Electronic Supplementary Information for

post-Spin Crossing Dynamics Determine the Regioselectivity in Open-shell Singlet Biradical Recombination

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1. Computational Methods

The computational studies were performed with Gaussian 16[1] or ORCA 4.2.1[2] packages. Density functional theory (DFT) calculations were carried out using the (U)B3LYP functional[3] including the D3 version of Grimme's empirical dispersion correction with Becke−Johnson damping.[4] It is known that the (U)B3LYP functional provides excellent open-shell singlet-triplet energy gaps when compared with experimental values.[5] The def2-SVP basis sets[6] were applied for all atoms. Optimizations were conducted without any constraint in the gas phase. Frequency analyses were carried out to confirm each structure being a minimum (no imaginary frequency) or a transition state (only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations were performed for transition states **2‡-OSS** and **5‡-OSS**, and the geometry of **4-T** with the wavefunction on the open-shell singlet state [using the "irc=downhill" and "guess=mix, stable=opt" options in Gaussian], which provided minimal energy paths connecting to the neighboring local minima. Single point calculations were performed at (U)B3LYP-D3(BJ)/def2-TZVP level of theory in MeCN (for the indole system) and DCM (for the pyrrole system), respectively (SMD model[7]). The relative electronic energies (ΔE) and Gibbs energies (ΔG) are discussed in kcal/mol. In order to confirm the validity of the results obtained by UDFT methods, multireference calculations were performed using N-electron valence state perturbation theory (DLPNO-NEVPT2[8]) in combination with def2-TZVPP basis sets [using RI-JK[9] approximation and def2/JK auxiliary basis sets[10] implemented in ORCA].

Quasi-classical Born–Oppenheimer molecular dynamics simulations were performed for the pyrrole system [using the "bomd" keyword in Gaussian]. The initial coordinates and momenta were generated from the normal mode sampling (at 298 K) using the structure of **4-T** on both the open-shell singlet and triplet states (abbreviated as OSS-sampling and T-sampling, respectively). Starting from each of the two ensembles of initial geometries and momenta, a series of trajectories (60 cases for OSS-sampling and 40 cases for T-sampling) were propagated until the fully formation of products **7** or **6**. For the cases of T-sampling, the wavefunction of the system is recalculated on the open-shell singlet state [using the "guess=mix, stable=opt" options in Gaussian] prior to the propagation of a trajectory. The changes of the $\langle S^2 \rangle$ values were monitored along all the IRC paths and the trajectories.

Various spin population analyses and the manipulations of wavefunction information were performed by Multiwfn.[11] The optimized structures are visualized by VMD.[12]

2. The Optimized Structures of All Stationary Points

The structures and key features of all stationary points discussed in the main text are shown in Figure S1.
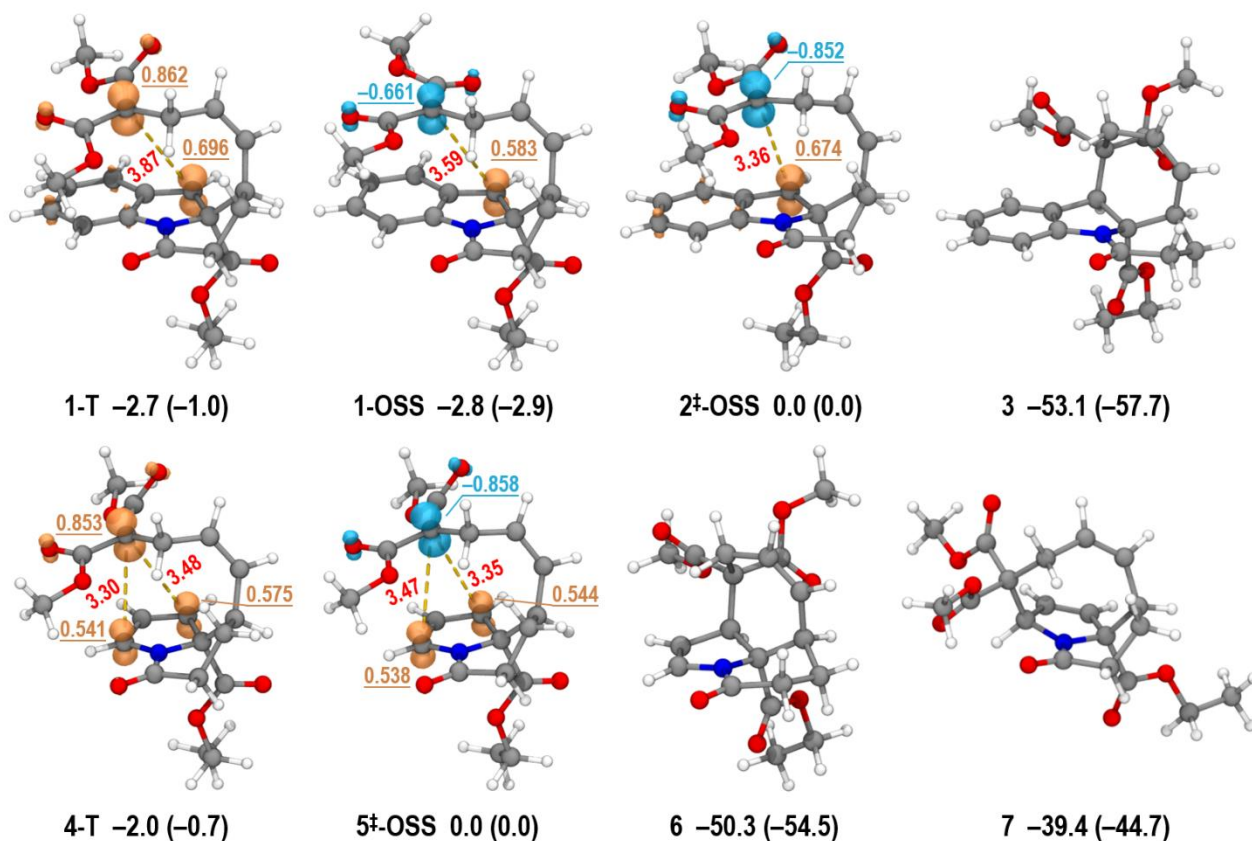

Figure S1. The optimized structures and energies for key intermediates, transition states and products for dearomative [5 + 2] or [5 + 4] cycloaddition reactions. Relative Gibbs energies and electronic energies (in parentheses) are in kcal/mol. The orange and blue lobes show the spin density distributions with the isovalues of 0.03 and –0.03, respectively. The underlined values are Mulliken spin populations at certain atoms. The red values are bond distances in Å.

3. The Calculated Energy Profile for the Formation of Biradical 1-T

The detailed energy profile for the formation of triplet biradical species in indole-tethered vinylcyclo-propanes have been studied in our previous work.[13] Herein we provide the calculated energies of selected stationary points for the precedent steps that lead to pyrrole-based biradical **1**-T (Figure S2). It can be found that the calculated results are in parallel with those of the indole-based system.
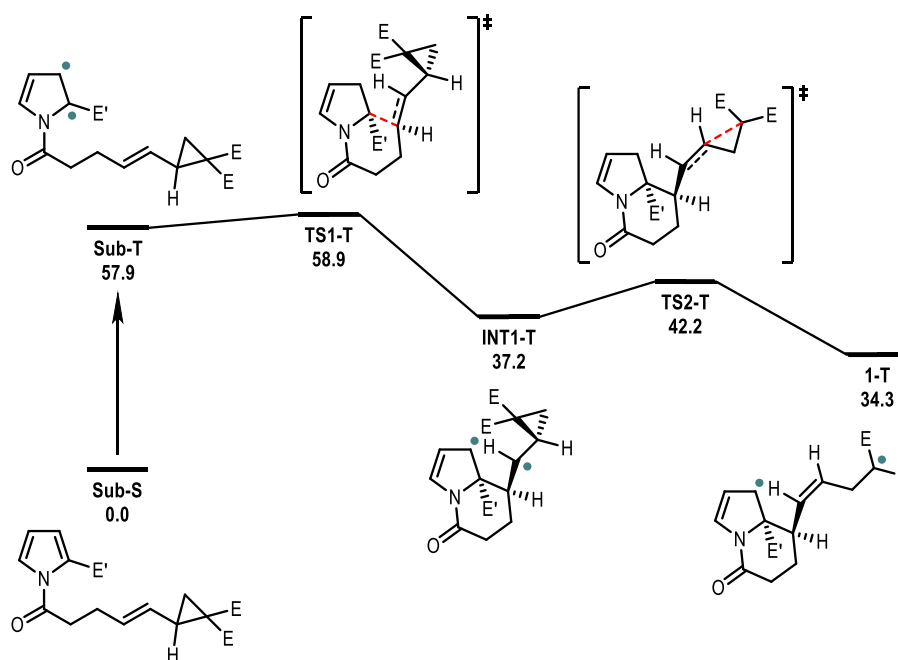

Figure S2. Energy profile for the formation of **1**-T calculated at the (U)B3LYP-D3(BJ)/def2-TZVP (DCM)//(U)B3LYP-D3(BJ)/def2-SVP (gas) level of theory. The relative Gibbs energies (ΔG_{sol}) are presented in kcal/mol. The green dots in triplet intermediates indicate the unpaired electrons. The red dashed lines indicate the forming or cleaving bonds in the transition states.

