

Supporting Information

Enhancing Intersystem Crossing to Achieve Thermally Activated Delayed Fluorescence in a Water-Soluble Fluorescein Derivative with a Flexible Propenyl Group

Yingnan Wu,^{a,d} Yanliang Zhao,^{a,d} Panwang Zhou,^a Daoyuan Zheng,^a Honglei Wang,^a Shanliang Tang,^b Jiarui Tian,^a Songqiu Yang,^c Weiqiao Deng,^a Keli Han^{a,c} and Fengling Song^{a,b}*

^a Institute of Molecular Sciences and Engineering, Shandong University, Qingdao 266237, China

^b State Key Laboratory of Fine Chemicals, Dalian University of Technology, No. 2 Linggong Road, High-tech District, Dalian, 116024, China

^c State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Science, Dalian 116023, China

^d These authors contributed equally to this work

Experimental Procedures

1. Computational Details

All electronic structure calculations were carried out using Gaussian 16 program suite.¹ DFT and linear-response TD-DFT were employed to calculate the ground (S_0) and excited states (S_1, T_1, T_2, T_3) of the target molecules.^{2,3} For all geometry optimizations and electron energy calculations, the CAM-B3LYP functionals was used, in combination with the 6-311G (d, p) basis set.⁴⁻⁶ All calculations were conducted using the integral equation formalism^{7,8} (IEF) version of the polarizable continuum^{9,10} (PCM) model, in which the solvent effect of acetonitrile ($\epsilon = 35.688$) was considered. The electron-hole analysis was based on TDDFT unrelaxed excited-state densities provided by the Multiwfn software.¹¹ The computations of spin-orbital coupling matrix elements were performed by PySOC+Gaussian 09 based on the stable geometry in the S_1 state.¹²

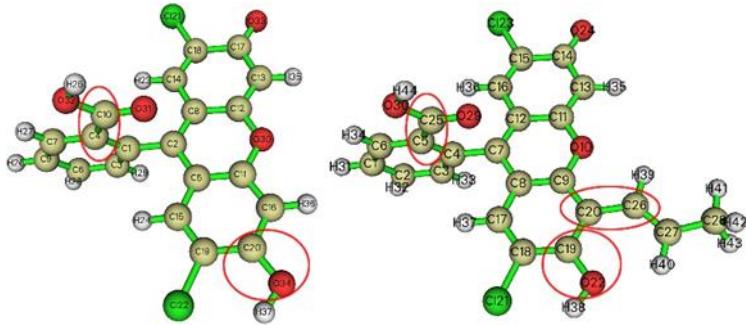
2. Theoretical Background

Boltzmann Distribution.

$$p_i = \frac{e^{-\Delta E_i / RT}}{\sum_j e^{-\Delta E_j / RT}} = \frac{Q_{i(\text{Relative})}}{Q_{(\text{Relative})}} \quad (1)$$

where ΔE is the relative free energy; T, temperature; R, gas constant.

Conformation searching and Boltzmann distribution were accomplished by Molclus (Tian Lu, molclus program, Version 1.6, <http://www.keinsci.com/research/molclus.html>). A simple and practical "systematic search method" was adopted, in which some dihedral angles of molecules are rotated according to specified rules and the resulting structure is used as the initial structure for optimization. As shown in the following figure, two bonds (C4-C10, C20-O34) of DCF and three bonds (C5-C25, C19-O22, C20-O26) of DCF-BXJ were set to be rotated, in which each bond rotates once at 45 degrees, resulting in producing $4^*4=16$ and $4^*4^*4=64$ initial configurations, respectively. After optimizing these initial configurations, 4 and 8 stable structures were obtained (shown in Figure S6 and S7) for DCF and DCF-BXJ in the S_0 state. The temperature was set at 300 K, and then we got Boltzmann distribution for each configuration. The cam-b3lyp/6-311G (d, p) level was performed for energy calculations, while IEFPCM model and acetonitrile solvent were considered.



Scheme S1. Conformation searching by rotate some dihedral angles.

Intersystem Crossing Rate

On the basis of the semiclassical Marcus theory,^{13, 14} the rate of ISC can be expressed as:

$$k_{ISC} = \frac{2\pi}{\hbar} |\hat{V}_{SOC}|^2 \frac{1}{\sqrt{4\pi\lambda k_B T}} \exp\left(-\frac{(\Delta G_{ST}^V)^2}{4\lambda k_B T}\right) \quad (2)$$

where V_{SOC} is the spin-orbital coupling (SOC) matrix element; \hbar , the reduced Plank constants; k_B , the Boltzmann constant; T , temperature; λ , the reorganization energy; ΔG_{ST}^V , the vertical free Gibss energy variation ($\approx \Delta E_{ST} = E_{Tm}(R_{minS1}) - E_{S1}(R_{minS1})$).¹⁵

Spin-orbital Coupling

The SOC matrix elements, as expected, were small in purely organic molecules in comparison to those in molecules containing a heavy metal atom. Based on the central-field approximation where the potential energy for an electron, V_{SOC} is a function of r between electron i and nucleus μ which can be expressed as¹⁶

$$\hat{V}_{SOC} = \sum_{\mu} \sum_i \frac{2c^2}{(2c^2 - V_{\mu i})^2} \frac{1}{r_{\mu i}} \frac{\partial V_{\mu i}}{\partial r_{\mu i}} \left[\frac{1}{2} (\hat{l}_{\mu i+} \cdot \hat{s}_{i-} + \hat{l}_{\mu i-} \cdot \hat{s}_{i+}) + \hat{l}_{\mu i z} \cdot \hat{s}_{i z} \right] \quad (3)$$

where $\hat{l}_{\pm}[\hat{s}_{\pm}]$ denotes raising (+) or lowering (-) operator for the orbital [spin] angular momentum of a given electron; $\hat{l}_z[\hat{s}_z]$ stands for the z component of orbital angular momentum operator [the spin angular momentum operator]. Due to the conservation of angular momentum, upon flipping the spin angular momentum of an electron up, the orbital angular momentum of the electron must be lowered.

3. The experimental details

All chemical reagents were commercially sourced. Absorption spectra were obtained using a UV-Vis spectrophotometer (Cary Eclipse from Agilent Tech) in a quartz cuvette at 25°C. Fluorescence spectroscopy was recorded on a fluorometer (Cary Eclipse from Agilent Tech) in a quartz cuvette at 25°C. The data were obtained under the control of a Windows-based PC running the manufacturers' supplied software. Microsecond fluorescence lifetimes were using HORIBA Jobin Yvon IBN photon counting fluorescence system with spectra-LED excitation at 462 nm. Nanosecond time-resolved transient absorption spectrum (TAS) was recorded on an LFP1000 spectrometer (nanosecond transient absorption spectroscopy, NTAS) at room temperature. A Xe lamp and a picosecond pulsed diode laser (532 nm, energy 2.8 mJ / pulse, frequency 3 Hz, pulse width 6 ns) were used as the excitation source. A tunable pulsed xenon lamp with a detection source of 450 W. The pH values were measured with a pH meter (STARRER 2100 from OHAUS). The pH of the solution was adjusted with 1M hydrochloric acid solution and 1M sodium hydroxide solution. The absolute quantum yields of the compounds were determined with an absolute PL quantum yield spectrometer (Hamamatsu, Quantaurus-QY, C11347).

All the reactions were carried out under a nitrogen atmosphere with dry, freshly distilled solvents under anhydrous conditions unless otherwise noted. Silica gel (200-300 mesh) was used for flash column chromatography, Ultrapure deionized water from a Milli-Q ultrapure system was used for all synthesis and storage steps.

4. Figures

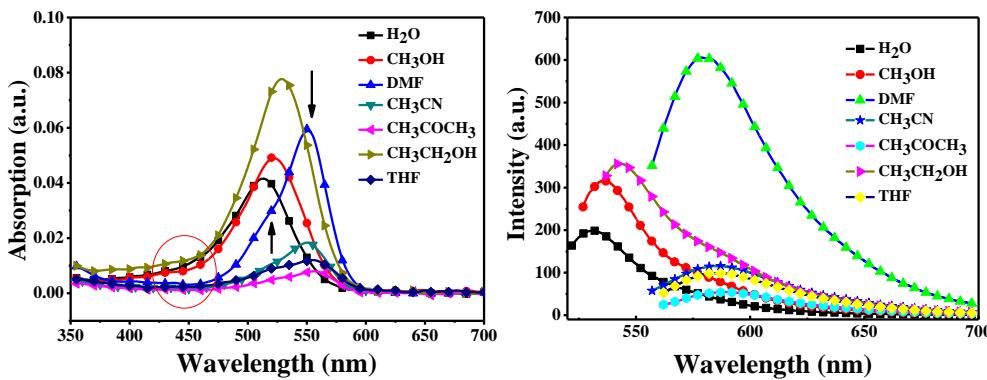


Figure S1. DCF-BXJ in different solvents UV-vis absorption spectrum (left) and steady-state fluorescence emission spectrum (right).

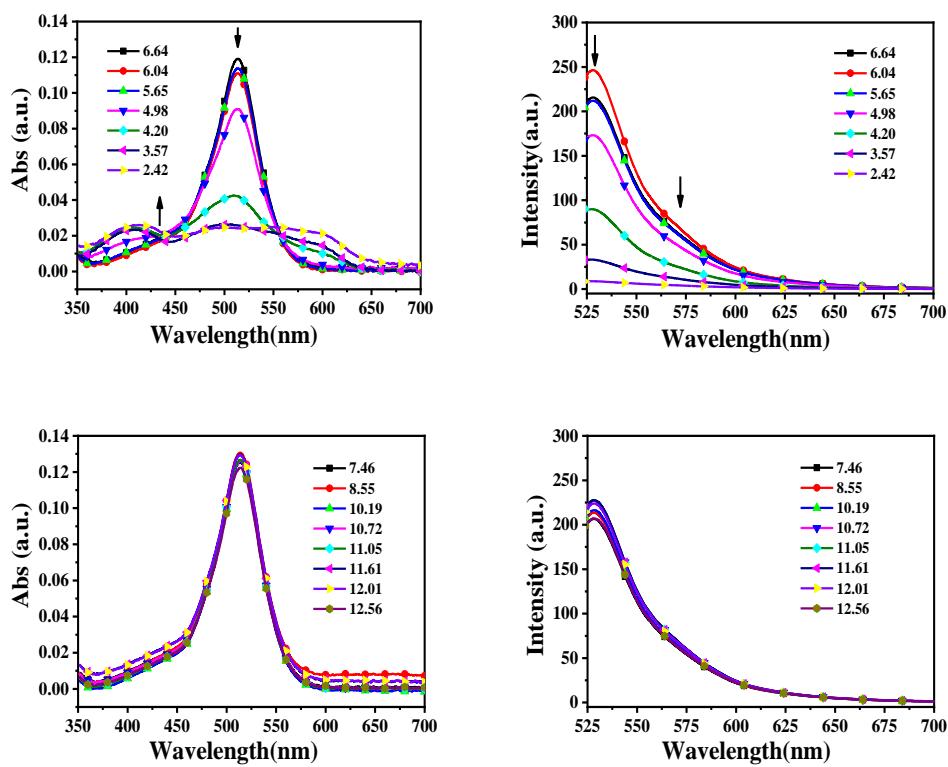


Figure S2. UV-vis absorption spectrum (left) and steady-state fluorescence emission spectrum (right) of DCF-BXJ in PBS buffer with different pH.

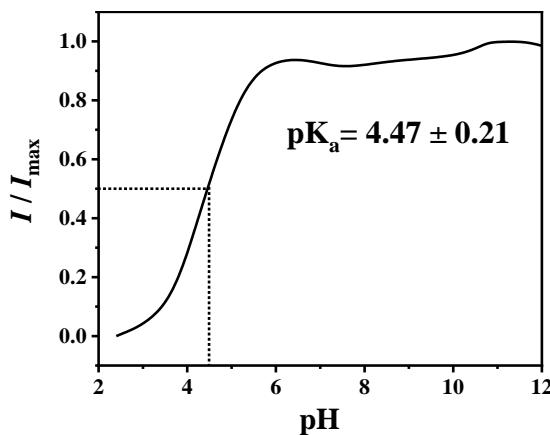


Figure S3. The sigmoidal fitting of the pH-dependent with I/I_{\max} of the DCF-BXJ .

