Supporting Information

Electron Switch in the Double-Cage Fluorinated Fullerene Anions, $e^-@C_{20}F_{18}(XH)_2C_{20}F_{18}$ (X = N, B): New Candidates for Molecular Quantum-Dot Cellular Automata

Xingyong Wang and Jing Ma*

School of Chemistry and Chemical Engineering, Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry of MOE, Nanjing University, Nanjing 210093, P. R. China

Contents:

- **Figure S9.** The SOMO, spin density, dipole moment (μ_x) and intercage charge difference (Δq) for **2** under the inducement of the driver composed of a single point charge in the axial driver model
- **Figure S10.** The SOMO, spin density, dipole moment (μ_x) and intercage charge difference (Δq) for **1** under the Coulomb perturbation of a neighboring molecule
- **Figure S11.** The SOMO, spin density, dipole moment (μ_x) and intercage charge difference (Δq) for **2** under the Coulomb perturbation of a neighboring molecule
- **Figure S12.** a) The energy profile for the change from **1-T** to **1-F** under the electric dipole field (0.0005 au); b) the energy barrier for the intercage electron transfer.
- **Equation (S1).** $\Delta E_{\text{ab initio}} = E_{\mathbf{T}} - E_{\mathbf{F}}$, where $E_{\mathbf{T}}$ and $E_{\mathbf{F}}$ are the ab initio energies for **T** and **F** in the electric dipole field, respetively
- **Equation (S2).** $\Delta E_{\text{model}} = \left(-\mu_{\mathbf{T}} \cdot E\right) - \left(-\mu_{\mathbf{F}} \cdot E\right)$, where $\mu_{\mathbf{T}}$ and $\mu_{\mathbf{F}}$ are the dipole moments of **T** and **F**, respectively, and E is the electric dipole field
- **Table S1.** The energy differences between **T** and **F** for **2**, derived from ab initio calculations and the dipole-field model, respectively
- **Table S2.** Cartesian coordinates for the optimized geometry of **1-T** and **1-F**
- **Table S3.** Cartesian coordinates for the optimized geometry of **2-T** and **2-F**

Computational Details. All geometry optimizations were carried out at the B3LYP/6-31G(d) level of theory, and the stationary points were tested at the same level. Extra diffuse basis functions were used to describe the diffuse characteristic of the excess electron located at the center of the $C_{20}F_{20}$ cage, as suggested by Wang et al..[1-3] Geometry optimizations in the presence of an electric dipole field or background point charges were done with the bridging N atoms in **1** and B atoms in **2** fixed. All calculations were performed with the Gaussian 09 program package.[4]

The degenerate ground states **T** and **F** of **1** are represented as **1-T** and **1-F**, respectively. Similarly, for **2** they are **2-T** and **2-F**. The isovalues for SOMO and spin density are 0.04 and 0.0012 electrons bohr^{-3}, respectively.

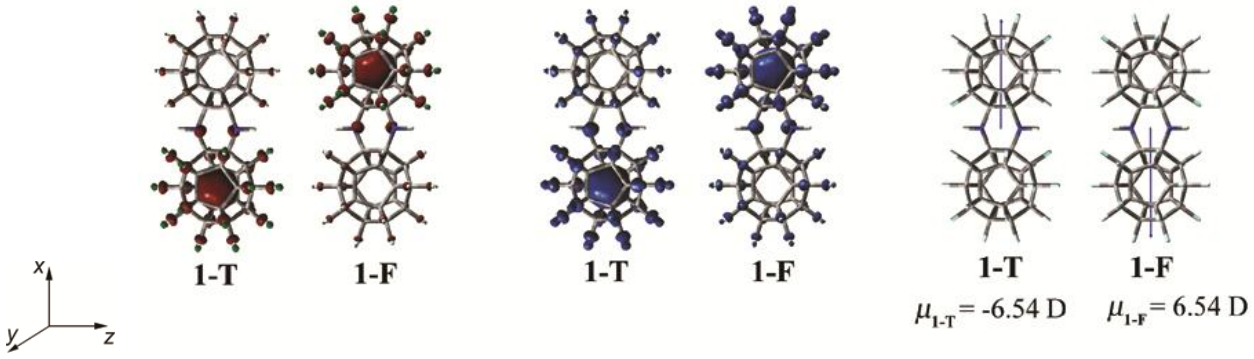

Figure S1. The SOMOs, spin densities and dipole moments for **1-T** and **1-F**.

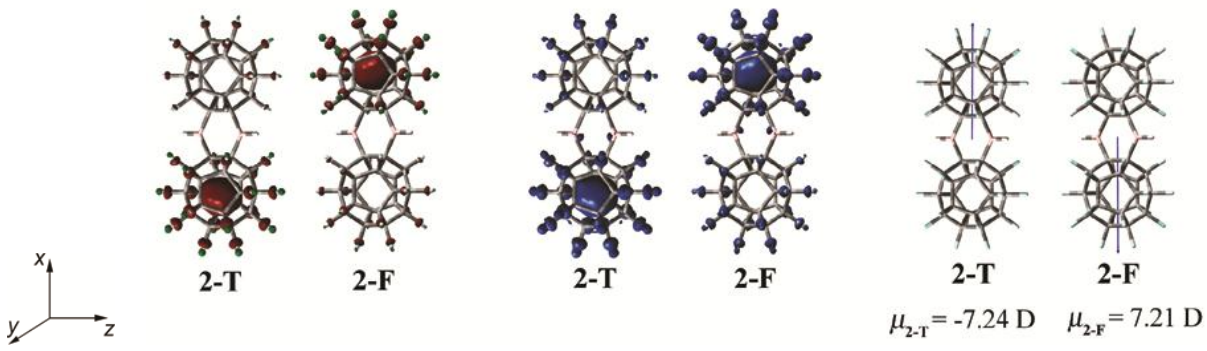

Figure S2. The SOMOs, spin densities and dipole moments for **2-T** and **2-F**.

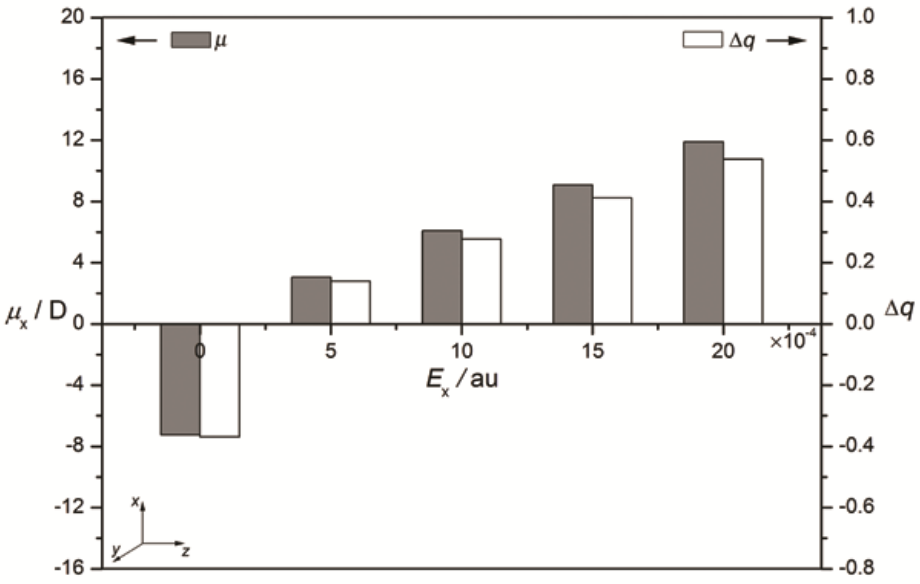

Figure S3. The influence of the electric dipole field on the dipole moment (μ_x) and intercage charge difference (Δq) of **2**.

