solution was stirred at 80 °C under an argon atmosphere for stated time, the reaction mixture was concentrated, and the residue purified through flash column chromatography (Hexane/EtOAc= 20/1 to 4/1 as eluent) to give the product.



3,3'-(2,2,2-trifluoro-1-phenylethane-1,1-diyl)bis(1*H*-indole): white solid, Yield: 98%; ¹H NMR (400 MHz, CDCl₃) δ (ppm): 6.82 (d, *J* = 2.4 Hz, 2H), 6.98 (t, *J* = 7.6 Hz, 2H), 7.20 (t, *J* = 7.6 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.31 (s, 1H), 7.33-7.36 (m, 4H), 7.58 (d, *J* = 7.2 Hz, 2H), 7.99 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 65.7, 111.2, 115.5, 119.7, 122.0, 122.4 (d, *J* = 3.0 Hz), 126.4 (d, *J* = 5.9 Hz), 127.6, 128.0, 129.6, 136.7, 139.3; ¹⁹F NMR (376 MHz, CDCl₃) δ (ppm): -62.4 (s, 3F); HRMS (EI): calcd for C₂₄H₁₆F₃N₂⁺ [M-H]⁺ 389.3924, found: 389.3921.



3,3'-(2,2-difluoro-1-phenylethane-1,1-diyl)bis(1H-indole): white solid, Yield: 95%; ^1H NMR (400 MHz, CDCl_3) δ (ppm): 6.90 (t, $J = 56$ Hz, 1H), 6.87 (d, $J = 2.4$ Hz, 2H), 6.92 (t, $J = 7.6$ Hz, 2H), 7.13-7.19 (m, 4H), 7.29 (t, $J = 3.2$ Hz, 3H), 7.35 (d, $J = 8$ Hz, 2H), 7.48-7.51 (m, 2H), 8.06 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 53.7, 111.2, 116.6, 118.7, 119.6, 122.0 (d, $J = 7.4$ Hz), 125.6, 126.6, 127.1, 128.0, 129.5, 136.8, 140.5; ^{19}F NMR (376 MHz, CDCl_3) δ (ppm): $\tilde{116.53}$ (d, $J = 259.5$ Hz, 2F); HRMS (EI): calcd for $\text{C}_{24}\text{H}_{17}\text{F}_2\text{N}_2$ $[\text{M}-\text{H}]^-$ 371.4020, found: 371.4022.