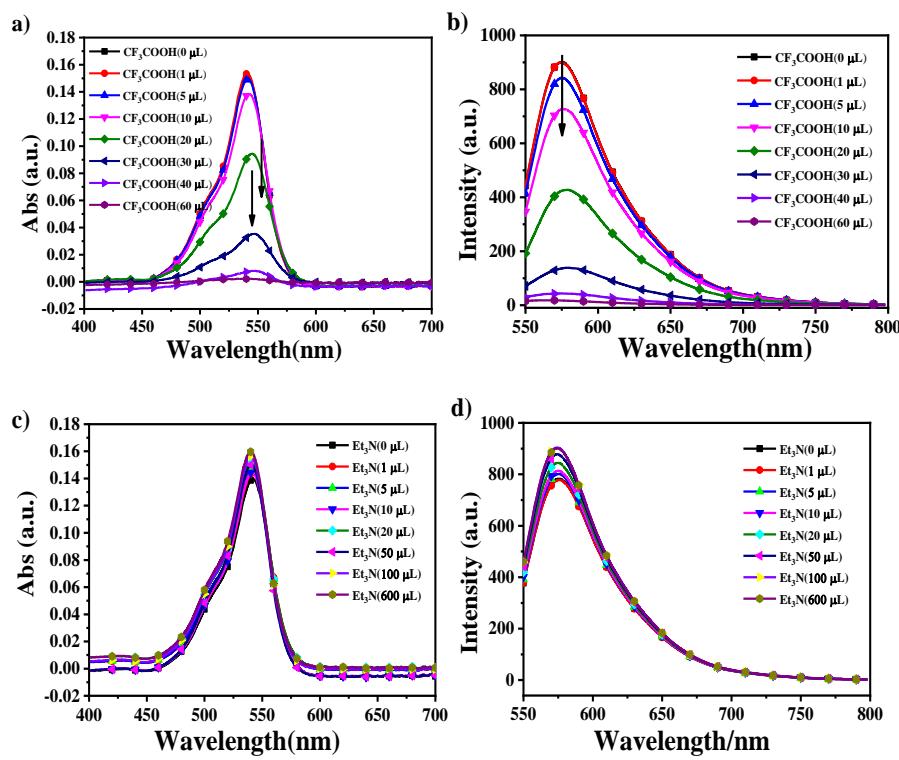


Figure S4. a) UV-vis absorption spectrum and b)steady-state fluorescence emission spectrum of DCF-BXJ (3 μ M) after adding trifluoroacetic acid solution (acetonitrile dilution, concentration 6.83×10^{-7} mol/L) to acetonitrile; c) UV-vis absorption spectrum and d)steady-state fluorescence emission spectrum of DCF-BXJ (3 μ M) adding triethylamine solution (acetonitrile dilution, concentration 5.4×10^{-6} mol/L) to acetonitrile.

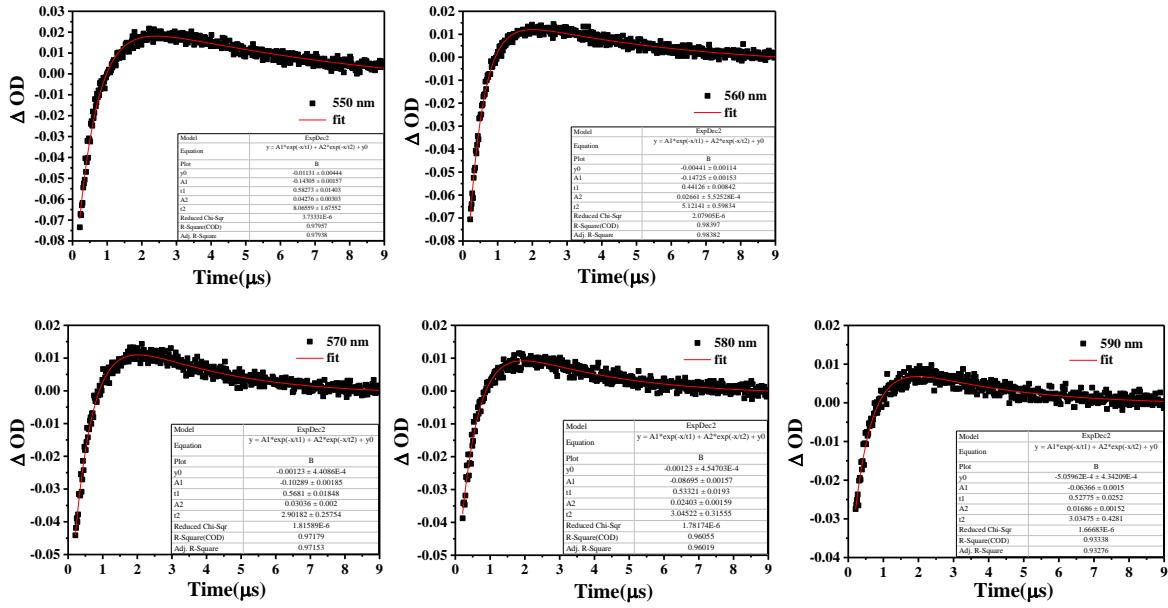


Figure S5. Kinetic attenuation and fitting curves of DCF-BXJ transient absorption at different wavelengths, 25.0

μM in acetonitrile after deoxygenating at room temperature, $\lambda_{\text{ex}}=532$ nm.

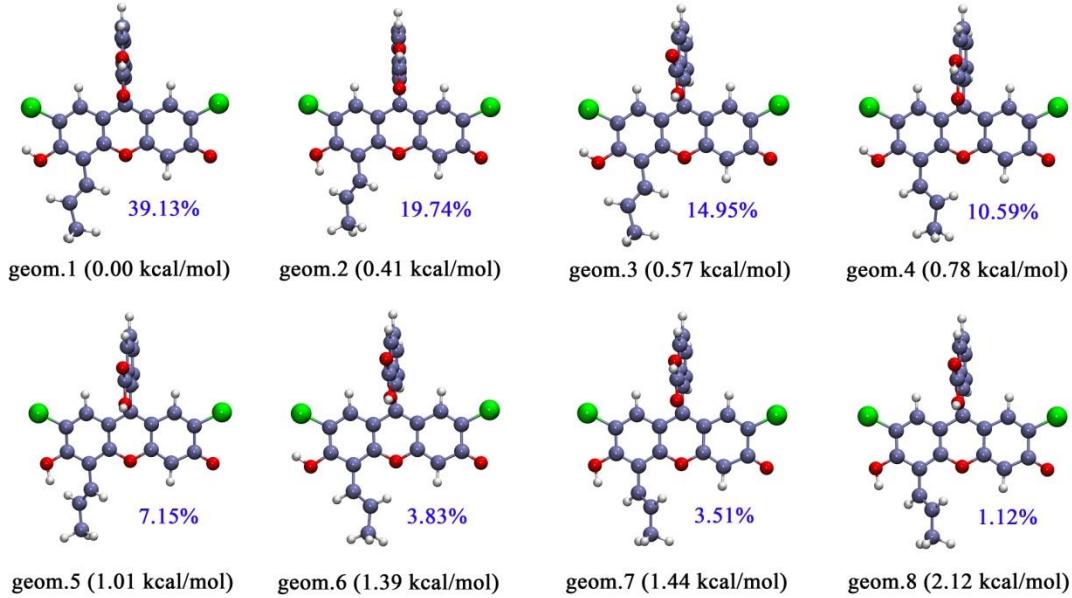


Figure S6. Calculated conformational population (%) and relative free energy (kcal/mol) of DCF-BXJ configurations in the ground state.

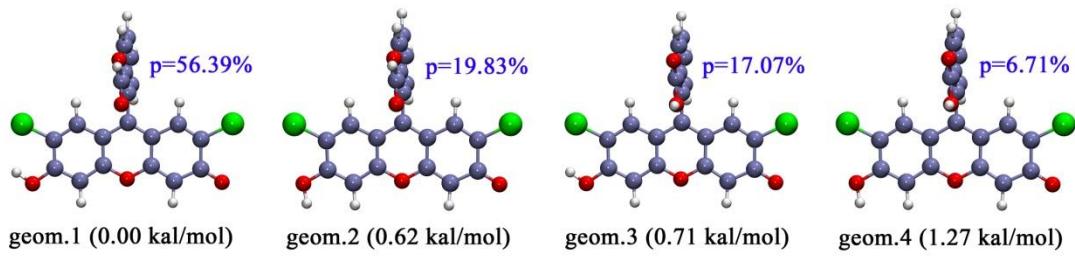


Figure S7. Calculated conformational population (%) and relative free energy (kcal/mol) of DCF configurations in the ground state.

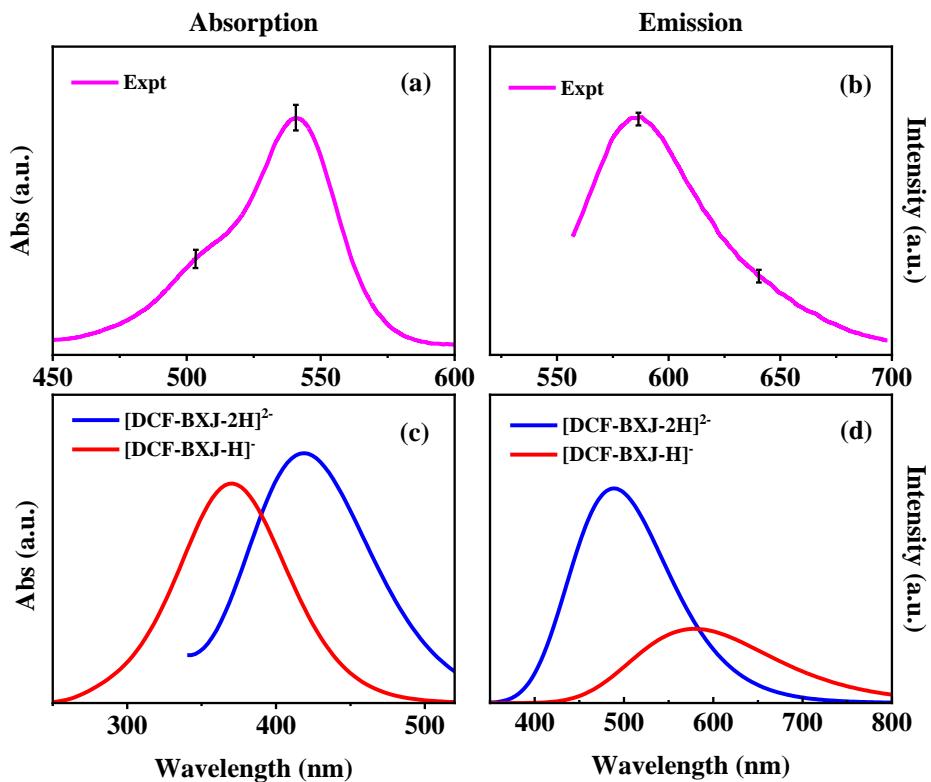


Figure S8. Absorption and fluorescence spectra of DCF-BXJ in acetonitrile [(a)(b): experimental, in acetonitrile; (c)(d): calculated].