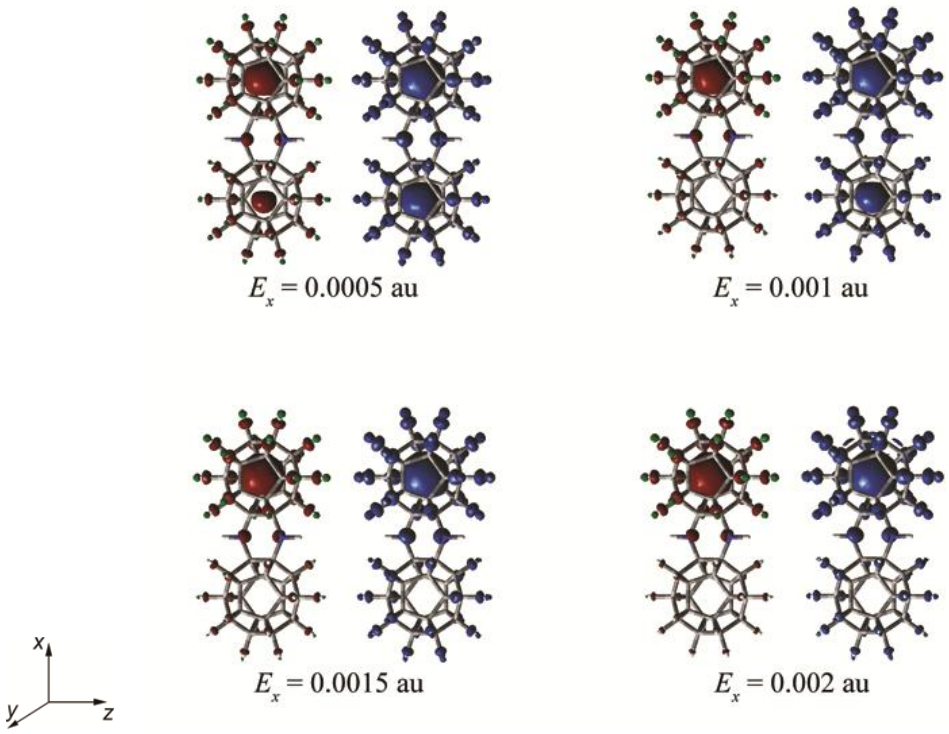

Figure S4. The SOMO and spin density for **1** under different electric dipole fields.

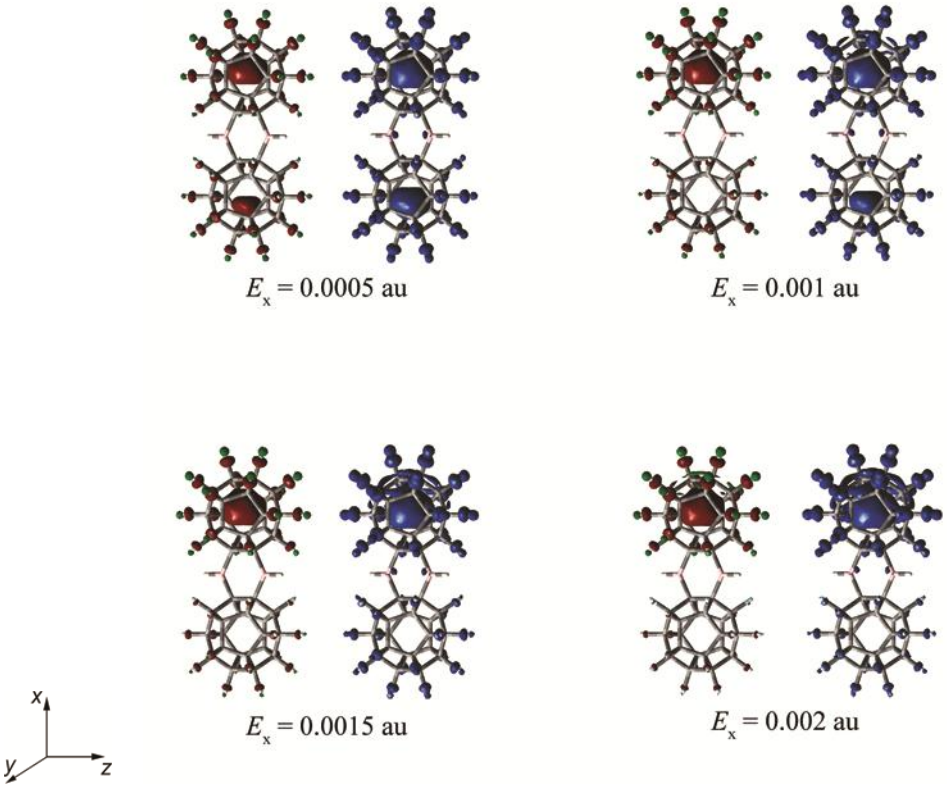

Figure S5. The SOMO and spin density for **2** under different electric dipole fields.