4. Detailed Results of Various Spin Population Analyses

The spin population analyses of structures of **1**-T, **1**-OSS, **2**‡-OSS, **4**-T and **5**‡-OSS were performed using different population schemes including Mulliken, Löwdin, SCPA, Hirshfeld and Becke. The detailed results are listed in Table S1. It can be seen that the calculated spin population values by different population schemes are quite parallel.
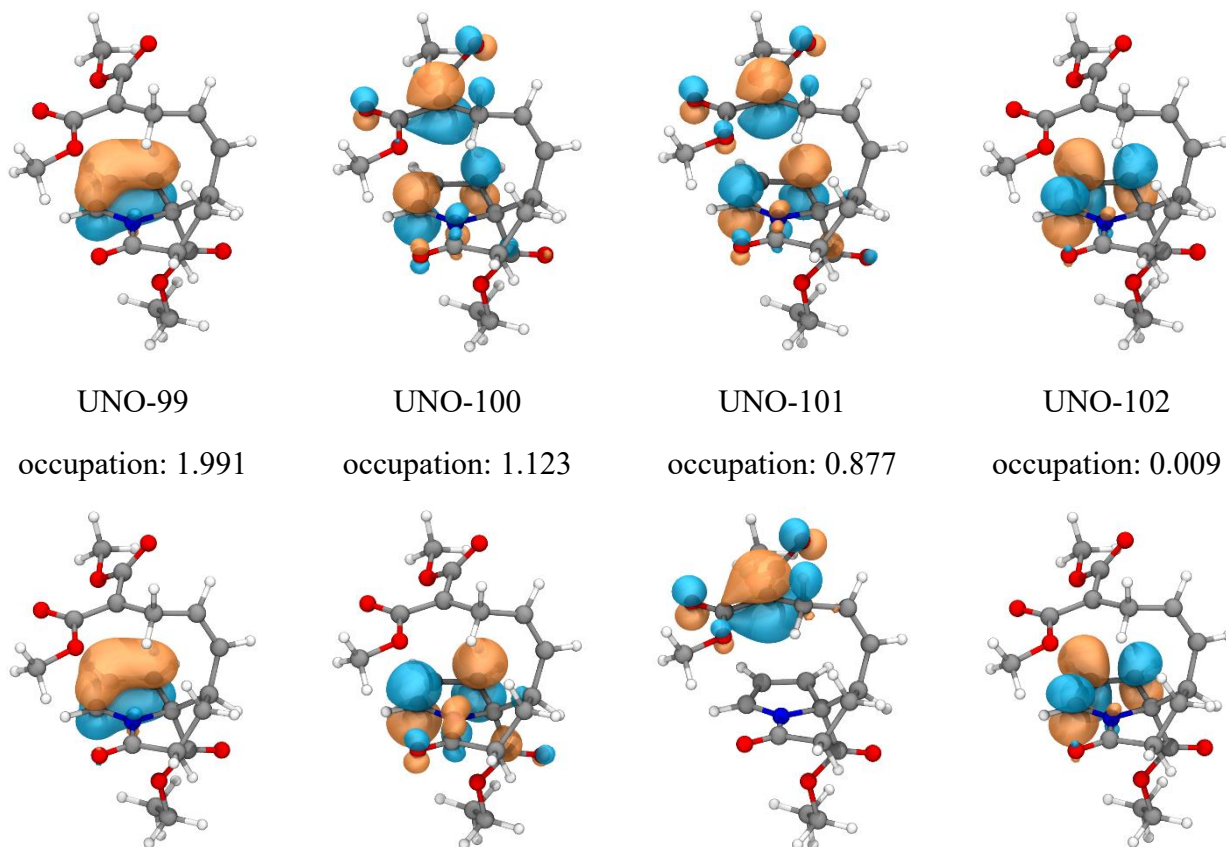
Table S1. Detailed results of various spin populations analyses.

Species/Atoms	Spin population				
	Mulliken	Löwdin	SCPA	Hirshfeld	Becke
1-T/C3	0.696	0.546	0.716	0.434	0.509
1-T/Cα	0.862	0.678	0.946	0.545	0.622
1-OSS/C3	0.583	0.455	0.634	0.359	0.424
1-OSS/Cα	−0.661	−0.514	−0.752	−0.411	−0.471
2‡-OSS/C3	0.674	0.524	0.677	0.411	0.485
2‡-OSS/Cα	−0.852	−0.668	−0.938	−0.534	−0.611
4-T/C3	0.575	0.455	0.546	0.359	0.422
4-T/C5	0.541	0.443	0.511	0.357	0.412
4-T/Cα	0.853	0.674	0.932	0.543	0.619
5‡-OSS/C3	0.544	0.426	0.519	0.329	0.391
5‡-OSS/C5	0.538	0.440	0.526	0.350	0.407
5‡-OSS/Cα	−0.858	−0.672	−0.941	−0.538	−0.616

5. Detailed Results of Multireference Calculations

In order to verify the results from UDFT calculations, a series of multireference calculations on a series of structures on the IRC paths of the transition states $2^{\ddagger}$-OSS and $5^{\ddagger}$-OSS have been performed based on the open-shell singlet and triplet wavefunctions, respectively. The key procedures are listed below (taking the calculations on the geometries of $2^{\ddagger}$-OSS and $5^{\ddagger}$-OSS as the examples).

(1) Single point calculations were first performed at the UB3LYP-D3(BJ)/def2-SVP level of theory to obtain the unrestricted natural orbitals (UNOs). For the structure of $5^{\ddagger}$-OSS (on both open-shell singlet and triplet states) the orbitals UNO-99~UNO-102 were included in the active space for the next-step calculations. There are four electrons occupying these orbitals (Figure S3). For the structure of $2^{\ddagger}$-OSS (on both open-shell singlet and triplet states), the orbitals UNO-113 and UNO-114 were included in the active space for the next-step calculations. There are two electrons occupying these orbitals (Figure S4).

| UNO-99 | UNO-100 | UNO-101 | UNO-102 |
| occupation: 1.991 | occupation: 1.123 | occupation: 0.877 | occupation: 0.009 |

UNO-99	UNO-100	UNO-101	UNO-102
occupation: 1.991	occupation: 1.000	occupation: 1.000	occupation: 0.009

Figure S3. The UNOs (at the isovalues of ±0.05) and occupations of structures **5‡-OSS** (on the open-shell singlet state, top; on the triplet sate, bottom).
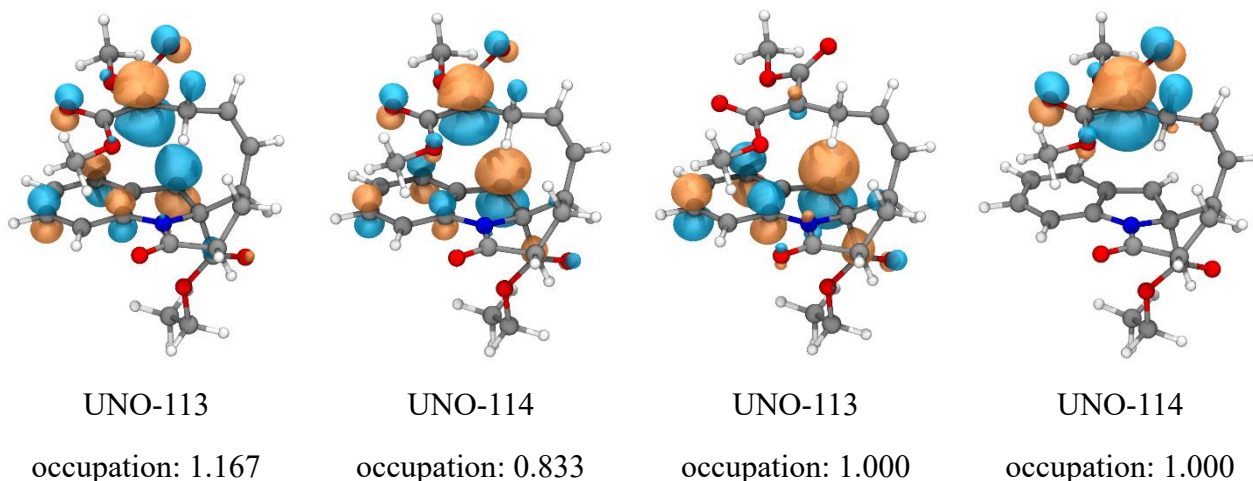

UNO-113	UNO-114	UNO-113	UNO-114
occupation: 1.167	occupation: 0.833	occupation: 1.000	occupation: 1.000

Figure S4. The UNOs (at the isovalues of ±0.05) and occupations of structures **2‡-OSS** (on the open-shell singlet state, the left two columns; and on the triplet state, the right two columns).