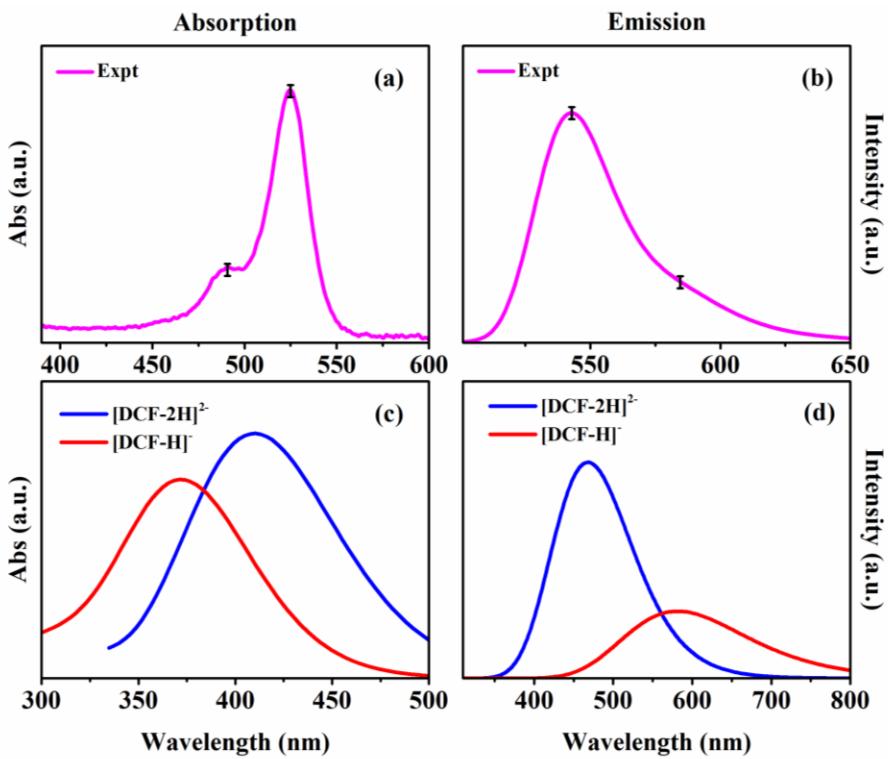


Figure S9. Absorption and fluorescence spectra of DCF in acetonitrile [(a)(b): experimental, in acetonitrile; (c)(d): calculated].

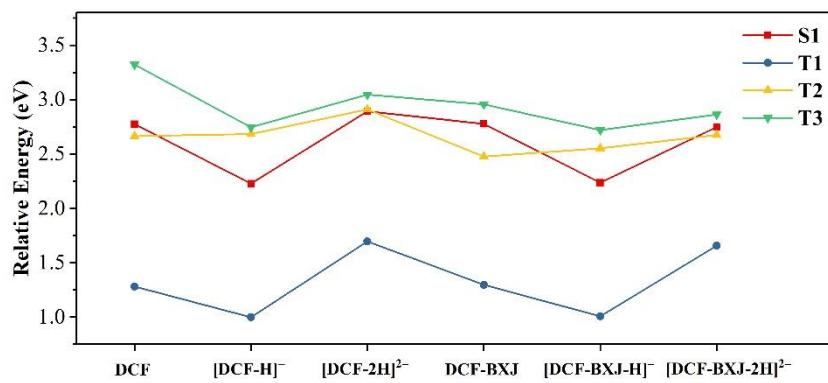


Figure S10. The vertical excitation energy (eV) in different forms for DCF and DCF-BXJ compounds.

Table S1. Calculated vertical excitation energy (eV) based on the stable geometry the S₁ state.

	S ₁ state	T ₁ state	ΔE _{S1T1}	T ₂ state	ΔE _{S1T2}	T ₃ state	ΔE _{S1T3}
DCF	2.7743	1.2820	-1.4923	2.6646	-0.1097	3.3218	0.5475
[DCF-H] ⁻	2.2280	0.9996	-1.2284	2.6830	0.4550	2.7459	0.5179
[DCF-2H] ²⁻	2.8924	1.6960	-1.1964	2.9106	0.0182	3.0462	0.1538
DCF-BXJ	2.7771	1.2974	-1.4797	2.4760	-0.3011	2.9561	0.1790
[DCF-BXJ-H] ⁻	2.2367	1.0079	-1.2288	2.5522	0.3155	2.7207	0.4840
[DCF-BXJ-2H] ²⁻	2.7477	1.6567	-1.0910	2.6756	-0.0721	2.8627	0.1150

Table S2. Photophysical data of DCF-BXJ in acetonitrile.

	Abs	PL (nm) 298K	PL (nm) 77K	Phosphorescence (nm)	τ ₁ (ns)	τ ₂ (μs)	Φ
DCF-BXJ	550	578	527/577	668	3.73	3.20	0.24

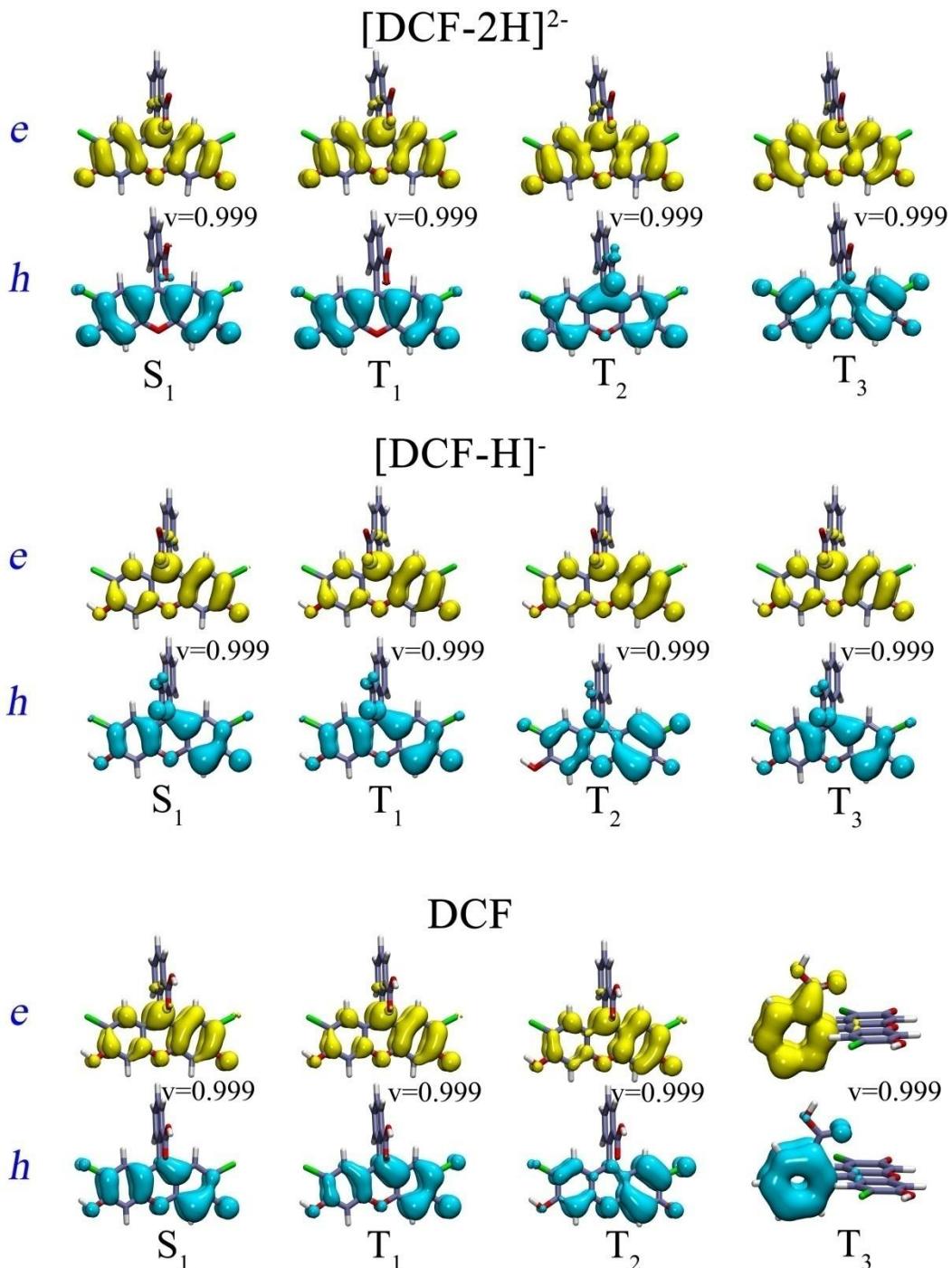


Figure S11. Electron–hole distribution for the S_1 , T_1 , T_2 , and T_3 excited states in DCF, $[DCF\cdot H]^-$, and $[DCF\cdot 2H]^{2-}$.

(The cyan and yellow regions represent the hole and electron, respectively.)

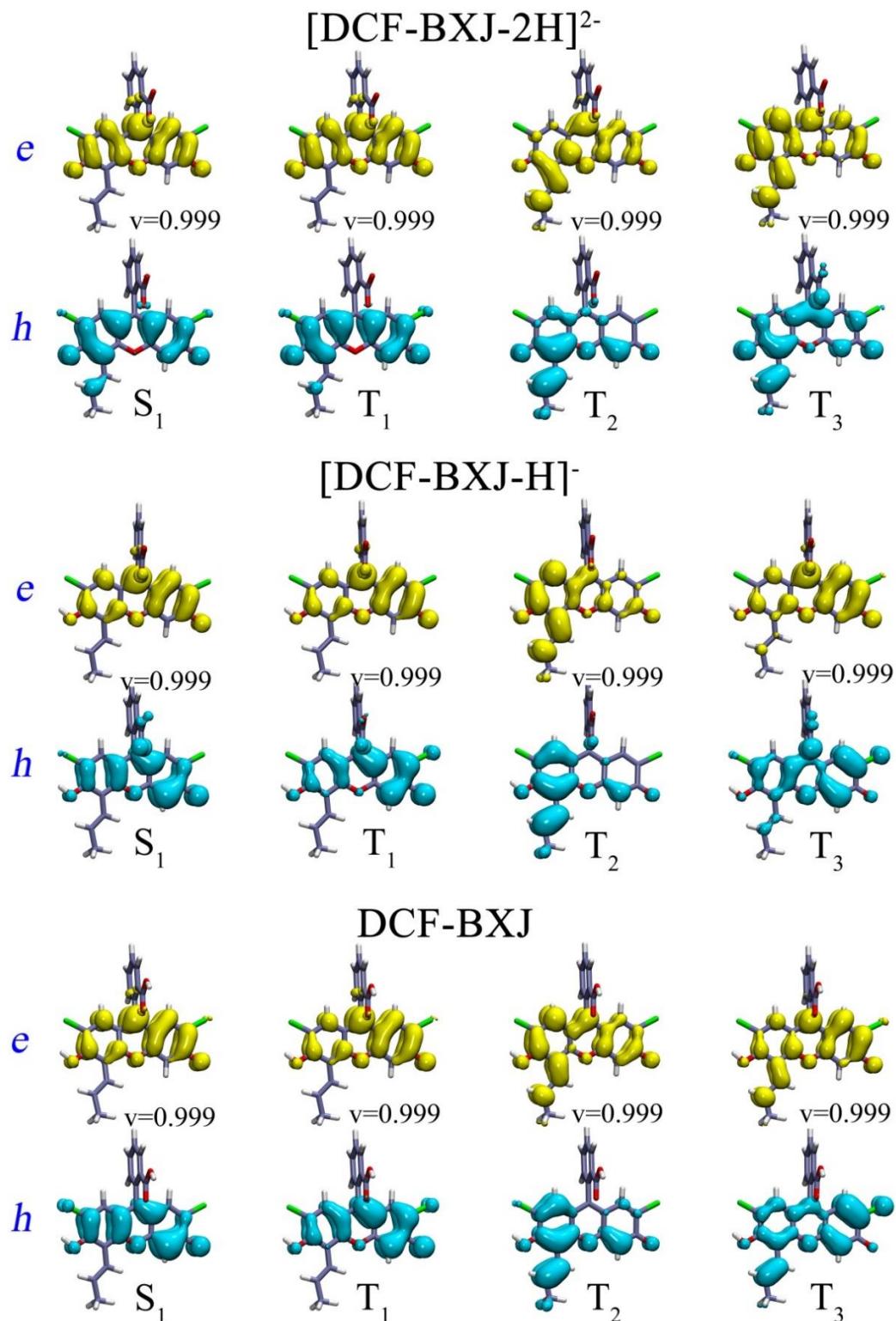


Figure S12. Electron–hole distribution for the S₁, T₁, T₂, and T₃ excited states in DCF–BXJ, [DCF–BXJ–H][−] and [DCF–BXJ–2H]^{2−}. The cyan and yellow regions represent the hole and electron, respectively.