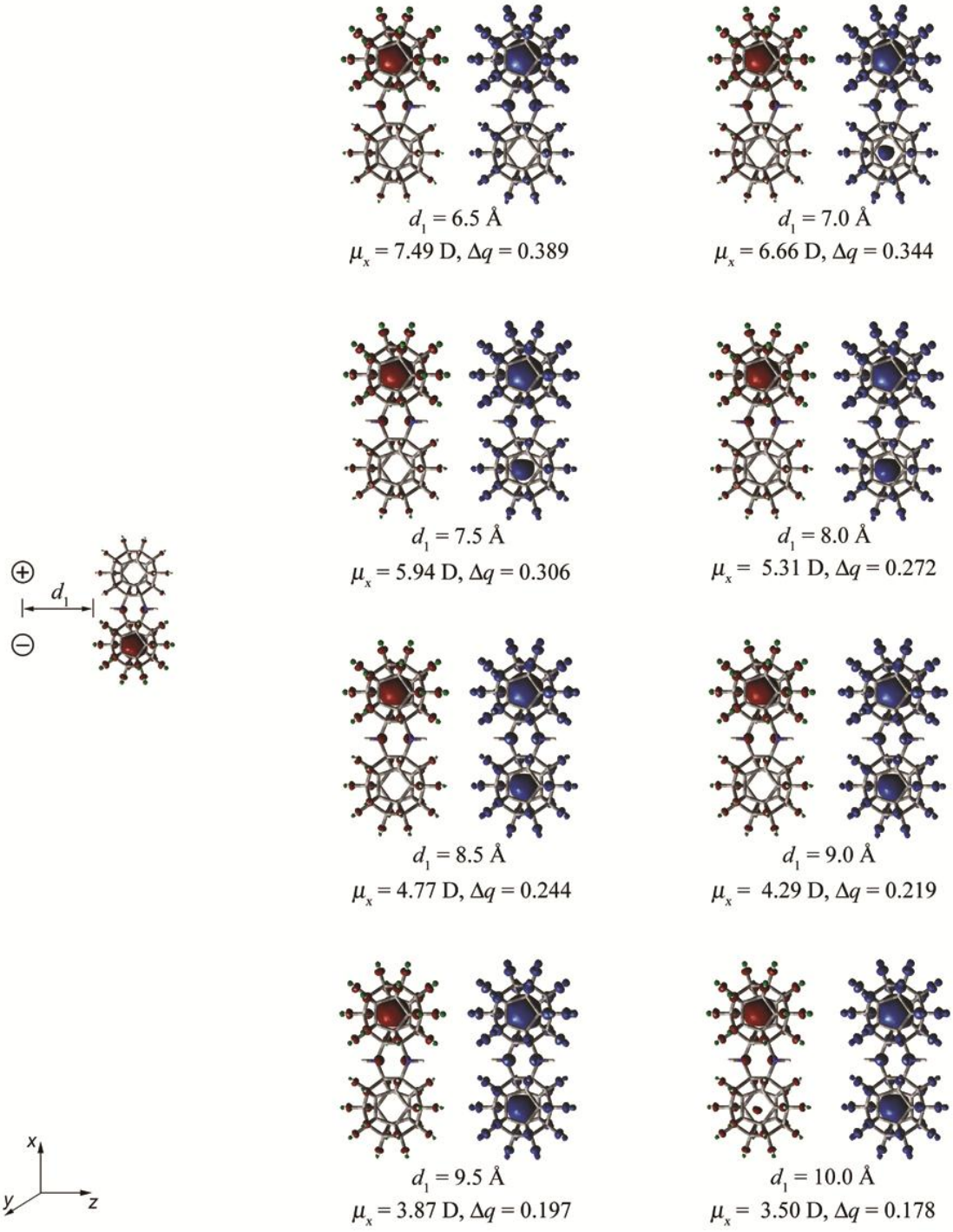

Figure S6. The SOMO, spin density, dipole moment (μ_x) and intercage charge difference (Δq) for **1** under the inducement of the driver composed of a dipole in the lateral driver model.

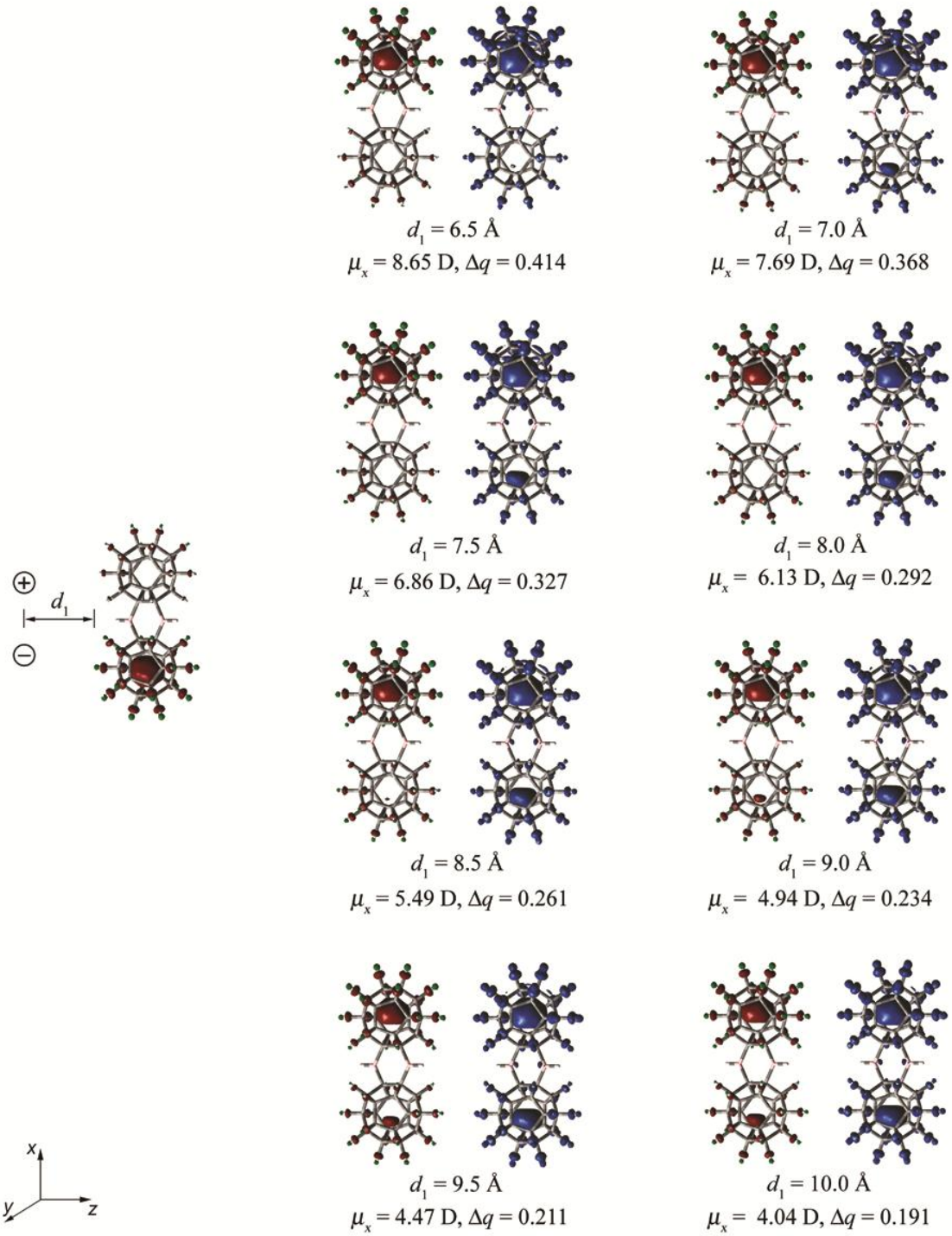

Figure S7. The SOMO, spin density, dipole moment (μ_x) and intercage charge difference (Δq) for **2** under the inducement of the driver composed of a dipole in the lateral driver model.