(2) Single point calculations at the CASSCF(4,4)/def2-TZVPP (for **5‡-OSS**) and CASSCF(2,2)/def2-TZVPP (for **2‡-OSS**) levels of theory (both with def2/JK auxiliary basis sets) by reading the CAS orbital information obtained in step (1).

(3) Single point calculations at the DLPNO-NEVPT2/def2-TZVPP (for **5‡-OSS** and **2‡-OSS**) levels of theory (both with def2/JK auxiliary basis sets) by reading the wavefunction information obtained in step (2)

The calculated energy plots for the geometries along the IRC paths are shown in Figures S5–S8.

Figure S5. The relative electronic energies (in kcal/mol) for the geometries along the IRC path for transition state **5‡-OSS** with respective to the Cα–C5 and Cα–C3 distances (in Å). Calculated at the UB3LYP-D3(BJ)/def2-SVP level of theory. Blue and green dots show the relative energies at the open-shell singlet and triplet states, respectively.

Figure S6. The relative electronic energies (in kcal/mol) for the geometries along the IRC path for

transition state **5‡**-OSS with respective to the Cα–C5 and Cα–C3 distances (in Å). Calculated at the DLPNO-NEVPT2/def2-TZVPP level of theory (see the text for the detailed procedures). Blue and green dots show the relative energies at the open-shell singlet and triplet states, respectively.
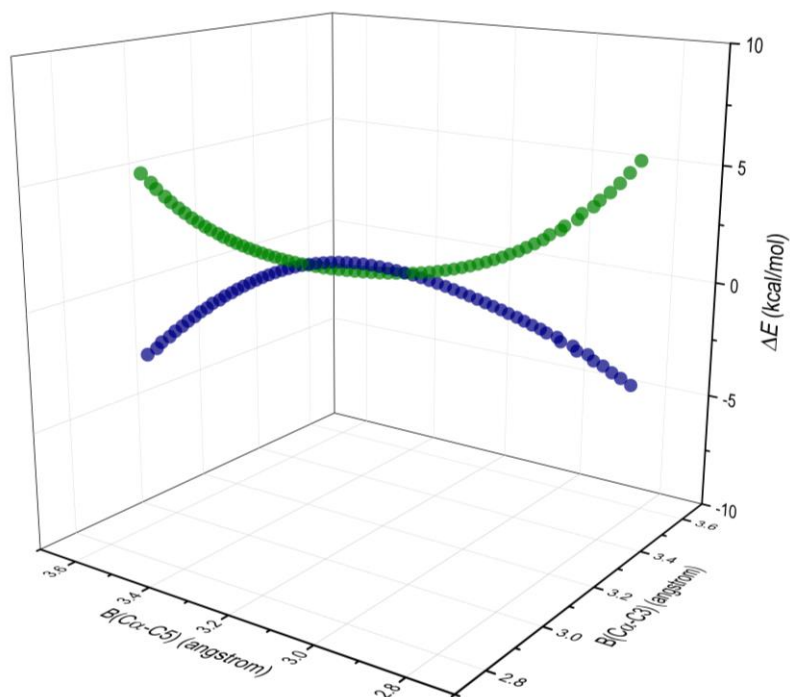

Figure S7. The relative electronic energies (in kcal/mol) for the geometries along the IRC path for transition state **2‡**-OSS with respective to the Cα–C5 and Cα–C3 distances (in Å). Calculated at the UB3LYP-D3(BJ)/def2-SVP level of theory. Blue and green dots show the relative energies at the open-shell singlet and triplet states, respectively.
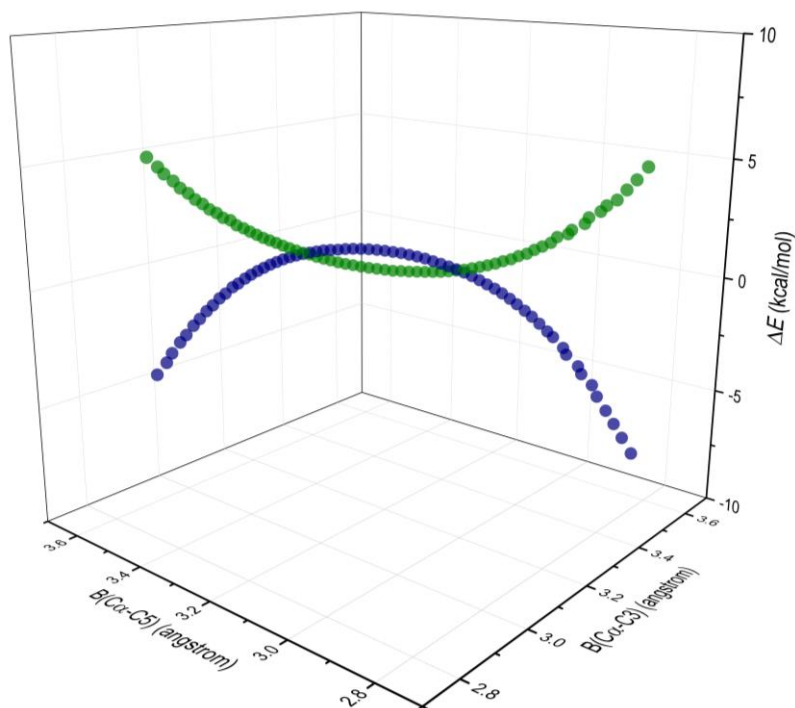
Figure S8. The relative electronic energies (in kcal/mol) for the geometries along the IRC path for transition state **2‡-OSS** with respective to the Cα–C5 and Cα–C3 distances (in Å). Calculated at the DLPNO-NEVPT2/def2-TZVPP level of theory (see the text for the detailed procedures). Blue and green dots show the relative energies at the open-shell singlet and triplet states, respectively.
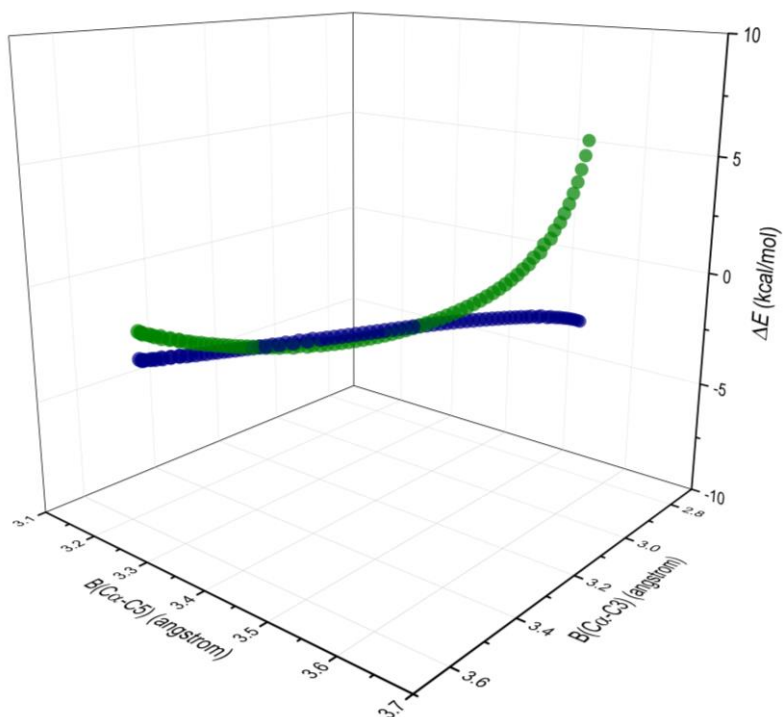
It is can be seen from Figures S4–S7 that the energy plots obtained using UDFT method are in qualitative agreement with those obtained using multireference method. This consistence well supports the validity of the results by UDFT method presented in the main text.

6. Detailed Results of Trajectory Calculations

Trajectory calculations were performed based on the geometry of **4**-T using the OSS-sampling and T-sampling, respectively. More details about the trajectory calculations are provided in this section. Figures S9 and S10 show the distribution of the initial geometries and the geometries at the transition from the open-shell singlet to closed-shell singlet state [with respect to $B(C\alpha–C5)$, $B(C\alpha–C3)$], for the trajectories starting from OSS-sampling and T-sampling, respectively. Figures 11 and 12 show the overlays of the initially sampled geometries.

Figure S9. The distribution of 60 sets of the initial geometries (green circles) and the geometries at the transition from the open-shell singlet to closed-shell singlet state (pink circles), for the trajectories started from the OSS-sampling using the geometry of **4**-T. The blue (on the open-shell singlet state) and orange (on the closed-shell singlet state) curves show the IRC path for **5**‡-OSS. Brown cross and purple square show the positions of **5**‡-OSS (3.47, 3.35) and **4**-T (3.30, 3.48).