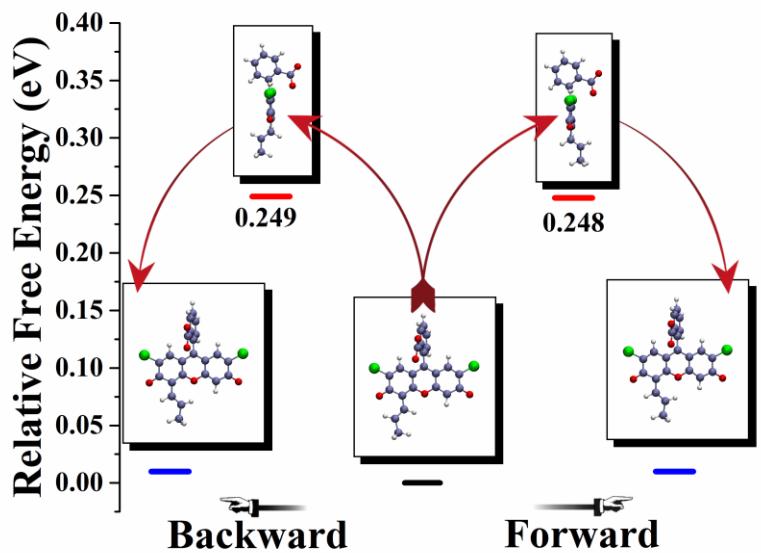


Figure S13. Energy profiles of transition states along the C–C bond twisting of $[DCF\text{--}BXJ\text{--}2H]^{2-}$ configuration in the S_1 state.

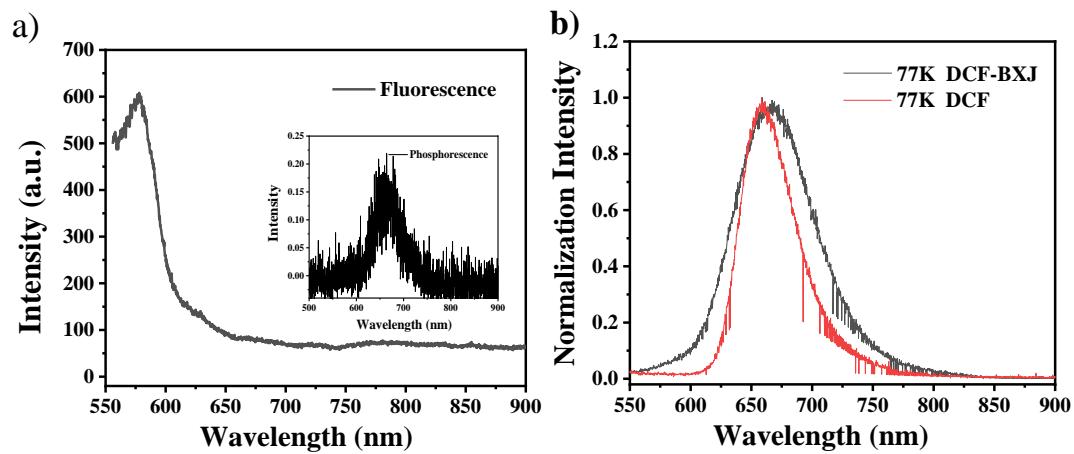


Figure S14. a) Fluorescence and phosphorescence spectra of DCF-BXJ, 77K, in acetonitrile. b) The normalized phosphorescent spectrum of DCF-BXJ and DCF, 77K, in acetonitrile. It's tested under the same conditions.

References

- (1) 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, 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 Jr., J. A.; 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 16 Rev. C.01*, Wallingford, CT, 2016.
- (2) Ferré, N.; Filatov, M.; Huix-Rotllant, M. Density-Functional Methods for Excited States. *Topics in Current Chemistry* **2016**, 368, VII-IX.
- (3) Bauernschmitt, R.; Ahlrichs, R. Treatment of electronic excitations within the adiabatic approximation of time dependent density functional theory. *Chem Phys Lett* **1996**, 256 (4–5), 454-464.
- (4) McLean, A. D.; Chandler, G. S. Contracted Gaussian basis sets for molecular calculations. I. Second row atoms, Z=11–18. *The Journal of Chemical Physics* **1980**, 72 (10), 5639-5648.
- (5) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. Self - consistent molecular orbital methods. XX. A basis set for correlated wave functions. *The Journal of Chemical Physics* **1980**, 72 (1), 650-654.
- (6) Yanai, T.; Tew, D. P.; Handy, N. C. A new hybrid exchange–correlation functional using the Coulomb-attenuating method (CAM-B3LYP). *Chem Phys Lett* **2004**, 393 (1-3), 51-57.
- (7) Mennucci, B.; Cancès, E.; Tomasi, J. Evaluation of solvent effects in isotropic and anisotropic dielectrics and in ionic solutions with a unified integral equation method: theoretical bases, computational implementation, and numerical applications. *The Journal of Physical Chemistry B* **1997**, 101 (49), 10506-10517.
- (8) Cancès, E.; Mennucci, B.; Tomasi, J. A new integral equation formalism for the polarizable continuum model: Theoretical background and applications to isotropic and anisotropic dielectrics. *The Journal of Chemical Physics* **1997**, 107 (8), 3032-3041.
- (9) Miertuš, S.; Scrocco, E.; Tomasi, J. Electrostatic interaction of a solute with a continuum. A direct utilization of AB initio molecular potentials for the prevision of solvent effects. *Chem Phys* **1981**, 55 (1), 117-129.
- (10) Cammi, R.; Tomasi, J. Remarks on the use of the apparent surface charges (ASC) methods in solvation problems: Iterative versus matrix-inversion procedures and the renormalization of the apparent charges. *Journal of Computational Chemistry* **1995**, 16 (12), 1449-1458.
- (11) Lu, T.; Chen, F. Multiwfn: a multifunctional wavefunction analyzer. *Journal of computational chemistry* **2012**, 33 (5), 580-592.
- (12) Chiodo, S. G.; Russo, N. One-electron spin-orbit contribution by effective nuclear charges. *Journal of Computational Chemistry* **2009**, 30 (5), 832-839.
- (13) Schmidt, K.; Brovelli, S.; Coropceanu, V.; Beljonne, D.; Cornil, J.; Bazzini, C.; Caronna, T.; Tubino, R.; Meinardi, F.; Shuai, Z.; Bredas, J. L. Intersystem crossing processes in nonplanar aromatic heterocyclic molecules. *J Phys Chem A* **2007**, 111 (42), 10490-10499.
- (14) Bredas, J. L.; Beljonne, D.; Coropceanu, V.; Cornil, J. Charge-transfer and energy-transfer processes in pi-conjugated oligomers and polymers: a molecular picture. *Chem Rev* **2004**, 104 (11), 4971-5004.
- (15) Liu, R.; Gao, X.; Barbatti, M.; Jiang, J.; Zhang, G. Promoting Intersystem Crossing of a Fluorescent Molecule via Single Functional Group Modification. *J Phys Chem Lett* **2019**, 10 (6), 1388-1393.
- (16) Samanta, P. K.; Kim, D.; Coropceanu, V.; Bredas, J. L. Up-Conversion Intersystem Crossing Rates in Organic Emitters for Thermally Activated Delayed Fluorescence: Impact of the Nature of Singlet vs Triplet Excited States. *J Am Chem Soc* **2017**, 139 (11), 4042-4051.

Cartesian coordinates of all optimized geometry are placed in below:

DCF-BXJ_geom.1 (S_0)

C	-2.70495300	-4.06188700	-1.09168700
C	-2.33669700	-3.20209600	-2.11515600
C	-1.66632200	-2.02250900	-1.82525800
C	-1.35260200	-1.68624100	-0.51222600
C	-1.72321200	-2.55739000	0.52154500
C	-2.40032100	-3.73730900	0.21919900
C	-0.62807600	-0.40175100	-0.28881400
C	0.81029400	-0.39976500	-0.26054500
C	1.48643000	0.81588700	-0.11712600
O	0.79031200	1.97413600	-0.01441000
C	-0.56330100	2.01160900	-0.05547000
C	-1.30076300	0.78345200	-0.20631800
C	-1.16294900	3.21988700	0.04827500
C	-2.59925400	3.35930600	0.01883400
C	-3.33927200	2.08428700	-0.12893400
C	-2.73610600	0.89143100	-0.23317900
C	1.57298400	-1.56846100	-0.36425100
C	2.93675800	-1.49103600	-0.32281700
C	3.60937800	-0.26443800	-0.17762300
C	2.88516500	0.93032700	-0.07130100
Cl	3.90003300	-2.94543800	-0.45132500
O	4.94664900	-0.21307700	-0.13880900
Cl	-5.07705700	2.19936300	-0.16210500
O	-3.17412200	4.43823200	0.10832300
C	-1.39800500	-2.22394500	1.93427700
C	3.48174900	2.26309100	0.08685300
C	4.76892100	2.61426500	0.11337100
C	5.22324900	4.02836000	0.28202600
O	-0.76357100	-1.25927500	2.28218100
O	-1.88260500	-3.11577200	2.80493600
H	-3.22969100	-4.98247500	-1.31253100
H	-2.57153000	-3.44505800	-3.14388400
H	-1.38188200	-1.35160000	-2.62630200
H	-2.68540600	-4.39859700	1.02501300
H	-0.57113800	4.11850300	0.15798600
H	-3.32201000	-0.01096200	-0.33904100
H	1.08922800	-2.52770200	-0.47816500
H	5.31631300	-1.10343100	-0.21943900
H	2.74986700	3.05494500	0.19204600
H	5.54461100	1.86875200	0.01056300

H	4.38256800	4.71739700	0.37737100
H	5.85486000	4.12888500	1.16978600
H	5.83340300	4.34321900	-0.56985100
H	-1.62347700	-2.83134500	3.69350300

DCF-BXJ_geom.2 (S_0)

C	-2.32565600	-4.30696000	-1.04643700
C	-1.99842100	-3.44216400	-2.07958700
C	-1.39818600	-2.22256700	-1.80194100
C	-1.11465600	-1.85057700	-0.49170300
C	-1.44351700	-2.72677100	0.55192500
C	-2.05025900	-3.94732700	0.26176300
C	-0.46398100	-0.52496900	-0.28270200
C	0.97040000	-0.44189000	-0.24250000
C	1.56755600	0.81481400	-0.11807500
O	0.81877700	1.93980300	-0.04185700
C	-0.53644400	1.89653300	-0.08726700
C	-1.20074200	0.62471300	-0.22372900
C	-1.20511900	3.06937400	-0.00390300
C	-2.64683700	3.12623000	-0.04318800
C	-3.31086900	1.80928300	-0.17843700
C	-2.63947000	0.65145700	-0.26183900
C	1.81196800	-1.56060300	-0.31929100
C	3.17072800	-1.41011100	-0.25901500
C	3.75741800	-0.13854700	-0.12900100
C	2.94910900	0.99942500	-0.07488000
Cl	4.20692500	-2.80999100	-0.33284700
O	5.09165700	-0.07379700	-0.04697300
Cl	-5.05235400	1.82408600	-0.22522600
O	-3.28281800	4.17181100	0.02856600
C	-1.14954500	-2.35546000	1.96205800
C	3.51716100	2.35353200	0.08175200
C	4.49262500	2.86169200	-0.66946900
C	5.06557300	4.23092400	-0.50111300
O	-0.57730900	-1.34952600	2.30089500
O	-1.58587400	-3.26325100	2.84171300
H	-2.79560200	-5.25887800	-1.25765300
H	-2.21072200	-3.71252700	-3.10637800
H	-1.14555600	-1.54788900	-2.61043400
H	-2.30371500	-4.61247900	1.07493700
H	-0.66494800	4.00114100	0.09513900
H	-3.17245100	-0.28419500	-0.35864100
H	1.38774200	-2.54911700	-0.42262800
H	5.35487200	0.84115300	0.13242900

H	3.07565600	2.96626800	0.86230600
H	4.89759100	2.27096400	-1.48894200
H	4.59446300	4.76422700	0.32535000
H	6.14153400	4.18095200	-0.31410900
H	4.93181700	4.81629000	-1.41472200
H	-1.35116000	-2.95168300	3.72800200

DCF-BXJ_geom.3 (S_0)