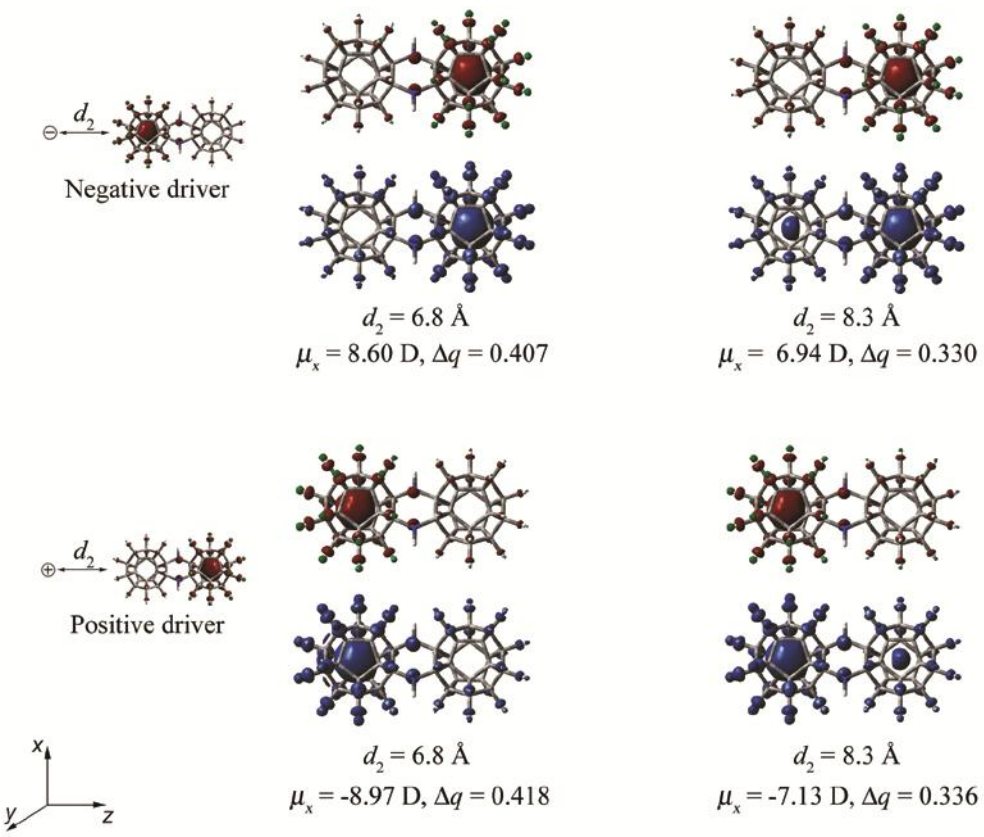

Figure S8. The SOMO, spin density, dipole moment (μ_x) and intercage charge difference (Δq) for **1** under the inducement of the driver composed of a single point charge in the axial driver model.

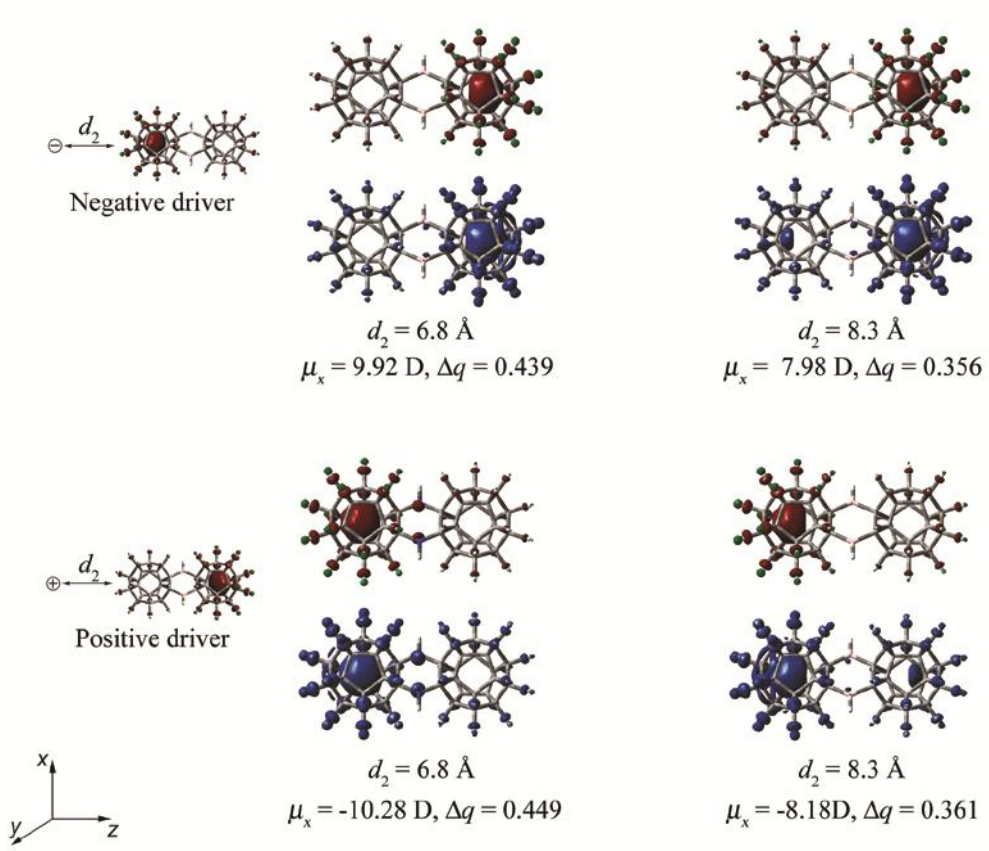

Figure S9. The SOMO, spin density, dipole moment (μ_x) and intercage charge difference (Δq) for **2** under the inducement of the driver composed of a single point charge in the axial driver model.