Figure S10. The distribution of 40 sets of the initial geometries (green circles) and the geometries at the transition from the open-shell singlet to closed-shell singlet state (pink circles) for the trajectories started from the T-sampling using the geometry of **4**-T. The blue (on the open-shell singlet state) and orange (on the closed-shell singlet state) curves show the IRC path for **5**‡-OSS. Brown cross and purple square show the positions of **5**‡-OSS (3.47, 3.35) and **4**-T (3.30, 3.48).

Figure S11. The overlay of the 60 sets of the initial geometries from the OSS-sampling using the geometry of **4**-T.

Figure S12. The overlay of the 40 sets of the initial geometries from the T-sampling using the geometry of **4**-T.

7. Reference

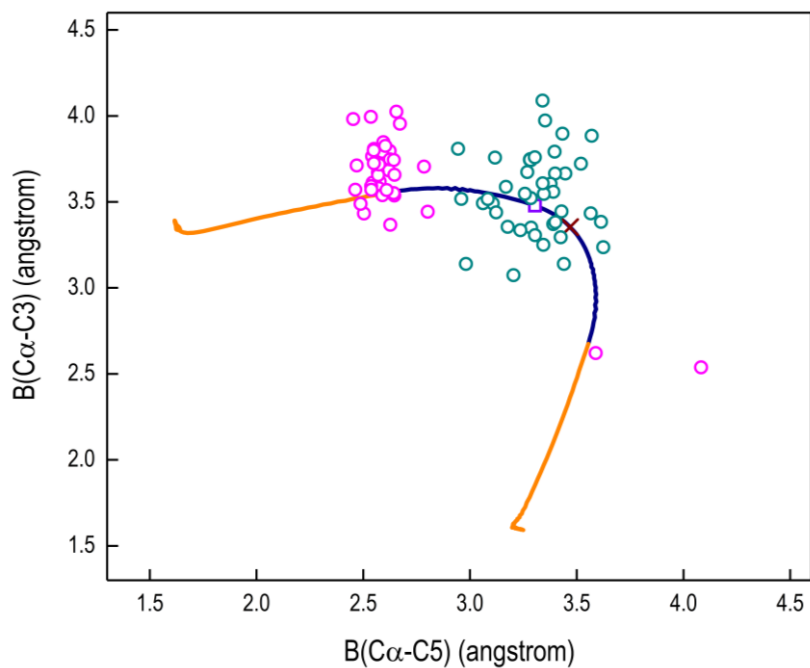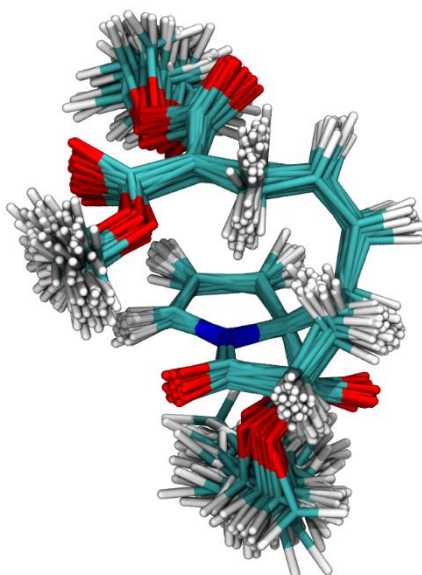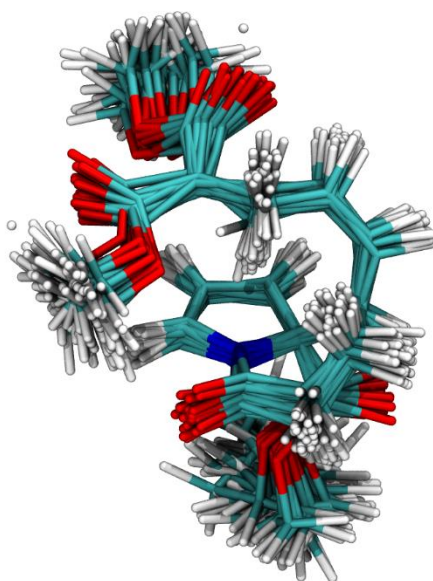1. Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

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8. Cartesian Coordinates and Energies of the Optimized Structures

1-T
Opt @ UB3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(UB3LYP) = -1471.82379071 a.u.
Zero-point correction = 0.448951 Hartree/Particle
Sum of electronic and thermal Free Energies = -1471.437967 a.u.
Sp @ UB3LYP-D3(BJ)/def2-TZVP in MeCN (SMD model)
SCF Done: E(UB3LYP) = -1473.48744439 a.u.

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1-OSS
Opt @ UB3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(UB3LYP) = -1471.82690216 a.u.
Zero-point correction = 0.449130 Hartree/Particle
Sum of electronic and thermal Free Energies = -1471.438167 a.u.
Sp @ UB3LYP-D3(BJ)/def2-TZVP in MeCN (SMD model)
SCF Done: E(UB3LYP) = -1473.49055778 a.u.

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H,0,2.6458420537,0.1545323795,-2.6169954856
H,0,0.7555389083,-2.175127245,-1.4757439528
H,0,-0.4709985741,1.6188249778,-0.8853795234
H,0,-1.7702044423,2.2170730233,-1.8552019581
H,0,-1.4168612135,0.4006711671,-3.5797016393
H,0,0.8400889548,-0.0389599657,-4.0077769666
H,0,5.369811079,-1.318537816,0.5641547628
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H,0,4.8168662463,-1.0381794852,2.2472505844
H,0,3.4545661422,-3.1697389268,2.1270115038
H,0,4.0653000709,-3.450110856,0.4679257333
H,0,5.1892665089,-3.4934940838,1.8504564785
H,0,-4.5579108198,-2.5558236652,-1.9577939642
H,0,-3.6235465478,-3.2691082779,-0.6189679197
H,0,-5.2823228936,-2.6406963239,-0.3060418411
H,0,-3.5394704722,3.3417909364,1.8939259841
H,0,-2.2194412494,2.491743223,2.7395678527
C,0,-1.0339431542,-2.1560828701,0.9572805363
C,0,-1.6502338858,-1.8016230628,2.1429405834
C,0,-1.2896084425,-0.6158471851,2.8226495919
C,0,-0.3120023928,0.2510004798,2.3244746102
H,0,-1.3099877493,-3.0652300866,0.4216081722
H,0,-2.4411224114,-2.4307506029,2.5545749687
H,0,-1.8001897893,-0.3617786285,3.7529799377
H,0,-0.035489379,1.1716192067,2.8314957408
H,0,-1.8608746297,4.00616811,1.8366679308
------------------------------------------------------------------------