C	-2.37422700	-4.31631100	-0.91319700
C	-2.09006300	-3.46981500	-1.97421400
C	-1.47985000	-2.24684000	-1.74083400
C	-1.14134300	-1.84670700	-0.45005400
C	-1.42640000	-2.70551800	0.62204300
C	-2.04364400	-3.93006300	0.37279800
C	-0.48452200	-0.51299900	-0.32026400
C	0.95098300	-0.42958100	-0.35716700
C	1.56122900	0.82773300	-0.30201200
O	0.80386100	1.94839800	-0.21896700
C	-0.54996500	1.90790600	-0.19390600
C	-1.22088300	0.63388300	-0.25396000
C	-1.21367600	3.08345100	-0.11180500
C	-2.65568500	3.13974200	-0.07461300
C	-3.32663200	1.81937800	-0.13279700
C	-2.66016700	0.65909800	-0.21490000
C	1.77512700	-1.55760400	-0.44126900
C	3.13255800	-1.40212000	-0.46662800
C	3.73848000	-0.13396600	-0.41089600
C	2.95141100	1.02244400	-0.32759800
Cl	4.17158200	-2.80503300	-0.57303300
O	5.07069200	-0.00566800	-0.43843900
Cl	-5.06753200	1.83509200	-0.08711900
O	-3.28725600	4.18723400	0.00001500
C	-1.12515500	-2.41386800	2.05404800
C	3.47529200	2.39345900	-0.27239000
C	4.74182500	2.81286300	-0.24353400
C	5.11930900	4.25812500	-0.18733400
O	-1.41403500	-3.15280900	2.96131200
O	-0.49566400	-1.25258100	2.24964500
H	-2.85201900	-5.27197300	-1.08649000
H	-2.34360600	-3.75664100	-2.98710600
H	-1.26093700	-1.58700600	-2.57118300
H	-2.25782300	-4.57144800	1.21692500
H	-0.67107500	4.01809200	-0.06983700
H	-3.19581600	-0.27918900	-0.25319900

H	1.34328500	-2.54668900	-0.48775400
H	5.48795500	-0.87625500	-0.50118000
H	2.70163200	3.15160300	-0.25102900
H	5.55667800	2.10307200	-0.25945100
H	4.24266600	4.90764900	-0.17349800
H	5.71874800	4.46734100	0.70373400
H	5.73767200	4.53045500	-1.04791400
H	-0.34130700	-1.15183200	3.20088700

DCF-BXJ_geom.4 (S_0)

C	-2.30622700	-4.34103200	-0.98188000
C	-2.02564100	-3.47735600	-2.02957200
C	-1.44832000	-2.24143200	-1.77646500
C	-1.14131000	-1.85182100	-0.47671700
C	-1.42346600	-2.72668800	0.58167000
C	-2.00750400	-3.96382900	0.31623900
C	-0.51758100	-0.50935000	-0.29341000
C	0.91629900	-0.39334100	-0.28586100
C	1.49537900	0.87715500	-0.16870900
O	0.71119700	1.97706300	-0.08368500
C	-0.64174500	1.90636300	-0.12022400
C	-1.28134000	0.62091900	-0.23177900
C	-1.33371900	3.06651900	-0.04536900
C	-2.77670200	3.09240300	-0.06512100
C	-3.41524300	1.75985400	-0.17146100
C	-2.72082900	0.61534900	-0.24785700
C	1.76330000	-1.50201200	-0.39165500
C	3.11932900	-1.32461800	-0.38396300
C	3.69042000	-0.04808900	-0.26395500
C	2.87839100	1.08826500	-0.14832600
Cl	4.18870600	-2.70102500	-0.52000500
O	5.01898900	0.13153000	-0.25233700
Cl	-5.15700200	1.73736600	-0.19362300
O	-3.43344400	4.12543600	0.00084900
C	-1.10473300	-2.33639100	1.98125600
C	3.53854500	2.39949800	-0.05711000
C	3.06819800	3.52510000	0.47796700
C	3.84397200	4.80146200	0.52805600
O	-0.55343900	-1.31196200	2.29865400
O	-1.49248000	-3.24960800	2.87791200
H	-2.75805100	-5.30570700	-1.17385600
H	-2.25666800	-3.76133600	-3.04862100
H	-1.23189000	-1.56779500	-2.59625900
H	-2.22489500	-4.62788100	1.14068300

H	-0.81352500	4.01147400	0.03289800
H	-3.23478400	-0.33273400	-0.32414000
H	1.34981600	-2.49590900	-0.48279000
H	5.47135400	-0.71601000	-0.36021100
H	4.54765800	2.40816200	-0.45485600
H	2.07822500	3.54922500	0.91583000
H	4.83091200	4.69335900	0.07558300
H	3.30990500	5.60048100	0.00532400
H	3.97136900	5.13684900	1.56148400
H	-1.24533800	-2.92426600	3.75578100

DCF-BXJ_geom.5 (S_0)

C	-2.32157000	-4.28952100	-1.05668100
C	-1.96999500	-3.42373500	-2.08130700
C	-1.37149600	-2.20822200	-1.78678500
C	-1.11156900	-1.83492500	-0.47000000
C	-1.46464100	-2.71320900	0.56538900
C	-2.06962000	-3.92980100	0.25455400
C	-0.46077700	-0.50636600	-0.27458600
C	0.97315900	-0.42446400	-0.22968300
C	1.57128800	0.83356600	-0.12033300
O	0.82288900	1.95971900	-0.06064200
C	-0.53236800	1.91664400	-0.10241000
C	-1.19739100	0.64291800	-0.22350400
C	-1.20077000	3.09003000	-0.03085500
C	-2.64282000	3.14605700	-0.06819700
C	-3.30770400	1.82751100	-0.18823500
C	-2.63652100	0.66900500	-0.26004100
C	1.81393800	-1.54521300	-0.28792500
C	3.17258100	-1.39504000	-0.22575200
C	3.75995400	-0.12202700	-0.11238200
C	2.95274200	1.01755900	-0.07639600
Cl	4.20775800	-2.79640700	-0.27636300
O	5.09375400	-0.05722500	-0.02750300
Cl	-5.04873700	1.84235900	-0.23245100
O	-3.27848600	4.19206000	-0.00624500
C	-1.25152600	-2.45057100	2.01864900
C	3.52202200	2.37313000	0.06181300
C	4.49990700	2.86884800	-0.69458400
C	5.07378000	4.23990600	-0.54568800
O	-1.61067400	-3.19887500	2.89253800
O	-0.61588500	-1.30443700	2.27451600
H	-2.79075300	-5.23955700	-1.27783600
H	-2.16169300	-3.68961700	-3.11331200

H -1.10037900 -1.53303600 -2.58888000
 H -2.33757000 -4.58662800 1.07097400
 H -0.66076700 4.02301900 0.05672200
 H -3.16911500 -0.26789600 -0.34589300
 H 1.38890000 -2.53460500 -0.37848200
 H 5.35740600 0.85994400 0.13943500
 H 3.07916000 2.99803800 0.83186600
 H 4.90639800 2.26535700 -1.50393100
 H 4.60154600 4.78605700 0.27167100
 H 6.14932700 4.19175000 -0.35593800
 H 4.94234500 4.81147100 -1.46832400
 H -0.52211600 -1.22202100 3.23534900

DCF-BXJ_geom.6 (S_0)

C -2.30193500 -4.32482200 -0.99440800
 C -2.00019900 -3.45712900 -2.03323100
 C -1.42389600 -2.22553700 -1.76222200
 C -1.13704100 -1.83769600 -0.45526500
 C -1.44022900 -2.71763300 0.59445600
 C -2.02301600 -3.95077900 0.30732500
 C -0.51310000 -0.49278800 -0.28441000
 C 0.92051000 -0.37831200 -0.27337100
 C 1.50055500 0.89332900 -0.17034000
 O 0.71671400 1.99441700 -0.09950000
 C -0.63632600 1.92398400 -0.13024800
 C -1.27656200 0.63700600 -0.22776100
 C -1.32804800 3.08439500 -0.06386600
 C -2.77137700 3.10947400 -0.07897900
 C -3.41064600 1.77565600 -0.17139800
 C -2.71644400 0.63077900 -0.23962500
 C 1.76691200 -1.48923100 -0.36271800
 C 3.12295800 -1.31270500 -0.35423400
 C 3.69476700 -0.03496800 -0.24951200
 C 2.88353100 1.10366600 -0.15020700
 Cl 4.19163700 -2.69123800 -0.47031700
 O 5.02317600 0.14370900 -0.23702300
 Cl -5.15198400 1.75342100 -0.18760800
 O -3.42792200 4.14258300 -0.01951200
 C -1.19437700 -2.44049800 2.03984700
 C 3.54482400 2.41534500 -0.07511100
 C 3.07430700 3.54897800 0.44262200
 C 3.85151900 4.82496800 0.47672900
 O -1.50104000 -3.19698800 2.92663900
 O -0.59375700 -1.27089200 2.27299800

H	-2.75340700	-5.28745600	-1.19716300
H	-2.21360200	-3.73415800	-3.05802200
H	-1.19113900	-1.54917200	-2.57529900
H	-2.25201900	-4.60882100	1.13454800
H	-0.80812900	4.03029400	0.00384400
H	-3.22986400	-0.31832000	-0.30558900
H	1.35268600	-2.48380100	-0.44197600
H	5.47537200	-0.70543900	-0.33255700
H	4.55497600	2.41732800	-0.47023900
H	2.08314900	3.58063600	0.87726900
H	4.83959300	4.70925600	0.02867100
H	3.31988000	5.61703300	-0.05887700
H	3.97637000	5.17491600	1.50562300
H	-0.47474300	-1.18099100	3.23037200

DCF-BXJ_geom.7 (S_0)

C	-2.29563500	-4.35133900	-0.93584000
C	-2.01892500	-3.50627700	-1.99963900
C	-1.44655700	-2.26351300	-1.76992100
C	-1.14071100	-1.84835100	-0.47782400
C	-1.41885500	-2.70440600	0.59681500
C	-1.99794600	-3.94869000	0.35483700
C	-0.52167200	-0.50048300	-0.32079500
C	0.91093900	-0.37841200	-0.31608600
C	1.47963000	0.89776700	-0.23162900
O	0.69709300	2.00016900	-0.17162400
C	-0.65543700	1.92032500	-0.19658100
C	-1.28915600	0.62922500	-0.28024400
C	-1.35354300	3.07816900	-0.13899400
C	-2.79633200	3.09701100	-0.15219800
C	-3.42822400	1.75965600	-0.23258300
C	-2.72846600	0.61717200	-0.29092000
C	1.77115500	-1.48189000	-0.39619900
C	3.12793500	-1.30427200	-0.38379400
C	3.68416400	-0.01865800	-0.28925200
C	2.85986200	1.10659200	-0.22331700
Cl	4.19212700	-2.68176000	-0.47043300
O	5.02051000	0.08379600	-0.26388100
Cl	-5.17019600	1.72759600	-0.24776500
O	-3.45834200	4.12783800	-0.10086500
C	-1.10147200	-2.28651100	1.98867000
C	3.48308200	2.44647200	-0.20248900
C	3.20816300	3.41233100	0.66841100
C	3.84252700	4.76317200	0.66381700

O	-0.55504400	-1.25367700	2.28666400
O	-1.48449200	-3.18462100	2.90249100
H	-2.74362100	-5.32125500	-1.10953200
H	-2.24911100	-3.81022300	-3.01311200
H	-1.23315200	-1.60442700	-2.60225400
H	-2.21234300	-4.59806700	1.19166500
H	-0.83614500	4.02609400	-0.08014700
H	-3.23846900	-0.33442700	-0.34751100
H	1.36327400	-2.48015500	-0.46480000
H	5.27944400	0.99265100	-0.06389000
H	4.22265100	2.63627700	-0.97953700
H	2.46904600	3.22796500	1.44291400
H	4.57883000	4.86141000	-0.13496000
H	3.08507800	5.54153600	0.53554400
H	4.33522400	4.96048200	1.61970500
H	-1.23858600	-2.84160000	3.77395000

DCF-BXJ_geom.8 (S_0)