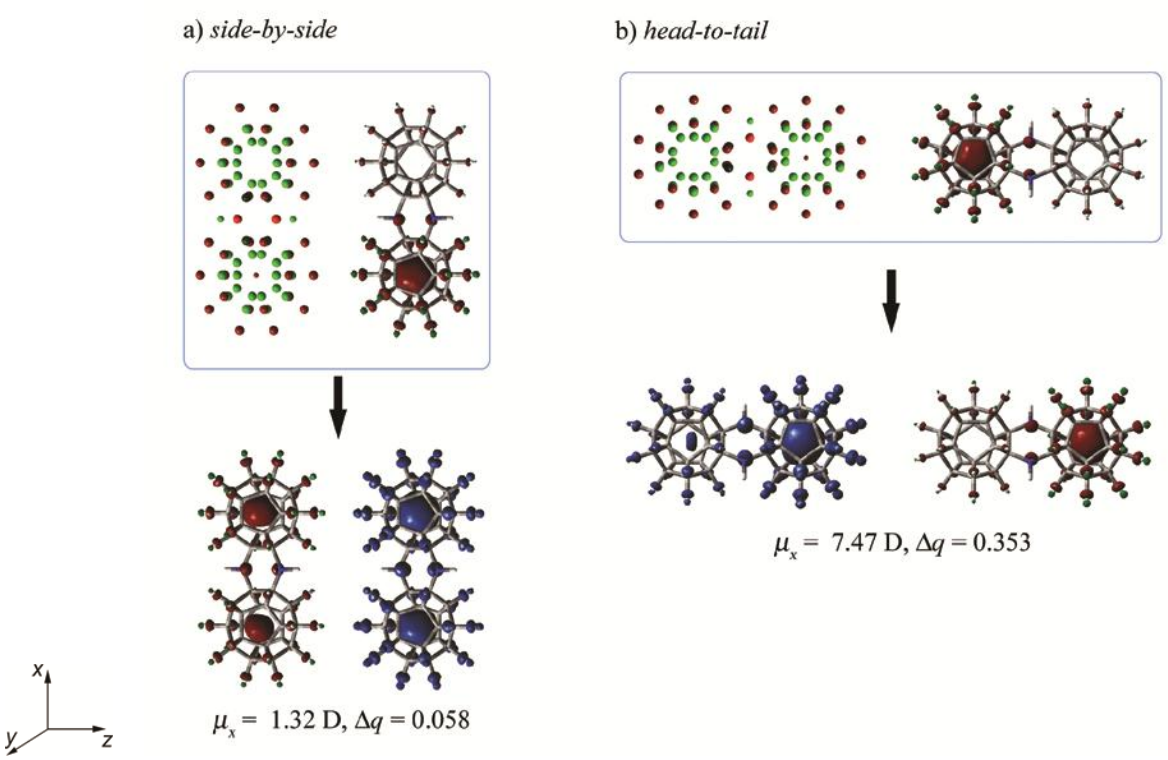

Figure S10. The SOMO, spin density, dipole moment (μ_x) and intercage charge difference (Δq) for **1** under the Coulomb perturbation of a neighboring molecule.

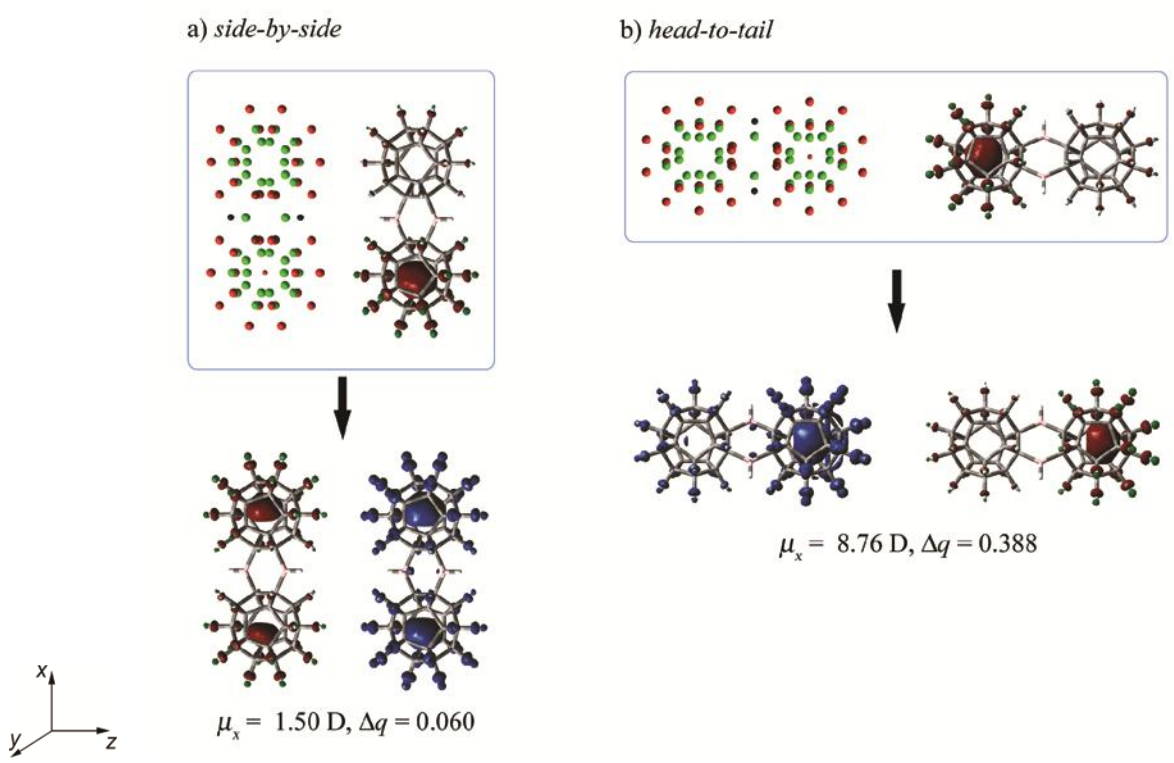

Figure S11. The SOMO, spin density, dipole moment (μ_x) and intercage charge difference (Δq) for **2** under the Coulomb perturbation of a neighboring molecule.

Electron tunnelling between the bistatble states

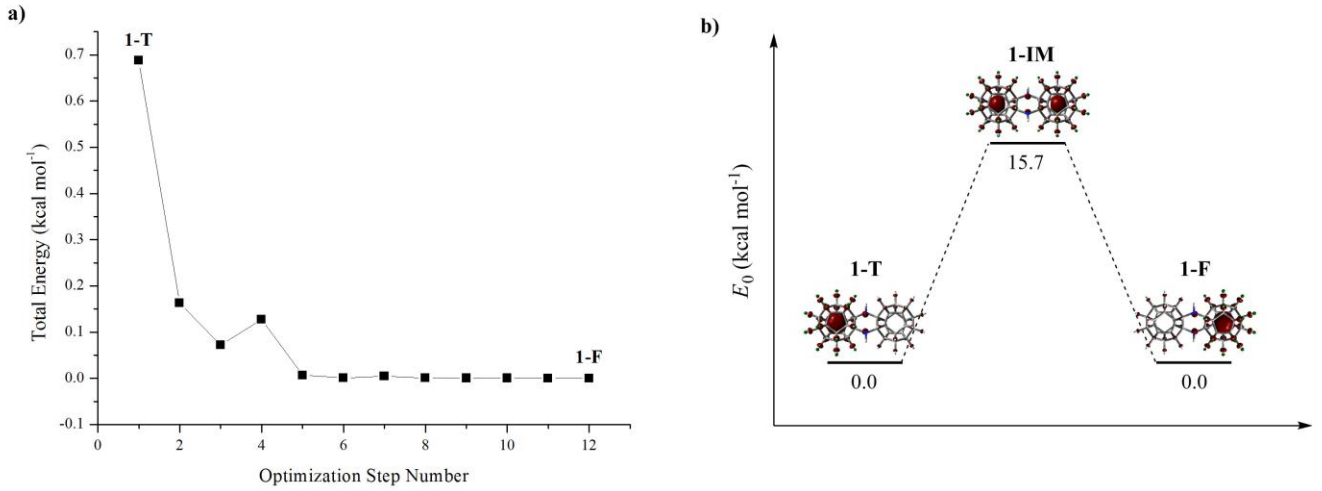

Figure S12. a) The energy profile for the change from **1-T** to **1-F** under the electric dipole field (0.0005 au); b) the energy barrier for the intercage electron transfer.