2‡-OSS
Opt @ UB3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(UB3LYP) = -1471.82232288 a.u.
Zero-point correction = 0.448900 Hartree/Particle
Sum of electronic and thermal Free Energies = -1471.433808 a.u.
Imaginary Frequency = -51.6557 cm⁻¹
Sp @ UB3LYP-D3(BJ)/def2-TZVP in MeCN (SMD model)
SCF Done: E(UB3LYP) = -1473.48588534 a.u.
Sp @ DLPNO-NEVPT2/def2-TZVPP in gas phase
FINAL SINGLE POINT ENERGY = -1470.008921853526 a.u.
------------------------------------------------------------------------
O,0,1.424447112,2.620218895,1.6859482308
O,0,3.4426078258,-1.3987743055,-1.2929613878
O,0,3.1688934077,-0.7407663638,0.844710485
O,0,-3.3201048437,-0.7102367163,-2.7460179656
O,0,-3.2983542736,-1.5131112008,-0.6474663987
O,0,-3.4789241411,0.68460181,1.053252033
O,0,-1.8551387991,2.1856244347,0.6014352548
N,0,1.0882816862,0.7399021157,0.4354952268
C,0,1.6470384688,1.9758019136,0.6761981455
C,0,2.5197083233,2.4589566707,-0.4670734743
C,0,1.834769451,2.2036274597,-1.8140700363
C,0,1.602324091,0.6967202996,-2.0757993356
C,0,1.4668043515,-0.0886833606,-0.7235705621
C,0,0.4650101478,-1.2180175349,-0.6410148789
C,0,-0.1289534764,-1.1977902777,0.6323474774
C,0,0.2772400324,-0.0004275054,1.3063267985
C,0,-2.3287828477,0.6040511791,-1.0462431069
C,0,-1.5083257892,1.4386317693,-1.9845140189
C,0,-0.7790640136,0.6978624841,-3.0727695675
C,0,0.5255877264,0.3972026252,-3.0990839499
C,0,2.8239353961,-0.8070629428,-0.4421263013
C,0,4.2798924769,-1.5510343202,1.2792373997
C,0,3.8292151077,-2.9723999467,1.5592390037
C,0,-3.0296420402,-0.5835098865,-1.5721113342
C,0,-4.0090221807,-2.6612489254,-1.0975673225
C,0,-2.6298001623,1.1171366204,0.3052606617
C,0,-2.0695243153,2.8214293953,1.8593026907
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H,0,2.7131438578,3.5262961277,-0.298333135
H,0,3.4919691166,1.9358697538,-0.4194570515
H,0,0.883735225,2.7532052788,-1.8310364678
H,0,2.4394531629,2.6160183211,-2.6352948619
H,0,2.5297179185,0.3034928905,-2.5084047566
H,0,0.4013798715,-1.9985288433,-1.3950736799
H,0,-0.8258694296,2.0295895258,-1.3672657984
H,0,-2.1936501234,2.1733661606,-2.4576314033
H,0,-1.3972952692,0.3630373965,-3.9082613973
H,0,0.8775718669,-0.1593237928,-3.9743391892
H,0,5.0624752454,-1.5221328682,0.5071829013
H,0,4.6446859681,-1.0530040773,2.1877579486
H,0,3.0084054001,-2.9829031751,2.2922881203
H,0,3.4852119386,-3.4593809768,0.6349337004
H,0,4.6681342342,-3.559751662,1.9644836098
H,0,-4.9929929568,-2.3779686473,-1.500667946
H,0,-3.4495912472,-3.1856373732,-1.8876716645
H,0,-4.1299750877,-3.3060395167,-0.2187292837
H,0,-2.9444545929,3.4886126504,1.8004339687
H,0,-2.2446868596,2.0736310946,2.6431382277
C,0,-0.9827302886,-2.1078224224,1.2967804984
C,0,-1.3884135665,-1.8236407861,2.595087717
C,0,-0.9548098762,-0.6544265017,3.2456962418
C,0,-0.112324371,0.2724279104,2.6098158592
H,0,-1.3115430998,-3.0153402192,0.7889794112
H,0,-2.0520886525,-2.5146934858,3.1188799237
H,0,-1.2823504466,-0.4576181257,4.2689495241
H,0,0.2278665618,1.1789718013,3.1028110383
H,0,-1.1559602211,3.3902241762,2.0673531776
----------------------------------------------------------------------
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3
Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -1471.91680779 a.u.
Zero-point correction = 0.454425 Hartree/Particle
Sum of electronic and thermal Free Energies = -1471.520928 a.u.
Sp @ B3LYP-D3(BJ)/def2-TZVP in MeCN (SMD model)
SCF Done: E(RB3LYP) = -1473.57790384 a.u.

```
O,0,-0.8706363176,6.4375947686,9.6784927434
O,0,-0.5449119227,5.226927247,6.0219538707
O,0,0.857377457,3.6297872154,5.2825704015
O,0,3.5764496693,2.2210981629,6.77923701
O,0,5.1722458118,2.4109901851,8.347160449
O,0,5.7730038844,5.781419849,8.4042916852
O,0,5.455157151,4.9298312067,6.3497640332
N,0,0.749441352,5.5215094269,8.3667282731
C,0,1.4357556685,6.7027739103,8.0203949347
C,0,1.132107852,8.0277815576,8.3438653383
C,0,1.9519583671,9.0311451197,7.8136772292
C,0,3.0334893316,8.7271363824,6.9814128955
C,0,3.3337646891,7.3924147859,6.680864291
C,0,2.5415387162,6.3810013046,7.2151462595
C,0,2.6817978436,4.8740108561,7.1082773245
C,0,3.8458707983,4.3341202184,7.9887395657
C,0,3.5865352446,4.4588981299,9.5015073489
C,0,2.7050637402,3.3736277298,10.0513624843
C,0,1.6621275789,2.7775469511,9.4634100363
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C,0,0.9660458533,3.056644223,8.1519838024
C,0,1.2325002207,4.4294167828,7.5014730074
C,0,-0.5557461156,2.967325562,8.3916548982
C,0,-1.0176917329,4.0802765734,9.3326057554
C,0,-0.4016251955,5.4595371001,9.126761067
C,0,0.4000159645,4.4993851821,6.1898341551
C,0,0.2076375094,3.6103695845,3.9967775629
C,0,0.7471915979,4.7058876498,3.0957289025
C,0,4.1454518346,2.8730625808,7.6165482556
C,0,5.5504121537,1.0536633503,8.1196955281
C,0,5.1277553998,5.11220477,7.6434142567
C,0,6.6527933246,5.5700242479,5.9071689131
H,0,0.2761937329,8.2501554164,8.974803164
H,0,1.7277139821,10.0747070445,8.047714503
H,0,3.646004128,9.5294823845,6.5646063746
H,0,4.1715444445,7.1490471359,6.0268351031
H,0,2.8869534511,4.5416669495,6.0864605391
H,0,4.5543751967,4.4276816643,10.0159847065
H,0,3.175032413,5.4606952272,9.7077159462
H,0,2.987455693,3.0035318822,11.0423711624
H,0,1.1915693759,1.9586907096,10.0204339045
H,0,1.2638593102,2.2916342918,7.4199813844
H,0,-1.093772239,3.028998395,7.4345550826
H,0,-0.8048651157,1.9846981485,8.8211853853
H,0,-2.1071763106,4.2229016016,9.3000934426
H,0,-0.7755133651,3.8207528039,10.3771352573
H,0,0.4215937772,2.6107351613,3.5943530225
H,0,0.5204290392,5.6975080135,3.5135433549
H,0,0.2806784156,4.6372875116,2.1003003014
H,0,1.8371973343,4.6106777779,2.9738263472
H,0,-0.8766336715,3.7191640698,4.1465989694
H,0,5.8279341594,0.8987548843,7.066617107
H,0,4.7182501474,0.3777107261,8.3670727625
H,0,6.4070423521,0.8610397778,8.7763207464
H,0,6.7693279115,5.302604027,4.8503444547
H,0,7.5157795874,5.2201227508,6.4924856954
H,0,6.5731485205,6.6613390309,6.0221590046
------------------------------------------------------------------------


4-T
Opt @ UB3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(UB3LYP) = -1318.25861613 a.u.
Zero-point correction = 0.401462 Hartree/Particle
Sum of electronic and thermal Free Energies = -1317.917050 a.u.
Sp @ UB3LYP-D3(BJ)/def2-TZVP in DCM (SMD model)
SCF Done: E(UB3LYP) = -1319.76050898 a.u.
------------------------------------------------------------------------
O,0,-0.2942777614,2.4910034111,-2.3406839475
O,0,-3.6668189715,0.2680911438,1.2299618251
O,0,-3.2874189251,0.4300406444,-0.9847141906
O,0,3.0866077879,-1.7343188359,2.2776350918
O,0,2.4325792452,-2.7669567717,0.3915837347
O,0,3.2766496051,-1.1389291278,-1.716863273
O,0,2.5731940723,0.9892756666,-1.4459914432
N,0,-0.7315430237,0.8729091757,-0.7980351518
C,0,-0.7416754399,2.1754318308,-1.2524886454
C,0,-1.3021858724,3.1356855761,-0.2211898017
C,0,-0.7108249302,2.8341504802,1.1649316697
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C,0,-1.0354989096,1.4023317489,1.6690160251
C,0,-1.3683361434,0.4578554559,0.4599408728
C,0,-0.9408105439,-0.99377952,0.5461571376
C,0,-0.3164999603,-1.3471734544,-0.6414923504
C,0,-0.2207891338,-0.2267590396,-1.4699122496
C,0,2.4841063447,-0.4005703903,0.4202894407
C,0,2.0799272684,0.8156615565,1.2007457716
C,0,1.2846685861,0.5842737677,2.4569607681
C,0,-0.0166509377,0.8432431354,2.6426492196
C,0,-2.9129085012,0.3932357513,0.2955720981
C,0,-4.6829660376,0.2082105542,-1.2731973208
C,0,-5.0026886564,-1.2745259452,-1.3042303234
C,0,2.7053901645,-1.6793368575,1.1252704605
C,0,2.6867651719,-4.0223047327,1.0177698202
C,0,2.82472347,-0.2651165938,-1.0080360219
C,0,2.7791976146,1.2611694649,-2.8308235706
H,0,-1.0608767021,4.153821269,-0.5535095544
H,0,-2.4030411567,3.0473961575,-0.2032696401
H,0,0.3771499813,2.9812509453,1.1157096661
H,0,-1.0822140629,3.5629210693,1.9003603762
H,0,-1.9798728343,1.4547522354,2.223607072
H,0,-1.1801151563,-1.6246384553,1.3981288567
H,0,0.0821908886,-2.3288437723,-0.8884950623
H,0,0.2000170235,-0.1073244998,-2.4623001059
H,0,1.55538216,1.4767654571,0.5036786302
H,0,3.0110357166,1.3595367491,1.4680413585
H,0,1.8430112116,0.1526897837,3.2904962868
H,0,-0.4205263778,0.6057082917,3.6326820333
H,0,-5.2876156735,0.7313714605,-0.5179970823
H,0,-4.8382905581,0.6784455865,-2.2537557526
H,0,-4.3553901145,-1.7974647692,-2.0245742208
H,0,-4.862637225,-1.7226869923,-0.3097747279
H,0,-6.0514472817,-1.4258848978,-1.6045761495
H,0,3.747995824,-4.1113299848,1.2941684955
H,0,2.0801814525,-4.1354126435,1.9293784856
H,0,2.420079236,-4.7888015172,0.2804288903
H,0,3.8358266896,1.5118651098,-3.0152711953
H,0,2.5189822048,0.3827237773,-3.4381830432
H,0,2.1232591721,2.1053415457,-3.0727992625
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5‡-OSS
Opt @ UB3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(UB3LYP) = -1318.25744073 a.u.
Zero-point correction = 0.401258 Hartree/Particle
Sum of electronic and thermal Free Energies = -1317.913754 a.u.
Imaginary Frquency = -90.5696 cm^{-1}
Sp @ UB3LYP-D3(BJ)/def2-TZVP in DCM (SMD model)
SCF Done: E(UB3LYP) = -1319.75941245 a.u.
Sp @ DLPNO-NEVPT2/def2-TZVPP in gas phase
FINAL SINGLE POINT ENERGY = -1316.678305906782 a.u.