C	-2.29197700	-4.33522700	-0.94641800
C	-1.99643500	-3.48439900	-2.00087000
C	-1.42510000	-2.24573700	-1.75260700
C	-1.13723200	-1.83376800	-0.45325500
C	-1.43408700	-2.69668800	0.61223700
C	-2.01182400	-3.93731000	0.34792800
C	-0.51775600	-0.48379900	-0.30859400
C	0.91462000	-0.36336700	-0.30191500
C	1.48456300	0.91353800	-0.23273400
O	0.70259100	2.01690500	-0.18603400
C	-0.65004100	1.93773600	-0.20358600
C	-1.28469300	0.64549500	-0.27236200
C	-1.34759200	3.09586500	-0.15380100
C	-2.79070400	3.11432300	-0.16089300
C	-3.42361700	1.77608000	-0.22651200
C	-2.72437400	0.63320500	-0.27731900
C	1.77403400	-1.46883700	-0.36644500
C	3.13083800	-1.29208600	-0.35538800
C	3.68806800	-0.00556200	-0.27811300
C	2.86479500	1.12135800	-0.22698100
Cl	4.19407500	-2.67115100	-0.42255200
O	5.02417700	0.09585200	-0.25365800
Cl	-5.16515100	1.74482200	-0.23387100
O	-3.45231100	4.14524600	-0.11549500
C	-1.18658800	-2.39332500	2.05200100
C	3.48934200	2.46073600	-0.22398800

C	3.21532800	3.43880300	0.63344900
C	3.85137400	4.78863300	0.61026300
O	-1.48522600	-3.13687300	2.95239500
O	-0.59451900	-1.21528100	2.26374300
H	-2.73953700	-5.30326300	-1.13134400
H	-2.21074900	-3.78020000	-3.02022000
H	-1.19700200	-1.58265200	-2.57786300
H	-2.23593700	-4.58185800	1.18703400
H	-0.83019500	4.04440400	-0.10622000
H	-3.23406300	-0.31911200	-0.32291100
H	1.36524200	-2.46750200	-0.42211300
H	5.28431300	1.00761300	-0.06891200
H	4.22913900	2.63916300	-1.00347800
H	2.47584700	3.26612500	1.41029400
H	4.58764500	4.87492400	-0.18990700
H	3.09489000	5.56610800	0.47142900
H	4.34450000	4.99837800	1.56327500
H	-0.47381100	-1.10846400	3.21915400

DCF-BXJ (S_1)

C	-2.75509500	-4.04949700	-1.12272300
C	-1.94444600	-3.45937900	-2.08102100
C	-1.22790600	-2.31313200	-1.77266700
C	-1.30522900	-1.72756600	-0.50874900
C	-2.12026300	-2.33773400	0.46105400
C	-2.83545700	-3.49154700	0.14127900
C	-0.53290300	-0.48306000	-0.28147500
C	0.86228700	-0.51242400	-0.16580400
C	1.60337900	0.70879700	-0.04725800
O	0.95526300	1.89028500	-0.05963700
C	-0.40386000	1.95542600	-0.16506500
C	-1.18724500	0.79673600	-0.27805000
C	-0.93946700	3.21620400	-0.16120000
C	-2.37488700	3.43917500	-0.27728200
C	-3.15703100	2.22033900	-0.39867800
C	-2.59059600	0.98102500	-0.39741900
C	1.61630900	-1.71233200	-0.13026700
C	2.97254600	-1.66300500	-0.00634700
C	3.68585600	-0.44485400	0.09901400
C	2.99263900	0.77432400	0.08020100
Cl	3.89274800	-3.14434200	0.04532700
O	5.01629900	-0.43286200	0.23256100
Cl	-4.88309400	2.39636100	-0.54887400
O	-2.85173200	4.57808000	-0.27133600

C	-2.19600600	-1.78557100	1.83979200
C	3.62952700	2.09216600	0.22109500
C	4.91082100	2.41533500	0.04446900
C	5.43642800	3.80434400	0.21155500
O	-1.64847500	-0.77885500	2.21625900
O	-2.94879300	-2.53229400	2.65918800
H	-3.31965000	-4.94304400	-1.35657500
H	-1.87090900	-3.88727100	-3.07322900
H	-0.60365100	-1.84905600	-2.52635600
H	-3.45413200	-3.95083400	0.89903100
H	-0.29943000	4.08368800	-0.07224100
H	-3.22146900	0.10818000	-0.49556500
H	1.11348400	-2.66531900	-0.19696900
H	5.35782800	-1.33808500	0.25809600
H	2.94173200	2.88736000	0.48468800
H	5.63087500	1.65904400	-0.23833000
H	4.64873200	4.50543200	0.49180700
H	6.21494500	3.83416800	0.97972400
H	5.90025300	4.15683000	-0.71446700
H	-2.94641900	-2.10425500	3.52753500

[DCF-BXJ-H] ⁻ (S₀)

C	-2.70215900	-4.04469500	-1.14993300
C	-2.35592800	-3.14231900	-2.14743900
C	-1.69170600	-1.97052100	-1.81723800
C	-1.36444500	-1.69296200	-0.48972700
C	-1.70826700	-2.59853200	0.51532700
C	-2.37939300	-3.76607500	0.16848700
C	-0.64091800	-0.42008300	-0.20929800
C	0.80093700	-0.40759000	-0.20109200
C	1.47729100	0.80847300	-0.08423200
O	0.78511900	1.97068500	0.00614000
C	-0.57013900	2.00420200	-0.04005800
C	-1.30583600	0.78046400	-0.16922700
C	-1.16770900	3.22011200	0.03171700
C	-2.60064400	3.36624600	-0.00894900
C	-3.33793800	2.09243400	-0.12976600
C	-2.73627900	0.89375500	-0.20298600
C	1.56285800	-1.57654600	-0.29066600
C	2.92699000	-1.49967100	-0.26581600
C	3.60187800	-0.27205900	-0.14752300
C	2.87847500	0.92304100	-0.05542200
Cl	3.88928900	-2.95846800	-0.37931900
O	4.94181000	-0.22131600	-0.12408900

Cl	-5.08063000	2.20530800	-0.17284400
O	-3.17300000	4.45305200	0.05033100
C	-1.36391900	-2.31384800	1.97732800
C	3.47686000	2.25919400	0.06481100
C	4.76391700	2.60849200	0.11358900
C	5.21810900	4.02772700	0.23673800
O	-0.73504400	-1.24899000	2.17602000
O	-1.73071200	-3.15351200	2.81938000
H	-3.22439100	-4.96013100	-1.40173400
H	-2.60376400	-3.34661300	-3.18201400
H	-1.42317600	-1.26397500	-2.59405900
H	-2.64034900	-4.44494500	0.96995200
H	-0.57109000	4.11809600	0.12091000
H	-3.32288000	-0.01065700	-0.28499700
H	1.07243800	-2.53522100	-0.37494100
H	5.30709900	-1.11423100	-0.19264200
H	2.74537300	3.05661200	0.11937900
H	5.53955100	1.85738700	0.06465200
H	4.37697700	4.72163400	0.27896700
H	5.82382300	4.16454400	1.13765600
H	5.85345200	4.30662300	-0.60935500

[DCF-BXJ-H] ⁻ (S₁)

C	-2.71767400	-4.15500500	-0.90419700
C	-1.95752400	-3.63251000	-1.94486200
C	-1.24310700	-2.45998800	-1.76454000
C	-1.27819300	-1.77248400	-0.54603500
C	-2.03331900	-2.31889000	0.50413900
C	-2.74240100	-3.50038400	0.31500900
C	-0.54977600	-0.50610200	-0.38013600
C	0.86559900	-0.43993100	-0.46271000
C	1.53126500	0.78358900	-0.21054900
O	0.82525100	1.89661500	0.12717900
C	-0.54587300	1.90308600	0.11070300
C	-1.26796400	0.71113000	-0.13361600
C	-1.14845400	3.10629600	0.32689900
C	-2.58706900	3.26552000	0.31534300
C	-3.29876600	2.03776400	0.01379500
C	-2.68033000	0.84389300	-0.20134300
C	1.68553000	-1.55816200	-0.71588800
C	3.04754300	-1.42303100	-0.76215400
C	3.68905000	-0.19742700	-0.54603100
C	2.92086500	0.94136400	-0.25087200
Cl	4.04642600	-2.82619500	-1.09921000

O	5.02954000	-0.08311800	-0.61204800
Cl	-5.04879500	2.13083100	-0.06580400
O	-3.13970500	4.35539500	0.53280700
C	-2.03907900	-1.70900800	1.87867800
C	3.48660600	2.27755600	-0.00845100
C	4.74621100	2.61359100	0.27166400
C	5.18599300	4.02410200	0.50352800
O	-1.57430300	-0.52685700	2.00927500
O	-2.46619800	-2.34447400	2.84392500
H	-3.27913900	-5.07064300	-1.04308300
H	-1.92839300	-4.13610800	-2.90374600
H	-0.66668200	-2.04918100	-2.58478400
H	-3.30028100	-3.89925600	1.15271300
H	-0.54751200	3.98821700	0.50854600
H	-3.27422600	-0.03219600	-0.42220500
H	1.24119300	-2.52932200	-0.87358100
H	5.41693900	-0.93736900	-0.84529700
H	2.75424000	3.07542000	-0.05291800
H	5.51085700	1.85201400	0.34569000
H	4.35589700	4.72713200	0.41551300
H	5.62771500	4.13534000	1.49840500
H	5.95996900	4.31390900	-0.21373200

[DCF-BXJ-2H] $^{2-}$ (S_0)

C	-2.67568300	-4.03985100	-1.18972500
C	-2.19722800	-3.18966400	-2.17817900
C	-1.52777400	-2.02994400	-1.81999800
C	-1.32636000	-1.70406200	-0.47732800
C	-1.80669200	-2.55635100	0.52072600
C	-2.47761800	-3.71671100	0.14240900
C	-0.59792100	-0.42904600	-0.20425300
C	0.80538700	-0.40489500	-0.20965600
C	1.49605500	0.82686700	-0.09255700
O	0.77865600	1.98113000	0.00606100
C	-0.57999600	1.99477300	-0.01272800
C	-1.29870600	0.77742000	-0.13302700
C	-1.19297200	3.21214600	0.08002700
C	-2.62160900	3.34966400	0.07053800
C	-3.33388000	2.07433300	-0.04512600
C	-2.71737500	0.87497900	-0.13952300
C	1.59609200	-1.57943500	-0.29783400
C	2.94348800	-1.49940200	-0.28222000
C	3.69125500	-0.24914500	-0.17793100
C	2.87720200	0.94944100	-0.07866100

Cl	3.89525400	-2.97194300	-0.39331400
O	4.93248600	-0.24202200	-0.17761700
Cl	-5.08823500	2.15308200	-0.05697700
O	-3.20679500	4.43958300	0.15056000
C	-1.61698700	-2.25635700	2.01262500
C	3.47350900	2.28356500	0.03252200
C	4.76558400	2.62316000	0.05940700
C	5.23882700	4.03949800	0.17448300
O	-0.98250700	-1.21513100	2.28279100
O	-2.11192600	-3.07703800	2.81149200
H	-3.20024300	-4.94923700	-1.45880600
H	-2.34347200	-3.42609600	-3.22539800
H	-1.15376500	-1.36399800	-2.58928600
H	-2.83839300	-4.35597200	0.93757000
H	-0.59859100	4.11291800	0.16348100
H	-3.30043300	-0.03259300	-0.21821300
H	1.10374300	-2.53891600	-0.37419600
H	2.74972100	3.08974000	0.09973300
H	5.51483000	1.84594900	-0.00450600
H	4.40393500	4.74154300	0.23181600
H	5.86094700	4.17837600	1.06477700
H	5.86025700	4.32026000	-0.68226700

[DCF-BXJ-2H] ²⁻ (S₁)