The energy profile in Fig. S12a shows the transformation from **1-T** to **1-F** induced by the electric dipole field (0.0005 au). The energy profiles for the other magnitudes of field are similar. The drop in energy indicates a direct electron transfer from one cage to the other, i.e., an electron tunnelling process. If the intercage electron transfer is considered as a reaction and an intermediate state (**1-IM**) with equivalent charge distributions in the two cages is suggested. The energy barrier (15.7 kcal mol^{-1}) is relatively high for the intercage electron transfer to take place at room temperature. In addition, the electrons were suggested to be able to tunnel between the two bistatble states in MQCA.[5] Therefore, this field induced intercage electron transfer is suggested to be an electron tunnelling process.

Table S1. The energy differences between **T** and **F** for **2**, derived from ab initio calculations and the dipole-field model, respectively.

	$E_x/10^{-4}$ au			
	5	10	15	20
$E_{\text{ab initio}}$/kcal mol^{-1}	1.780	3.55	5.28	8.84
E_{model}/kcal mol^{-1}	1.780	3.57	5.35	7.14

Table S2. Cartesian coordinates for the optimized geometry of **1-T** and **1-F**.[a]

1-T				**1-F**			
Bq	-3.39265400	0.03615600	-0.02453100	Bq	3.39401100	0.03597400	-0.02464400
C	3.39674000	0.84454000	-1.99223400	C	3.40195000	0.78522800	-2.00774700
C	4.65676300	1.30209800	-1.20073900	C	4.65747500	1.25982000	-1.23056900
C	5.43592700	0.02709100	-0.76450600	C	5.43161800	-0.00057200	-0.76399300
C	4.65684200	-1.21451200	-1.29157800	C	4.65279800	-1.24989600	-1.25754100
C	3.39445200	-0.70701800	-2.04979000	C	3.39498500	-0.76127800	-2.02621700
C	4.17312400	2.03617700	0.08373400	C	4.17644800	2.02511400	0.03104200
C	2.61339300	2.03543400	0.08294700	C	2.62295100	2.02491300	0.03119900
C	2.14065500	1.30074800	-1.19890200	C	2.15302100	1.26239400	-1.22733000
C	4.64988500	1.21344100	1.31471800	C	4.65065300	1.23596600	1.27782400
C	5.43198000	-0.02797100	0.79164500	C	5.42857800	-0.01509900	0.78737600
C	4.65090500	-1.30318900	1.22388500	C	4.64970500	-1.27383300	1.25090100
C	4.17403800	-2.03739800	-0.06306200	C	4.17190700	-2.03807400	-0.01262600
C	2.61432700	-2.03709800	-0.07038500	C	2.61828600	-2.03460100	-0.01896600
C	2.13194700	-1.22173800	-1.29728500	C	2.13405400	-1.25168600	-1.26212900
C	1.29299200	0.03163300	-0.78039400	C	1.30436200	0.01073900	-0.77796700
C	3.38379200	0.70559600	2.06643600	C	3.38863000	0.75002700	2.04146500
C	3.38678100	-0.84593500	2.00891000	C	3.39198600	-0.79651700	2.02318200
C	2.13492300	-1.30240100	1.20897700	C	2.14480600	-1.27094900	1.23777500
C	1.28917900	-0.03380300	0.78624200	C	1.30094500	-0.01756800	0.78442600
C	2.12504500	1.22002600	1.30741900	C	2.13195000	1.24303700	1.27221000

F	1.40193000	-2.16270800	1.98887300	F	1.39928400	-2.11313800	2.04517200
F	1.38295900	2.00720400	2.13244500	F	1.37748300	2.05372500	2.07800600
F	5.44455700	2.11646200	-1.96151400	F	5.44857400	2.06001100	-2.01823600
F	6.71247700	0.04513400	-1.24769900	F	6.71564300	0.00243400	-1.25257500
F	5.44706400	-1.97115100	-2.10741700	F	5.44330800	-2.03441500	-2.06107800
F	2.13737700	-3.31494700	-0.10781100	F	2.12838400	-3.31752800	-0.02479500
F	4.66409200	-3.31007000	-0.10690300	F	4.65805200	-3.32191800	-0.02414400
F	5.43499700	-2.11734000	1.98870200	F	5.43565200	-2.07576900	2.04168200
F	6.70604000	-0.04568600	1.28139500	F	6.71054500	-0.02128400	1.28118600
F	5.43567600	1.97030900	2.13461700	F	5.43965900	2.01850700	2.08474900
F	4.66258200	3.30899600	0.13013200	F	4.66544300	3.30798700	0.04465400
F	2.13589600	3.31320900	0.11796800	F	2.13566300	3.30897100	0.03522200
F	1.41134000	2.16053400	-1.98249200	F	1.41271700	2.10636800	-2.03783900
F	1.39421000	-2.00915300	-2.12617000	F	1.38094200	-2.06079600	-2.07075700
F	-4.66027200	-3.31539800	-0.06400400	F	-4.66857600	-3.30167000	-0.09372400
C	-4.17285100	-2.03214500	-0.04300000	C	-4.17624900	-2.02950600	-0.06111600
C	-2.61920200	-2.03047600	-0.04329100	C	-2.61652000	-2.03233100	-0.06092900
C	-4.64770900	-1.23637100	-1.28525900	C	-4.65139700	-1.21873800	-1.30046900
C	-4.65468500	-1.27441800	1.22295500	C	-4.65788100	-1.28079200	1.21574300
C	-2.15027900	-1.27476900	1.21974700	C	-2.14218700	-1.28552000	1.21314600
C	-2.12860000	-1.24095400	-1.27972300	C	-2.12619100	-1.23075200	-1.29388400
F	-2.13070200	-3.31387300	-0.05480400	F	-2.14193800	-3.31147800	-0.08257000
C	-3.38614800	-0.74494800	-2.04609600	C	-3.38427500	-0.72178500	-2.05786800