```
O,0,1.3857645578,2.6261922442,1.6631096509
O,0,3.3695608659,-1.4862206425,-1.2663346864
O,0,3.1610300708,-0.7406022954,0.8492960344
O,0,-3.4130206753,-0.6363408598,-2.7494939139
O,0,-3.21597673,-1.539976906,-0.7005785796
O,0,-3.386893214,0.587569007,1.1005630403
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```
O,0,-1.8898442563,2.203642201,0.6018137343
N,0,1.0734191194,0.7402641222,0.4272068644
C,0,1.6425020926,1.9729383681,0.6669500954
C,0,2.5405110656,2.4224694402,-0.4682644431
C,0,1.8519361227,2.1629430184,-1.816033426
C,0,1.5871886248,0.6583563621,-2.0707173168
C,0,1.4388015059,-0.1163931991,-0.7096383927
C,0,0.3971218699,-1.2127512027,-0.5978003549
C,0,-0.2598299904,-1.0796030901,0.6169109375
C,0,0.1672432031,0.0883818447,1.2502932071
C,0,-2.3608942674,0.6385967098,-1.0597878425
C,0,-1.527868011,1.4702052937,-1.9901645992
C,0,-0.7992305026,0.7105392448,-3.0675745591
C,0,0.4987142852,0.379573124,-3.0876979426
C,0,2.7814161239,-0.8512919928,-0.4249476962
C,0,4.2979007414,-1.5215027302,1.27155178
C,0,3.8866893596,-2.9441533424,1.6009915103
C,0,-3.0503172457,-0.5540415786,-1.5928318802
C,0,-3.9176243793,-2.6907605592,-1.1650091184
C,0,-2.6207783341,1.1023739832,0.3141169589
C,0,-1.9949948906,2.7498370212,1.9162834753
H,0,2.7559235951,3.4881492222,-0.316364965
H,0,3.500477375,1.878493361,-0.4108781562
H,0,0.9111736823,2.730175989,-1.8390168496
H,0,2.4650508878,2.5569692813,-2.6399550019
H,0,2.5032181845,0.2422311027,-2.5062264242
H,0,0.3096338021,-2.012541369,-1.3283457621
H,0,-0.8438473159,2.0554017354,-1.368395587
H,0,-2.2006227985,2.2094494688,-2.4730548009
H,0,-1.4191989028,0.381539889,-3.9046830175
H,0,0.8356869809,-0.1919719371,-3.9592356555
H,0,5.0571503686,-1.4989551302,0.4762170673
H,0,4.680211084,-0.9933357039,2.1556322688
H,0,3.0889194136,-2.9532332822,2.3591433965
H,0,3.5268909658,-3.4625454746,0.7002893339
H,0,4.7498981507,-3.5021263518,1.9966461524
H,0,-4.931850716,-2.4211730913,-1.4955194562
H,0,-3.3895595037,-3.1566221976,-2.0111184997
H,0,-3.9655844099,-3.3810563626,-0.3144036541
H,0,-2.8147921297,3.4847606404,1.9520521353
H,0,-2.2039264652,1.9557912829,2.6462905165
H,0,-1.0300528667,3.227085832,2.1256426387
H,0,-0.1265308255,0.5387180279,2.1923954554
H,0,-1.0376856285,-1.7382935783,0.9972289178
------------------------------------------------------------------------


6
Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -1318.34661492 a.u.
Zero-point correction = 0.406606 Hartree/Particle
Sum of electronic and thermal Free Energies = -1317.996283 a.u.
Sp @ B3LYP-D3(BJ)/def2-TZVP in DCM (SMD model)
SCF Done: E(RB3LYP) = -1319.84625822 a.u.
------------------------------------------------------------------------
O,0,3.5441659849,0.4948083747,-2.2384124825
O,0,2.8685274217,-0.1192031285,1.5209349272
O,0,1.0667534302,-1.1495786039,2.389390412
O,0,-1.8756884907,-1.9744977808,1.0273486823
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O,0,-3.4131836831,-1.5980845173,-0.5655787517
O,0,-2.9747646703,1.7847142577,-1.2309527875
O,0,-2.909982546,1.2219922098,0.9431906895
N,0,1.7378601004,0.1589031558,-0.9088273099
C,0,1.3503972809,1.4974445201,-0.8068012706
C,0,0.2241575739,1.6257198587,-0.0902268153
C,0,-0.309569718,0.2571712815,0.2956364424
C,0,-1.5887831953,-0.097871004,-0.5155462744
C,0,-1.3269489349,-0.3161706267,-2.0161455744
C,0,-0.7566846639,-1.6666871988,-2.346719091
C,0,0.1167704487,-2.3975425089,-1.6451488229
C,0,0.8786876968,-2.0993205315,-0.3757505572
C,0,0.9662206016,-0.6234033468,0.0632360561
C,0,2.3334490962,-2.5927418114,-0.5545430406
C,0,3.0709352207,-1.7804817735,-1.6232137294
C,0,2.8469421381,-0.274289662,-1.6055872813
C,0,1.762118668,-0.5793843647,1.3995600794
C,0,1.6667566641,-1.1667520894,3.6983349971
C,0,1.4410656984,0.1482094644,4.4215886386
C,0,-2.2729489082,-1.3298411217,0.0910956077
C,0,-4.1448093942,-2.7403088362,-0.1215192461
C,0,-2.5694009664,1.0739571415,-0.3497274892
C,0,-3.8138254739,2.2861881402,1.2427088126
H,0,-0.5923253865,0.1904828063,1.3512272477
H,0,-2.2767423671,-0.1889663457,-2.549911181
H,0,-0.6742946422,0.4964089705,-2.3753488161
H,0,-1.1383991303,-2.115740015,-3.2696443642
H,0,0.3571177735,-3.3875059586,-2.0510912679
H,0,0.4099410188,-2.6545074158,0.450593927
H,0,2.8707000499,-2.5304037238,0.4030623916
H,0,2.3273853104,-3.6575209303,-0.8345090936
H,0,4.1578574161,-1.9403685626,-1.5838512971
H,0,2.750486408,-2.0995333723,-2.6300161706
H,0,1.1774440699,-2.0034466936,4.2156032567
H,0,1.9431871427,0.9713442418,3.8927473064
H,0,1.8540892945,0.0920469703,5.4411596758
H,0,0.3661046928,0.374012215,4.4960552038
H,0,2.7405967655,-1.3806404604,3.592953761
H,0,-4.4204841412,-2.6373822676,0.9384396685
H,0,-3.5409713317,-3.6523767387,-0.2403521968
H,0,-5.0421682809,-2.7916974169,-0.7494384586
H,0,-3.9840532073,2.2467209413,2.3250921977
H,0,-4.7605458094,2.154582473,0.698222162
H,0,-3.3789547082,3.2557364813,0.9574278498
H,0,-0.2865086377,2.5634473906,0.1188834913
H,0,1.9694585106,2.248765023,-1.2924402443
------------------------------------------------------------------------
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7
Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -1318.33287485 a.u.
Zero-point correction = 0.407135 Hartree/Particle
Sum of electronic and thermal Free Energies = -1317.980800 a.u.
Sp @ B3LYP-D3(BJ)/def2-TZVP in DCM (SMD model)
SCF Done: E(RB3LYP) = -1319.83064821 a.u.

```
O,0,7.7811410091,4.7026046231,9.3527073905
O,0,9.4857922936,8.3569145689,10.0016394171
```

```
O,0,11.6981665699,8.5716188106,9.6674412268
O,0,10.1326276565,3.4255822276,4.6192812743
O,0,8.6084011652,5.055666015,4.4002047509
O,0,6.6589977091,4.3235230838,6.4860226049
O,0,7.6797077287,2.5309807524,7.3726642763
N,0,9.4065661748,6.0110056403,8.4574767471
C,0,8.8295079213,5.3163089265,9.4827211372
C,0,9.6779043878,5.2892442992,10.7401928712
C,0,11.1469680315,4.9430087495,10.4102878961
C,0,11.7443743424,5.7126518058,9.1882066974
C,0,10.6706254092,6.7126699539,8.625429885
C,0,10.9376383405,7.2086968486,7.2224078892
C,0,10.0253381298,6.7411481116,6.3715882079
C,0,9.0228500618,5.8477493522,7.0555065763
C,0,9.0861752203,4.3265646637,6.6211375157
C,0,10.1475054354,3.5034357435,7.3942213787
C,0,11.5809359207,3.9618632425,7.2951740991
C,0,12.2541799426,4.8287348467,8.0677105027
C,0,10.5136868326,7.9561214061,9.5218239244
C,0,11.7038530556,9.7924112333,10.4311407661
C,0,13.124217723,10.3104513746,10.4690124866
C,0,9.3571052408,4.204918727,5.1157901042
C,0,8.7356949605,4.9732418901,2.9808470824
C,0,7.6603797072,3.7508343516,6.8281271737
C,0,6.4102356801,2.0136176737,7.7711090324
H,0,9.2380418334,4.5400308483,11.4109791628
H,0,9.601847378,6.2642924954,11.2419032281
H,0,11.2199304903,3.8642222789,10.213774327
H,0,11.7663065254,5.1327380639,11.2993939632
H,0,12.5885517642,6.3211590334,9.5343700753
H,0,11.7798156072,7.8611910042,6.9965139559
H,0,9.9785567814,6.9466408232,5.3044675121
H,0,7.9885836162,6.1776319932,6.8770624526
H,0,9.8214072403,3.4361989274,8.4363574963
H,0,10.0909655378,2.4831391073,6.9974901658
H,0,12.1427507163,3.5027005198,6.4762295571
H,0,13.3030391628,4.9967124115,7.800387839
H,0,11.3101759009,9.5805605658,11.4378880947
H,0,11.0113250079,10.5065567214,9.9580775808
H,0,13.497004809,10.5116108491,9.4530786008
H,0,13.796940309,9.5813244595,10.9460073023
H,0,13.1665508173,11.2477561318,11.0446174947
H,0,8.472788935,3.9654664136,2.6273620522
H,0,9.7677623873,5.1941850313,2.6689778641
H,0,8.0413838835,5.7156953537,2.5702482457
H,0,5.7164671001,1.9768855136,6.9186996781
H,0,5.9862634851,2.6563114139,8.5564195318
H,0,6.5999640619,1.0054211183,8.1588209052
```