C	-2.75975100	-4.02733600	-1.17166200
C	-2.52171000	-3.05668800	-2.13611600
C	-1.83551300	-1.90488400	-1.78750800
C	-1.36185000	-1.69463100	-0.48630700
C	-1.61288900	-2.67291400	0.48991000
C	-2.31421400	-3.82148000	0.12304700
C	-0.62999000	-0.42646200	-0.23982500
C	0.79195100	-0.38939200	-0.15757800
C	1.47912200	0.83773000	-0.07492400
O	0.77782200	2.01931000	-0.05830600
C	-0.58997400	2.03035300	-0.10701200
C	-1.31827600	0.80790300	-0.20249300
C	-1.19339300	3.25201000	-0.06427400
C	-2.62434400	3.41600000	-0.10767700
C	-3.34304400	2.15514900	-0.18841800
C	-2.73344400	0.93444000	-0.22888200
C	1.59151200	-1.57154200	-0.17115200
C	2.94203700	-1.50510700	-0.12689700
C	3.68893400	-0.25779100	-0.04730600
C	2.86418400	0.95826400	-0.01800500

Cl	3.88238600	-2.98294400	-0.15120800
O	4.92760500	-0.24078800	-0.00926700
Cl	-5.09375900	2.23935100	-0.22783500
O	-3.18390200	4.52891400	-0.07394300
C	-1.18166600	-2.53842200	1.95794000
C	3.45448200	2.28541500	0.06322900
C	4.75042900	2.62252100	0.13240400
C	5.22231800	4.03770200	0.21350200
O	-0.34911800	-1.64676300	2.22678300
O	-1.70155300	-3.34550200	2.75850100
H	-3.29499100	-4.93463700	-1.42731200
H	-2.86632200	-3.19498700	-3.15439800
H	-1.64892500	-1.14413100	-2.53742400
H	-2.50776500	-4.54703200	0.90207500
H	-0.58896300	4.14796400	0.00491600
H	-3.33327100	0.03620200	-0.28095000
H	1.09336100	-2.52868600	-0.21981100
H	2.73184700	3.09401300	0.06902300
H	5.49930800	1.84263200	0.13066500
H	4.39095300	4.74531600	0.20799200
H	5.80852200	4.20326200	1.12335000
H	5.88392200	4.27828700	-0.62515300

[DCF-BXJ-2H] $^{2-}$ _TSf (Transition state of Twist Forward in S₁)

C	-2.83187600	-4.02359700	-0.95489000
C	-2.69544200	-3.06948000	-1.95480800
C	-1.97064900	-1.91638500	-1.70102300
C	-1.36523100	-1.68608800	-0.45952500
C	-1.51461400	-2.64634700	0.55472300
C	-2.24859900	-3.80014600	0.28103500
C	-0.59270600	-0.42665300	-0.31647700
C	0.83000300	-0.42042000	-0.36269500
C	1.54756000	0.80849300	-0.34749000
O	0.87423300	2.00347600	-0.29871000
C	-0.49302200	2.03429600	-0.23908800
C	-1.24928200	0.82328900	-0.24740200
C	-1.07110000	3.26564800	-0.17389600
C	-2.50030900	3.45450100	-0.10322000
C	-3.24652100	2.20577200	-0.09361300
C	-2.66114200	0.97529900	-0.15634700
C	1.60904500	-1.60547600	-0.43624700
C	2.96731300	-1.55617400	-0.50219600
C	3.72867600	-0.31906000	-0.49108700
C	2.91479500	0.88991400	-0.39088700

Cl	3.88014400	-3.04709200	-0.60187600
O	4.96747800	-0.28420800	-0.56657800
Cl	-4.99082400	2.32163500	0.01471700
O	-3.03324600	4.57769400	-0.05019100
C	-0.93814300	-2.48404300	1.97111000
C	3.60464000	2.20160300	-0.39566700
C	4.09124700	2.79620700	0.68460500
C	4.80096700	4.11374900	0.69095700
O	-0.20912200	-1.49147500	2.17766400
O	-1.25500200	-3.36797700	2.79642300
H	-3.39325700	-4.93269700	-1.13776400
H	-3.14622400	-3.22266600	-2.92852200
H	-1.85702400	-1.17182700	-2.48122700
H	-2.35053500	-4.51574800	1.08614900
H	-0.44789900	4.15116100	-0.17311900
H	-3.27632600	0.08635800	-0.13575500
H	1.10004000	-2.55854400	-0.44083200
H	3.71739400	2.69122200	-1.36291200
H	3.97685400	2.30331500	1.64779300
H	4.86671000	4.53635600	-0.31329600
H	4.28591600	4.83379700	1.33339400
H	5.81565000	4.00955000	1.08625100

[DCF-BXJ-2H] $^{2-}$ _TSb (Transition state of Twist Backward in S₁)

C	-2.83751600	-4.02872100	-0.95556300
C	-2.70268200	-3.07439700	-1.95546200
C	-1.97840300	-1.92084200	-1.70210100
C	-1.37217700	-1.69042900	-0.46108900
C	-1.51993700	-2.65075900	0.55311000
C	-2.25325600	-3.80511600	0.27987600
C	-0.60142800	-0.42942600	-0.31946600
C	0.82050000	-0.41862500	-0.37988400
C	1.53359000	0.81333300	-0.38437600
O	0.85727300	2.00553400	-0.31502900
C	-0.50885100	2.03136400	-0.23165300
C	-1.26115800	0.81791500	-0.23641400
C	-1.09012900	3.26016100	-0.14939300
C	-2.51883900	3.44329800	-0.05540400
C	-3.26069400	2.19197800	-0.04414100
C	-2.67206200	0.96406000	-0.12455600
C	1.60266100	-1.60180800	-0.45068300
C	2.96068000	-1.54908400	-0.52095800
C	3.71752900	-0.30941100	-0.51946600
C	2.89880300	0.89879300	-0.46362600

Cl	3.87854500	-3.03815700	-0.59799300
O	4.95777700	-0.27019800	-0.55987300
Cl	-5.00348900	2.30086100	0.09067400
O	-3.05471800	4.56418200	0.01396100
C	-0.94179300	-2.48809500	1.96883400
C	3.59193700	2.20848200	-0.44193800
C	3.96041900	2.88051600	-1.52343100
C	4.67468800	4.19567500	-1.51184500
O	-0.21414500	-1.49443800	2.17456900
O	-1.25619100	-3.37298000	2.79409500
H	-3.39846400	-4.93816500	-1.13808100
H	-3.15442600	-3.22763600	-2.92872200
H	-1.86622300	-1.17585500	-2.48211200
H	-2.35373900	-4.52103600	1.08488600
H	-0.47024600	4.14799700	-0.15282300
H	-3.28358000	0.07263900	-0.10135900
H	1.09640900	-2.55634100	-0.44452900
H	3.81673100	2.62518900	0.53977600
H	3.73713200	2.45927300	-2.50148100
H	4.85385300	4.54284500	-0.49264100
H	5.63883000	4.12209700	-2.02340800
H	4.09705600	4.96095400	-2.03834700

DCF_geom.1 (S_0)

C	0.07214100	1.60737200	-0.54799100
C	0.08083400	0.14246500	-0.26907600
C	0.18023100	2.00367500	-1.87723500
C	-0.04670500	2.58682400	0.44773200
C	-1.16507800	-0.57170800	-0.20580900
C	0.17197100	3.34797800	-2.22018000
C	-0.04975500	3.93428700	0.09219500
C	1.25159300	-0.55547800	-0.17095300
C	0.05685000	4.31601800	-1.23427100
C	-0.16431100	2.19096100	1.87670700
C	-1.13695600	-1.95877500	-0.01794100
C	1.22540600	-1.98393300	0.02893900
C	2.34833100	-2.72776100	0.15075500
C	2.55087400	0.06199500	-0.22898700
C	-2.41953000	0.04350100	-0.31645100
C	-2.29124400	-2.71625000	0.05598800
C	3.66362400	-2.13541000	0.09208800
C	3.66904900	-0.66778400	-0.10788700
C	-3.56786100	-0.69949900	-0.24185900
C	-3.52323800	-2.09420100	-0.05512800

Cl	5.23250200	0.09672900	-0.18019100
Cl	-5.13125400	0.06850500	-0.37645900
H	2.60927400	1.13199700	-0.37194900
H	-2.48445200	1.11249000	-0.46275900
H	-0.29365000	2.89802200	3.60809400
H	0.05165300	5.36620200	-1.49635700
H	-0.13663600	4.68058900	0.86898100
H	0.25766000	3.63523700	-3.26066400
H	0.27201800	1.24940500	-2.64884700
O	0.03336800	-2.62834200	0.09915100
O	-0.21717500	1.05231900	2.27022300
O	-0.21104900	3.23914100	2.70563500
O	4.69961100	-2.78177100	0.19808300
O	-4.62352900	-2.85186300	0.01930100
H	2.28188100	-3.79727400	0.29751400
H	-2.23593000	-3.78630800	0.19945200
H	-5.41505000	-2.30477400	-0.07458500

DCF_geom.2 (S_0)

C	0.07240600	1.60245200	-0.54514400
C	0.08649800	0.13764800	-0.26599400
C	0.17400400	1.99916200	-1.87475400
C	-0.04619500	2.58139600	0.45106800
C	-1.15654000	-0.58046600	-0.20175500
C	0.15936200	3.34344900	-2.21757600
C	-0.05549800	3.92885900	0.09566600
C	1.26003000	-0.55655800	-0.16919600
C	0.04446800	4.31103000	-1.23118500
C	-0.15773500	2.18494500	1.88033400
C	-1.12274300	-1.96483000	-0.01235200
C	1.23870400	-1.98451700	0.03240900
C	2.36399800	-2.72544600	0.15182000
C	2.55715500	0.06440400	-0.23142000
C	-2.41542500	0.02873300	-0.31571300
C	-2.27724100	-2.72594000	0.06077500
C	3.67734400	-2.12965000	0.08808400
C	3.67777200	-0.66236900	-0.11321400
C	-3.56372200	-0.71383100	-0.24516300
C	-3.51137400	-2.10877000	-0.05677700
Cl	5.23882500	0.10663900	-0.19169300
Cl	-5.11716500	0.06102700	-0.39146300
H	2.61225200	1.13439700	-0.37581800
H	-2.48301700	1.09730400	-0.46393300
H	-0.28227400	2.89126400	3.61237000

H	0.03413700	5.36119000	-1.49321500
H	-0.14227200	4.67478200	0.87283100
H	0.23969500	3.63107000	-3.25838700
H	0.26539400	1.24527500	-2.64679200
O	0.04806700	-2.63184000	0.10687900
O	-0.20689300	1.04609700	2.27377700
O	-0.20337900	3.23280000	2.70974000
O	4.71566800	-2.77309700	0.19087900
O	-4.67087100	-2.77591200	-0.00216800
H	2.30087800	-3.79499400	0.29979800
H	-2.19993800	-3.79575800	0.20733900
H	-4.51596800	-3.72046800	0.11490100

DCF_geom.3 (S_0)

C	0.06937000	1.59243300	-0.52425200
C	0.07803300	0.12240300	-0.26863000
C	0.15022100	1.98831300	-1.85755500
C	-0.01783200	2.57736500	0.47077700
C	-1.16792300	-0.59162300	-0.21508800
C	0.14747300	3.33003500	-2.20711800
C	-0.01456900	3.92227700	0.10494800
C	1.24832600	-0.57505300	-0.17229800
C	0.06516100	4.30273800	-1.22210600
C	-0.10876900	2.30643100	1.93516900
C	-1.14023900	-1.98175100	-0.04851800
C	1.22217500	-2.00707900	0.00565200
C	2.34481000	-2.75152300	0.12232300
C	2.54754900	0.04455500	-0.21595100
C	-2.42237100	0.02595400	-0.31527500
C	-2.29463800	-2.73979800	0.01366100
C	3.65991400	-2.15671500	0.07972700
C	3.66551000	-0.68595600	-0.09998600
C	-3.57082100	-0.71782100	-0.25270800
C	-3.52646200	-2.11546800	-0.08777300
Cl	5.22859200	0.07957000	-0.15480100
Cl	-5.13378500	0.05242600	-0.37639300
H	2.60527400	1.11644800	-0.34400000
H	-2.48649100	1.09715000	-0.44449600
H	-0.23967500	0.93141400	3.20615900
H	0.06447400	5.35242300	-1.48624000
H	-0.07603400	4.66220700	0.89139500
H	0.21215300	3.61120700	-3.25078300
H	0.21794800	1.23083400	-2.62855200
O	0.03005000	-2.65276000	0.05937600