C	-5.42680300	0.01110900	-0.78782000	C	-5.43059000	0.02985700	-0.79021100
F	-5.43575800	-2.01522900	-2.09668400	F	-5.43912600	-1.98242600	-2.11216000
C	-3.39965600	-0.80305000	2.00288200	C	-3.39673800	-0.81783000	2.00208000
C	-5.42984400	-0.01211200	0.76333100	C	-5.43417900	-0.00867700	0.76642400
F	-5.44486800	-2.07990200	2.00591900	F	-5.44732200	-2.08528700	1.98531500
C	-1.30265600	-0.02049000	0.77766300	C	-1.29112900	-0.02342100	0.78134800
F	-1.40987500	-2.12360800	2.02528200	F	-1.41562600	-2.13947900	2.00585800
C	-1.29916800	0.01804600	-0.78471600	C	-1.28772400	0.02689500	-0.78600300
F	-1.37274000	-2.04585700	-2.08996800	F	-1.38546600	-2.02818500	-2.11045300
C	-3.39131000	0.80129800	-2.01909400	C	-3.38410000	0.83029800	-2.01651100
F	-3.38486700	-1.20850700	-3.33928500	F	-3.39153300	-1.16835200	-3.34821700
C	-4.64933600	1.27306300	-1.24430000	C	-4.64679800	1.29864700	-1.23595800
F	-6.70888300	0.01861500	-1.28153000	F	-6.70476200	0.04517300	-1.27978100
C	-3.39404500	0.74327200	2.02993100	C	-3.39043000	0.73421400	2.04343500
F	-3.39815200	-1.31291800	3.27972000	F	-3.40344300	-1.33511500	3.26645100
C	-4.65227800	1.23509100	1.26386400	C	-4.65197200	1.23657200	1.28023700
F	-6.71381400	-0.01930900	1.25205100	F	-6.71061700	-0.01849200	1.25017900
C	-2.13335600	1.23888600	1.26866900	C	-2.12662000	1.23783000	1.28531000
C	-2.14485100	1.27259800	-1.23105500	C	-2.13123200	1.29263000	-1.22180200
F	-3.38440100	1.31101900	-3.29607500	F	-3.38273300	1.34760100	-3.28089500
C	-4.17224900	2.03055700	0.02348200	C	-4.16775600	2.04528900	0.04309900
F	-5.43612400	2.07885000	-2.03049800	F	-5.42925200	2.10653500	-2.00910300
F	-3.39809800	1.20662900	3.32315600	F	-3.40175200	1.18081700	3.33373600

F	-5.44345400	2.01413400	2.07212300	F	-5.44014500	2.00361800	2.08832900
C	-2.61872500	2.02836600	0.02996700	C	-2.60805300	2.04146800	0.05008000
F	-1.38101500	2.04409700	2.08164400	F	-1.38650100	2.03221900	2.10531100
F	-1.40057100	2.12065600	-2.03360600	F	-1.39744900	2.14341100	-2.01118200
F	-4.65937000	3.31405800	0.04252800	F	-4.65479200	3.31953600	0.07345200
F	-2.12989500	3.31173500	0.04364700	F	-2.12810200	3.31857200	0.07389500
N	-0.00269800	-0.09201400	1.39642600	N	-0.00206900	-0.08183600	1.39771000
N	0.00392600	0.08955700	-1.39648200	N	0.00418100	0.07898000	-1.39654500
H	-0.00201700	0.69956700	-2.20243800	H	0.01488900	0.68475000	-2.20566800
F	3.38966000	1.13846600	3.36143800	F	3.38813900	1.22066000	3.33205900
F	3.38629000	-1.37659800	3.26771200	F	3.38482500	-1.29902800	3.30286300
F	3.40264800	1.37516600	-3.25107700	F	3.40103500	1.28765600	-3.28766600
F	3.40719600	-1.13985100	-3.34475600	F	3.39870300	-1.23207600	-3.31680600
H	-0.01271700	-0.70685200	2.19866400	H	0.00264600	-0.68998000	2.20510700

[a] The Bq atom is used to add the extra diffuse basis functions.

Table S3. Cartesian coordinates for the optimized geometry of **2-T** and **2-F**.

2-T				**2-F**			
Bq	-3.46358200	0.04673700	-0.01919700	Bq	3.46207400	0.04654800	-0.01890400
C	3.46615600	0.77587700	-2.03411900	C	3.45966300	0.77168300	-2.02572500
C	4.72415300	1.25792800	-1.24813200	C	4.71316700	1.25185900	-1.24317600
C	5.50215500	-0.00012400	-0.76471900	C	5.48801900	-0.00120900	-0.76165000
C	4.72469000	-1.25858900	-1.24794200	C	4.71389100	-1.25491800	-1.24291700
C	3.46649500	-0.77714700	-2.03400600	C	3.46006300	-0.77558400	-2.02557100
C	4.23949800	2.03451100	0.01064100	C	4.23145300	2.02651600	0.01064100
C	2.68202600	2.03087100	0.00675800	C	2.68032100	2.02212300	0.00741500
C	2.20527400	1.24826900	-1.24814100	C	2.20338500	1.24362400	-1.24283800
C	4.71800200	1.25811600	1.27183700	C	4.70795000	1.25224300	1.26665100
C	5.49836800	-0.00002700	0.79245800	C	5.48484200	-0.00099400	0.78869900
C	4.71851100	-1.25841000	1.27205400	C	4.70866500	-1.25460600	1.26708500
C	4.24034400	-2.03520000	0.01091800	C	4.23256900	-2.02961900	0.01120700
C	2.68286600	-2.03219100	0.00710600	C	2.68128500	-2.02604800	0.00798900
C	2.20569400	-1.25000200	-1.24798600	C	2.20395600	-1.24803900	-1.24254700
C	1.40647100	-0.00107100	-0.78186800	C	1.39612300	-0.00238800	-0.77926500
C	3.45618300	0.77613700	2.05166600	C	3.45101000	0.77224300	2.04408100
C	3.45648000	-0.77683100	2.05179700	C	3.45140200	-0.77500900	2.04435700
C	2.19960400	-1.24975700	1.25963600	C	2.19836700	-1.24762600	1.25625200
C	1.40267900	-0.00079500	0.78923100	C	1.39228100	-0.00217600	0.78872100
C	2.19905500	1.24845200	1.25945300	C	2.19783600	1.24390100	1.25582800