Sub-S
Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -1318.31724259 a.u.
Zero-point correction = 0.402615 Hartree/Particle
Sum of electronic and thermal Free Energies = -1317.973447 a.u.
Sp @ B3LYP-D3(BJ)/def2-TZVP in DCM (SMD model)
SCF Done: E(RB3LYP) = -1319.81737370 a.u.

```
O,0,4.1046172085,-0.517445877,-0.8642771661
O,0,0.531726885,-2.3302810189,-2.1671264635
O,0,1.9647445864,-2.2373270854,-0.4229296313
N,0,2.0933160927,0.5738957766,-0.6466699275
C,0,1.5951573106,1.8584473497,-0.5575701175
C,0,0.3491015642,1.8949331466,-1.1492575031
C,0,0.0659604696,0.5814208935,-1.6069465169
C,0,1.1492762893,-0.2228659866,-1.2888765041
C,0,3.6896636551,0.5692739955,1.2426500716
C,0,3.3864877337,0.1600526293,-0.1804902854
C,0,1.1854453983,-1.6889010606,-1.3718656194
C,0,2.104308706,-3.6686788268,-0.3970833012
C,0,1.2158092384,-4.2688903208,0.6766810015
H,0,-0.8559203069,0.2243764677,-2.0570401543
H,0,4.7274566159,0.2716429217,1.4436987726
H,0,1.8528202095,-4.0637833475,-1.3906692665
H,0,0.1595886254,-4.0292911432,0.4900651953
H,0,1.4828215761,-3.8791799701,1.6717879769
H,0,1.3374023114,-5.3638343949,0.6946787168
H,0,3.1708765842,-3.8486796992,-0.1961967711
H,0,3.6227231926,1.664001837,1.3562042665
C,0,2.7214070159,-0.1136262776,2.2456615834
H,0,3.1503481202,0.0356557459,3.2524175271
H,0,2.7106880023,-1.1975891899,2.0565859665
C,0,1.32434588,0.4335122384,2.209513111
C,0,0.2170995706,-0.2666490568,1.9329070301
H,0,1.2284963052,1.509142819,2.4053444701
H,0,0.2758998515,-1.337831697,1.7245634972
C,0,-1.1205171973,0.3640371016,1.8970900173
C,0,-2.2740571062,-0.1498759286,1.0287669392
C,0,-2.3274049509,-0.2514769885,2.541376599
H,0,-1.0933838184,1.457138713,1.9067051193
H,0,-3.033132428,0.3991756141,3.0635386327
H,0,-2.229275288,-1.265194978,2.9367507054
C,0,-2.1255380747,-1.4441035935,0.2867037282
O,0,-1.643362,-2.4492019775,0.7592296809
O,0,-2.5959245681,-1.3571792266,-0.9607363709
C,0,-3.1306124846,0.9038102624,0.3734239954
O,0,-2.7549576408,1.9964908073,0.0230052463
O,0,-4.399629852,0.486098288,0.2603252187
C,0,-2.5923850445,-2.559885018,-1.7459186766
H,0,-3.0776436501,-3.3741214896,-1.1889635014
H,0,-3.1625371756,-2.3216072197,-2.6516962948
H,0,-1.5622080354,-2.8375529935,-2.0018097866
C,0,-5.2959606885,1.3701828568,-0.4103519082
H,0,-6.2745198132,0.8752193114,-0.4063517177
H,0,-5.3528699878,2.3386814253,0.1087816987
H,0,-4.9621813038,1.5479578666,-1.4439211453
H,0,-0.3065089132,2.7586925376,-1.2193780109
H,0,2.1907017495,2.6579032708,-0.1254522876
```

Sub-T
Opt @ UB3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(UB3LYP) = -1318.20656203 a.u.
Zero-point correction = 0.398375 Hartree/Particle
Sum of electronic and thermal Free Energies = -1317.872086 a.u.
Sp @ UB3LYP-D3(BJ)/def2-TZVP in DCM (SMD model)

SCF Done: E(UB3LYP) = -1319.71584008 a.u.

O,0,3.9932175434,-0.9336430427,2.0261615349
O,0,0.7536418151,2.4414612822,-1.19917753
O,0,2.4793321946,2.6202544898,0.2711310696
N,0,2.7403203915,-0.2627822637,0.2707965688
C,0,3.0984261685,-0.2095734956,1.622570149
C,0,2.2532476225,0.6376682721,2.5498758527
C,0,0.7978698567,0.1175475414,2.6587511371
C,0,-0.0977242927,0.486633413,1.5152033187
C,0,1.8040952989,0.4869508513,-0.4753760253
C,0,1.3606524236,-0.3841304678,-1.598819184
C,0,2.1994765136,-1.4697062442,-1.6194341079
C,0,3.0866997776,-1.3920765331,-0.5159511127
C,0,-2.1757648682,-0.847775393,-1.4173362314
C,0,-3.1818181994,-0.3042851781,-0.4276791141
C,0,-1.6707502514,0.0640554228,-0.3501707653
C,0,-0.7892015378,-0.3807769674,0.7477849128
C,0,1.6297695604,1.9191114276,-0.5180031166
C,0,2.3548272531,4.0520302797,0.2438661553
C,0,3.0767823823,4.6537535128,-0.9487538743
H,0,2.7428013209,0.5592438434,3.5291999563
H,0,2.2590237995,1.6917912699,2.2438371575
H,0,0.8041754414,-0.9751354062,2.8032052679
H,0,0.3701524492,0.5517098135,3.5805342724
H,0,-0.2379454321,1.5594976261,1.3400122563
H,0,-1.4821890928,1.0946925227,-0.6673747833
H,0,-0.6953082682,-1.4545967818,0.9212745544
H,0,1.2873882564,4.3179865363,0.2303253163
H,0,2.7990609169,4.3871044603,1.1922083955
H,0,4.1344064506,4.3484460899,-0.959070137
H,0,2.6030194441,4.3332887912,-1.8877091591
H,0,3.0333238454,5.7533352765,-0.8981781076
H,0,0.5877970941,-0.0982244543,-2.3052417452
C,0,-3.8450813888,-1.2451821934,0.5291191991
O,0,-5.0099405683,-1.2058212928,0.8365930735
O,0,-3.0031876562,-2.2007847679,0.9769056304
C,0,-4.0276272814,0.8469190595,-0.9067197293
O,0,-4.1219634631,1.1884337738,-2.0612358748
O,0,-4.5954027874,1.4991753767,0.1123228567
C,0,-3.5703594828,-3.1693592405,1.8581750979
H,0,-3.9750854616,-2.6855991632,2.7593740989
H,0,-4.385371249,-3.7172668911,1.3623415861
H,0,-2.7555830207,-3.8536328262,2.1242406468
C,0,-5.4338367094,2.5995127356,-0.2342987098
H,0,-6.2645903441,2.267196594,-0.8745606363
H,0,-5.8194024149,2.9986060108,0.7114504937
H,0,-4.8634276509,3.3703313894,-0.7744748944
H,0,-1.93772811,-1.9086878753,-1.3244840481
H,0,-2.2634147373,-0.4556092881,-2.4325426267
H,0,2.2076715659,-2.2708161211,-2.3572653562
H,0,3.881267282,-2.0477369148,-0.1737085091