O	-0.12335200	3.17091300	2.77480500
O	-0.18116300	1.00885900	2.24210400
O	4.69563300	-2.80319700	0.18311400
O	-4.62663600	-2.87381000	-0.02451200
H	2.27893800	-3.82316300	0.25278800
H	-2.23985900	-3.81193200	0.14085700
H	-5.41838800	-2.32532200	-0.10810500

DCF_geom.4 (S_0)

C	0.06409300	1.58707100	-0.52336500
C	0.08301700	0.11775900	-0.26419100
C	0.13344900	1.98017500	-1.85812100
C	-0.02205600	2.57382000	0.46987200
C	-1.15768700	-0.60411200	-0.20736300
C	0.12031200	3.32101700	-2.21079500
C	-0.02894200	3.91787200	0.10093700
C	1.25840100	-0.57197300	-0.16882400
C	0.03924400	4.29560700	-1.22752900
C	-0.10246800	2.30568900	1.93533800
C	-1.11969100	-1.99133600	-0.03816600
C	1.24190100	-2.00330800	0.01305400
C	2.36940300	-2.74090200	0.12825700
C	2.55340200	0.05533000	-0.21858200
C	-2.41865100	0.00348200	-0.30950900
C	-2.27176400	-2.75680400	0.02410800
C	3.68057900	-2.13830700	0.07924400
C	3.67625300	-0.66823400	-0.10464200
C	-3.56455000	-0.74348700	-0.24930400
C	-3.50777300	-2.14127900	-0.08323600
Cl	5.23437900	0.10688100	-0.16790800
Cl	-5.12035200	0.02868600	-0.38137000
H	2.60426400	1.12716000	-0.35010600
H	-2.48907100	1.07406200	-0.44065900
H	-0.22356100	0.93306100	3.20984500
H	0.03038300	5.34462600	-1.49415200
H	-0.08936000	4.65928800	0.88607000
H	0.17578500	3.60005600	-3.25556300
H	0.20017100	1.22128100	-2.62782300
O	0.05332600	-2.65586600	0.07187300
O	-0.11209200	3.17175400	2.77341400
O	-0.17179100	1.00862500	2.24526000
O	4.72081900	-2.77818400	0.18039400
O	-4.66511000	-2.81226200	-0.03800200
H	2.31045000	-3.81259500	0.26158400

H	-2.19144400	-3.82844700	0.15481700
H	-4.50774200	-3.75833000	0.06255800

DCF (S_1)

C	0.02760900	1.60634800	-0.52659400
C	-0.06438700	0.15251900	-0.25661900
C	-0.31122400	2.04778500	-1.80604400
C	0.45168700	2.55836300	0.41756900
C	-1.30430100	-0.48549500	-0.14924400
C	-0.21861100	3.38651700	-2.15461800
C	0.53918200	3.90273400	0.05734600
C	1.11978300	-0.66559800	-0.20711700
C	0.21263000	4.31805900	-1.22190900
C	0.76724400	2.14982000	1.81202600
C	-1.36471300	-1.90876600	0.01693300
C	0.98596700	-2.05474100	-0.04356300
C	2.06020300	-2.90212200	0.00710500
C	2.44157500	-0.16061200	-0.32870500
C	-2.55305400	0.19437600	-0.16465800
C	-2.55436700	-2.59168200	0.13299700
C	3.42812300	-2.41503900	-0.10921000
C	3.53256800	-0.97551300	-0.28386400
C	-3.72729600	-0.49222500	-0.05116800
C	-3.75684600	-1.90134400	0.09744100
Cl	5.13334200	-0.30727000	-0.43553500
Cl	-5.24915800	0.35631500	-0.07657300
H	2.57895700	0.90327700	-0.46562400
H	-2.56999900	1.26966200	-0.26461400
H	1.25997600	2.83665900	3.48514700
H	0.28997300	5.36470300	-1.48717700
H	0.86247900	4.62258800	0.79572500
H	-0.47987200	3.69864400	-3.15827500
H	-0.63772100	1.32163000	-2.54037400
O	-0.24035700	-2.64771300	0.06862100
O	0.75725100	1.01558900	2.22258800
O	1.06907600	3.18805100	2.60345900
O	4.39252300	-3.18454900	-0.06197800
O	-4.89187000	-2.59570100	0.21117700
H	1.91125600	-3.96596000	0.13429900
H	-2.55317100	-3.66631400	0.25286000
H	-5.65661600	-2.00436600	0.17428600

[DCF-H]⁻ (S_0)

C	0.07715100	1.62235000	-0.52659900
---	------------	------------	-------------

C	0.08241600	0.16788300	-0.20052500
C	0.21064400	1.98346700	-1.86767700
C	-0.06762700	2.61036700	0.44853200
C	-1.16114700	-0.55845200	-0.16295700
C	0.19817000	3.31914700	-2.24049900
C	-0.07316200	3.94529900	0.05896700
C	1.25391800	-0.54833000	-0.14505600
C	0.05533700	4.30538300	-1.27283500
C	-0.20859000	2.23953000	1.92468700
C	-1.13293200	-1.94784000	-0.01052500
C	1.22724800	-1.97361700	0.02709100
C	2.35211000	-2.72552200	0.12102000
C	2.55129100	0.06297000	-0.20263400
C	-2.41489600	0.05778400	-0.25852200
C	-2.28867400	-2.70838400	0.03998200
C	3.66753900	-2.13952600	0.06172500
C	3.67093700	-0.67302400	-0.10873200
C	-3.56355200	-0.68694400	-0.20969900
C	-3.52016200	-2.08529500	-0.05827500
Cl	5.23732100	0.09671100	-0.18197400
Cl	-5.12818600	0.08565400	-0.33113200
H	2.60910200	1.13625900	-0.31877300
H	-2.47363700	1.13117600	-0.36881900
H	0.04777000	5.35065100	-1.55840600
H	-0.17938600	4.68847800	0.83862600
H	0.30223500	3.58673200	-3.28505100
H	0.32417300	1.21271700	-2.62124300
O	0.03601400	-2.62340600	0.09253800
O	-0.22873900	1.01003300	2.16295100
O	-0.29190700	3.17764700	2.73796600
O	4.70533200	-2.79386100	0.14389100
O	-4.62280700	-2.84577000	-0.00701500
H	2.28109900	-3.79803500	0.24348200
H	-2.23273600	-3.78185100	0.15580800
H	-5.41255000	-2.29382200	-0.08315400

[DCF-H]⁻ (S₁)

C	-0.03149400	1.63637100	-0.59866800
C	-0.03382800	0.18965400	-0.33787300
C	-0.42735400	2.13413500	-1.84530100
C	0.37146900	2.55278900	0.38593300
C	-1.22978900	-0.57174800	-0.34949500
C	-0.39248500	3.49161300	-2.11691900
C	0.39764400	3.91475000	0.10516900

C	1.19628300	-0.50070100	-0.06546900
C	0.02854900	4.38903900	-1.14164300
C	0.70061000	2.11759900	1.78711000
C	-1.18571400	-1.94642500	-0.00786400
C	1.16870200	-1.87865200	0.26182300
C	2.29461800	-2.60842700	0.50060800
C	2.48666400	0.08040200	-0.18578400
C	-2.51148200	-0.03979000	-0.61136500
C	-2.31429000	-2.73760000	0.02754100
C	3.62125900	-2.03401600	0.43161100
C	3.62102300	-0.63376300	0.05265500
C	-3.63190700	-0.83268700	-0.57772500
C	-3.55964400	-2.19611100	-0.26360400
Cl	5.18306400	0.15120800	-0.09255900
Cl	-5.20692600	-0.14269700	-0.91868400
H	2.56238400	1.12145700	-0.46762700
H	-2.61677400	1.01024200	-0.84150600
H	0.05938100	5.45094000	-1.35214900
H	0.69974200	4.59200900	0.89391600
H	-0.68630000	3.85025300	-3.09618500
H	-0.73953400	1.43874200	-2.61524700
O	-0.02206000	-2.55762500	0.33619000
O	0.88316500	0.87148500	1.99770800
O	0.77263000	2.94299600	2.69896600
O	4.64742000	-2.69192100	0.66496300
O	-4.63456600	-3.00559500	-0.21968500
H	2.21342300	-3.66019100	0.74376700
H	-2.23244000	-3.78287600	0.29329100
H	-5.43244700	-2.50486800	-0.43364600

[DCF-2H]²⁻ (S₀)

C	0.04823800	1.61354500	-0.52025100
C	0.04500100	0.15077400	-0.22156500
C	0.09268900	1.97874800	-1.86692400
C	0.00666600	2.60445800	0.46454200
C	-1.15954200	-0.56265300	-0.20560600
C	0.09568100	3.31334700	-2.24200000
C	0.00972800	3.93981900	0.06949800
C	1.25103600	-0.55500200	-0.13534600
C	0.05337600	4.30136000	-1.26690700
C	-0.04140400	2.26792100	1.95992500
C	-1.14116900	-1.97226800	-0.03684000
C	1.23160800	-1.96496600	0.03083700
C	2.36866800	-2.71414500	0.14205900

C	2.53195600	0.06005700	-0.17157900
C	-2.44001600	0.04431800	-0.31622100
C	-2.27824200	-2.72819100	0.01130900
C	3.67824300	-2.12758000	0.10467300
C	3.66319300	-0.67320000	-0.06334300
C	-3.57120000	-0.69548200	-0.27004800
C	-3.58712700	-2.14951400	-0.09997300
Cl	5.22544400	0.12772900	-0.12179900
Cl	-5.13245600	0.09607700	-0.41673300
H	2.58931400	1.13394300	-0.28719000
H	-2.49737000	1.11768400	-0.43656700
H	0.05484400	5.34759200	-1.54971000
H	-0.02399000	4.68376000	0.85485500
H	0.13044300	3.57800900	-3.29210100
H	0.12470700	1.20529200	-2.62583000
O	0.04486000	-2.63001600	0.08159300
O	-0.03737300	1.05217300	2.24593000
O	-0.07954300	3.23644400	2.74555400
O	4.72722000	-2.78177000	0.20323700
O	-4.63621400	-2.80968200	-0.05832100
H	2.29671300	-3.78737700	0.26352100
H	-2.20704400	-3.80079700	0.13859300

[DCF-2H]²⁻ (S₁)

C	-0.01549900	1.62534000	-0.53652700
C	0.00170300	0.16818800	-0.25808200
C	-0.27457900	2.01609500	-1.85564300
C	0.24069200	2.61513100	0.42564100
C	-1.19422300	-0.59072100	-0.27704700
C	-0.28186700	3.35015600	-2.23004800
C	0.24359400	3.95142000	0.02772700
C	1.21850800	-0.53751800	-0.05934600
C	-0.01694400	4.32754400	-1.27965200
C	0.48163200	2.30721400	1.91313100
C	-1.15225700	-2.01229900	-0.15255200
C	1.21450800	-1.95867300	0.06105700
C	2.35132300	-2.68688000	0.23715300
C	2.49154600	0.08998100	0.01917400
C	-2.49104100	-0.01620400	-0.38730700
C	-2.27072400	-2.78790000	-0.17068800
C	3.66054800	-2.08020200	0.31573000
C	3.63650300	-0.63028800	0.19116800
C	-3.61671500	-0.78603800	-0.41024300
C	-3.59913800	-2.23759300	-0.31149200

Cl	5.17354000	0.20019900	0.27647400
Cl	-5.18229300	-0.01804400	-0.55569700
H	2.54110900	1.16683200	-0.06140500
H	-2.57412000	1.05968700	-0.45383600
H	-0.01387000	5.37533000	-1.55748800
H	0.45542400	4.68901600	0.79075300
H	-0.48501500	3.62274600	-3.25921000
H	-0.46505900	1.24939300	-2.59855300
O	0.04336400	-2.66668700	-0.01358900
O	0.23305400	1.14610000	2.29740200
O	0.89287400	3.26130900	2.60876100
O	4.70099800	-2.74147200	0.47266200
O	-4.62249200	-2.94291200	-0.33832200
H	2.29299100	-3.76495900	0.31834300
H	-2.18113700	-3.86288300	-0.07717600

..