F	1.43892000	-2.08617900	2.04929700	F	1.41848400	-2.08233800	2.04693800
F	1.43806300	2.08458800	2.04897300	F	1.41709700	2.07822600	2.04630900
F	5.51509800	2.04686400	-2.03308600	F	5.50458200	2.04842700	-2.03782000
F	6.77970200	0.00010600	-1.24839700	F	6.77462200	-0.00109000	-1.25192500
F	5.51593900	-2.04727100	-2.03282400	F	5.50560000	-2.05136200	-2.03713200
F	2.20219200	-3.30804400	0.00605900	F	2.18581200	-3.30576700	0.00718800
F	4.72618400	-3.31082000	0.01222600	F	4.71489200	-3.31689000	0.01248800
F	5.50585300	-2.04705000	2.06089500	F	5.49688000	-2.05068800	2.06498800
F	6.77352300	0.00021700	1.28241600	F	6.76926800	-0.00074000	1.28450400
F	5.50503900	2.04709200	2.06066600	F	5.49587300	2.04890300	2.06451800
F	4.72482100	3.31034200	0.01174700	F	4.71313500	3.31426600	0.01154900
F	2.20081600	3.30654700	0.00549000	F	2.18397200	3.30171000	0.00624300
F	1.44792900	2.08438500	-2.04144800	F	1.42578900	2.07784500	-2.03667100
F	1.44888000	-2.08664600	-2.04102500	F	1.42720000	-2.08314000	-2.03607600
F	-4.72119700	-3.31684500	-0.01126000	F	-4.73189700	-3.31421400	-0.01295800
C	-4.23923400	-2.02944100	-0.01028600	C	-4.24667800	-2.03835700	-0.01198100
C	-2.68794300	-2.02545900	-0.00759000	C	-2.68920600	-2.03459200	-0.00743400
C	-4.71607900	-1.25459800	-1.26600200	C	-4.72466900	-1.26234000	-1.27364700
C	-4.72027200	-1.25484200	1.24399400	C	-4.73196300	-1.26143800	1.24634200
C	-2.21025100	-1.24719700	1.24272500	C	-2.21299500	-1.25160400	1.24751200
C	-2.20578100	-1.24707500	-1.25612800	C	-2.20576100	-1.25245000	-1.26010200
F	-2.19213700	-3.30504100	-0.00678200	F	-2.20791400	-3.31020300	-0.00558300
C	-3.45929800	-0.77479200	-2.04372800	C	-3.46252300	-0.78048100	-2.05304300

C	-5.49238100	-0.00117400	-0.78736700	C	-5.50533500	-0.00411600	-0.79494400
F	-5.50447400	-2.05098400	-2.06344300	F	-5.51126200	-2.05167000	-2.06253800
C	-3.46620500	-0.77504300	2.02622300	C	-3.47435100	-0.77904800	2.03275000
C	-5.49501600	-0.00136100	0.76299700	C	-5.50981400	-0.00355800	0.76222200
F	-5.51135900	-2.05141000	2.03862500	F	-5.52317200	-2.05019300	2.03118600
C	-1.40304600	-0.00133500	0.77892400	C	-1.41406100	-0.00242900	0.78122300
F	-1.43287500	-2.08197900	2.03594700	F	-1.45619200	-2.08755500	2.04137500
C	-1.39978500	-0.00135000	-0.78908500	C	-1.40969100	-0.00296200	-0.78985200
F	-1.42601500	-2.08164600	-2.04701500	F	-1.44435400	-2.08887700	-2.04902900
C	-3.45920100	0.77240100	-2.04351700	C	-3.46295300	0.77250100	-2.05357900
F	-3.45004900	-1.27146800	-3.32366700	F	-3.46292900	-1.27473500	-3.32423700
C	-4.71593000	1.25220100	-1.26562300	C	-4.72535900	1.25419200	-1.27452400
F	-6.77700800	-0.00124200	-1.28258200	F	-6.78028000	-0.00467400	-1.28547900
C	-3.46633400	0.77229300	2.02628400	C	-3.47476700	0.77395800	2.03220300
F	-3.46142200	-1.27195400	3.30608600	F	-3.48223200	-1.27239200	3.30427500
C	-4.72031900	1.25198700	1.24417700	C	-4.73264500	1.25508300	1.24544700
F	-6.78129900	-0.00162800	1.25383500	F	-6.78758900	-0.00376600	1.24532500
C	-2.21050800	1.24446800	1.24273000	C	-2.21365200	1.24663500	1.24664400
C	-2.20579600	1.24446100	-1.25596200	C	-2.20646400	1.24573700	-1.26096000
F	-3.45002900	1.26910000	-3.32358200	F	-3.46365500	1.26579000	-3.32515600
C	-4.23920200	2.02666700	-0.00989500	C	-4.24778700	2.03136400	-0.01341300
F	-5.50439200	2.04866700	-2.06326100	F	-5.51241200	2.04248600	-2.06400200
F	-3.46143500	1.26875500	3.30636700	F	-3.48295000	1.26813100	3.30341600

F	-5.51162400	2.04829000	2.03903400	F	-5.52431300	2.04393300	2.02974200
C	-2.68805600	2.02268000	-0.00738600	C	-2.69030900	2.02847300	-0.00884400
F	-1.43277300	2.07892300	2.03619900	F	-1.45719000	2.08342400	2.03994900
F	-1.42565800	2.07889700	-2.04683500	F	-1.44543900	2.08191400	-2.05052000
F	-4.72119500	3.31430700	-0.01054400	F	-4.73372600	3.30695500	-0.01530600
F	-2.19204700	3.30239700	-0.00653300	F	-2.20973300	3.30437700	-0.00791200
F	3.45723100	1.26996400	3.32304300	F	3.44113300	1.26898100	3.32404000
F	3.45771900	-1.27055000	3.32319900	F	3.44181800	-1.27159000	3.32428700
F	3.47351700	1.26952800	-3.30553200	F	3.45517900	1.26811000	-3.30593100
F	3.47404300	-1.27103000	-3.30532600	F	3.45585900	-1.27258800	-3.30546300
B	-0.00272700	-0.00150700	-1.55183700	B	0.00396200	-0.00283800	-1.55101500
H	0.01290700	-0.00153500	-2.73355900	H	-0.00369900	-0.00328700	-2.73277200
B	-0.01084100	-0.00089000	1.55057300	B	-0.00491000	-0.00205500	1.55150400
H	-0.00331100	-0.00135500	2.73233000	H	-0.02060200	-0.00192300	2.73320700

References

1 Y. F. Wang, Z. R. L, D. Wu, Y. Li, C. Sun, F. L. Gu, *J. Phys. Chem. A* 2010, **114**, 11782.

2 K. D. Jordan,W. Luken, *J. Chem. Phys.* 1976, **64**, 2760; K. M. Griffing, J. Kenney, J. Simons, K. D. Jordan, *J. Chem. Phys.* 1975, **63**, 4073.

3 P. Skurski, M. Gutowski, J. Simons, *Int. J. Quantum. Chem.* 2000, **80**, 1024; I. Anusiewicz, P. Skurski, J. Simons, *J. Phys. Chem. A* 2002, **106**, 10636.

4 Gaussian 09 (Revision B.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

5 S. B. Braun-Sand and O. Wiest, J. Phys. Chem. A, 2003, 107, 285; S. B. Braun-Sand and O. Wiest, J. Phys. Chem. B, 2003, 107, 9624; Y. Lu and C. S. Lent, J. Comput. Electron., 2005, 4, 115.