TS1-T
Opt @ UB3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(UB3LYP) = -1318.20631967 a.u.
Zero-point correction = 0.398142 Hartree/Particle

Sum of electronic and thermal Free Energies = -1317.870450 a.u.
Imaginary Frequency = -114.8811 cm^{-1}
Sp @ UB3LYP-D3(BJ)/def2-TZVP in DCM (SMD model)
SCF Done: E(UB3LYP) = -1319.71558621 a.u.

O,0,4.0808781863,-0.7528999686,2.0913331361
O,0,0.7401877821,2.4586033962,-1.1390916484
O,0,2.4805915597,2.619328632,0.3116690464
N,0,2.7471742825,-0.2195164914,0.340170914
C,0,3.1166817652,-0.1289688574,1.6843724675
C,0,2.1686895976,0.6240422283,2.5934583129
C,0,0.743710897,0.022320381,2.5521204392
C,0,-0.0856738987,0.3986143752,1.3604335138
C,0,1.7341309806,0.484934531,-0.3560731412
C,0,1.3231556155,-0.3937565084,-1.4819334004
C,0,2.2221255639,-1.4402762287,-1.5300405433
C,0,3.1208546358,-1.3290151365,-0.4514361558
C,0,-2.292580571,-0.9159614262,-1.4997703246
C,0,-3.2489902044,-0.3489880673,-0.4762701798
C,0,-1.7228686611,-0.0152778349,-0.4556549418
C,0,-0.8191638951,-0.4738994215,0.6128812452
C,0,1.6052461345,1.9276351925,-0.455573606
C,0,2.4062910987,4.0536031084,0.2486048834
C,0,3.1498136101,4.5982094102,-0.9580224697
H,0,2.5886069877,0.5200169219,3.6022065496
H,0,2.1384334032,1.6931058308,2.3421439854
H,0,0.7996759073,-1.0746188326,2.6456365323
H,0,0.2117654662,0.381775888,3.4518206762
H,0,-0.2617204704,1.4692896723,1.2140288949
H,0,-1.526604217,1.012577119,-0.777754686
H,0,-0.7348835405,-1.5470908422,0.7910823559
H,0,1.3487166675,4.3558363391,0.2263137092
H,0,2.8615744615,4.3967837462,1.1887185898
H,0,4.1959562817,4.2555158083,-0.9587367704
H,0,2.6657310219,4.2699202304,-1.8890292031
H,0,3.1451518306,5.6995978541,-0.936522193
H,0,0.5425891041,-0.1325462796,-2.18915179
C,0,-3.8951352974,-1.2722210866,0.5090014961
O,0,-5.0454000696,-1.2053919908,0.8627597714
O,0,-3.0577535556,-2.245892883,0.9255544642
C,0,-4.0808650676,0.8244852122,-0.9239203898
O,0,-4.1997436226,1.1739550004,-2.0738476266
O,0,-4.6018307215,1.4852860242,0.114170476
C,0,-3.6117953744,-3.2010879435,1.8297966895
H,0,-3.9701582453,-2.7078151631,2.7453444657
H,0,-4.4575542208,-3.7307058686,1.3667465648
H,0,-2.8028578681,-3.9034173862,2.0647493798
C,0,-5.4207376654,2.6093218711,-0.2027093458
H,0,-6.2774842602,2.3026011326,-0.821059272
H,0,-5.7689263467,3.0123490895,0.7557527778
H,0,-4.8455270994,3.3682223681,-0.7544939902
H,0,-2.0756740486,-1.9819681706,-1.4134909569
H,0,-2.4072252161,-0.5225756889,-2.5117978248
H,0,2.2535698142,-2.2321490323,-2.2771921535
H,0,3.9435125422,-1.9572553942,-0.1231478341

INT1-T

Opt @ UB3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(UB3LYP) = -1318.25285850 a.u.
Zero-point correction = 0.400284 Hartree/Particle
Sum of electronic and thermal Free Energies = -1317.914297 a.u.
Sp @ UB3LYP-D3(BJ)/def2-TZVP in DCM (SMD model)
SCF Done: E(UB3LYP) = -1319.75281152 a.u.

O,0,2.9070771292,-0.7761745857,-2.0391908967
N,0,1.9711655252,-0.6059402912,0.0140922447
C,0,2.2789904813,0.7285333725,0.2414400436
C,0,1.6458082954,1.1446325111,1.416400802
C,0,0.9447050229,0.0856047785,1.9726149045
C,0,1.2034935001,-1.1514929216,1.1411564615
C,0,2.2220052016,-1.277946249,-1.1625336254
C,0,1.5265734146,-2.6184181679,-1.3552610399
C,0,0.561595789,-3.1002739927,-0.2573024206
C,0,-0.0082602729,-1.9366201897,0.5875691681
C,0,-0.9165930957,-1.0278292486,-0.1808550629
C,0,-1.9707340166,-1.5699731873,-1.0267914185
C,0,-1.9730347369,-1.3483007636,-2.5815609925
H,0,0.9975435596,-2.5063241388,-2.3138274894
H,0,2.3165912403,-3.3628576705,-1.5387962843
H,0,1.0733216579,-3.8022377882,0.4191498451
H,0,-0.2585893338,-3.6676730022,-0.7199582402
H,0,-0.5433326491,-2.377255455,1.449437897
H,0,-0.7167353228,0.0443132828,-0.2047434353
H,0,-2.2729295338,-2.5993580791,-0.8139189045
C,0,-3.0145471745,-0.7242207181,-1.6820764426
H,0,0.3734059033,0.0650087219,2.8972184937
C,0,2.1099281904,-2.0958443212,1.9606684451
O,0,3.2403518846,-2.3919749455,1.6734671924
O,0,1.4538165104,-2.5387200043,3.0442270461
C,0,2.1785001017,-3.3981540065,3.9469031982
C,0,3.043763833,-2.5942735305,4.8997551998
H,0,2.7866230356,-4.0983458183,3.3554945198
H,0,1.3987328444,-3.9584843142,4.4812438425
H,0,3.5293035249,-3.2675920308,5.6237185435
H,0,3.8298409698,-2.0574106395,4.3494233286
H,0,2.4378643566,-1.8643971495,5.4583489458
C,0,-2.3872005223,-2.5438091183,-3.3917077407
O,0,-2.5508801828,-3.6572489925,-2.9490823612
O,0,-2.6145664496,-2.2151288457,-4.6693336742
C,0,-0.9145299024,-0.4387477827,-3.1271441808
O,0,-0.753366009,0.7063082722,-2.7758772376
O,0,-0.1238307904,-1.0760747999,-4.0002922033
H,0,-2.9275080606,0.3595494024,-1.5728521695
H,0,-4.0307412106,-1.1199389779,-1.7481130838
C,0,0.9438495138,-0.3180187816,-4.5909937052
H,0,1.2711318145,-0.8959563348,-5.4638564443
H,0,0.5814833531,0.6733118756,-4.8959503525
H,0,1.768657485,-0.2154606868,-3.8719406058
C,0,-2.9815151772,-3.2840800016,-5.5408690437
H,0,-3.914554005,-3.7601889241,-5.2040235296
H,0,-3.1159446677,-2.8363063169,-6.5327236587
H,0,-2.1905036006,-4.0484016071,-5.5701351985
H,0,1.6972523765,2.1570545856,1.8155140974
H,0,2.8719103693,1.271893147,-0.4880405173

TS2-T
Opt @ UB3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(UB3LYP) = -1318.24036033 a.u.
Zero-point correction = 0.399619 Hartree/Particle
Sum of electronic and thermal Free Energies = -1317.901442 a.u.
Imaginary Frequency = -405.2716 cm^{-1}
Sp @ UB3LYP-D3(BJ)/def2-TZVP in DCM (SMD model)
SCF Done: E(UB3LYP) = -1319.74524593 a.u.

O,0,2.6744480702,-0.3800317993,-3.2794759513
O,0,2.0431524893,-2.0615889139,1.8152176866
O,0,3.6300934795,-0.8704807663,0.7439844248
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