Theoretical Calculation

All density functional theory (DFT) calculation was performed using the Gaussian 16 program[1]. The B3LYP functional was used for geometry optimization in the ground state. The 6-31G(d) basis set was used. All geometry optimization was done in the gas phase and based on the single crystal structures. In order to simulate the UV-Vis spectra of the molecules TD-DFT calculations were carried by using B3LYP functional and 6-31G(d) basis set. For better comparison to the experimental absorption spectra the polarity of the solvent dichloromethane was added.

Singlet biradical character index (*y*0) was estimated using a symmetry-broken UCAM-B3LYP/6-31G(d) or UHF/6-31G(d) method along with geometry optimization. The index *y*0, related to the HOMO and LUMO for singlet states, is defined by the weight of the doubly-excited configuration in the multi-configurational MC-SCF theory, and is formally expressed in the case of the spin-projected UHF (PUHF) theory[2,3] as

,

where T is the orbital overlap between the corresponding orbital pairs, and can be calculated using the occupation numbers of UHF natural orbitals:

The singlet-triplet energy gap *ΔE*S-T was evaluated as

,

where *ΔE*S(*qs*) and *ΔE*T(*qT*) are the total energies of the singlet biradical (open-shell) and triplet ground state, respectively, i.e., *ΔE*S-T denotes the minimum-to-minimum energy difference.

Anisotropy of the induced current density (ACID) plots were calculated by Herges’s method.[4] Nucleus

independent chemical shifts (NICS) values were calculated using the standard gauge invariant atomic

orbital (GIAO)[5] method at B3LYP functional. The 6-311+G(d,2p) basis set was used for the C, and H atoms. All NICS values were averaged by two positions (above and below the plane) of each molecule.

For transition state (TS) calculation all the structure were optimized in gas phase by using B3LYP level of density functional theory with the 6-31G\* basis. To confirm the accuracy of the transition state we did frequency calculation. The Gibbs free energies of reaction (Δr*G*o) at room temperature (298 K) can be calculated by the following equations[6]

where *H*corr is the thermal correction to Enthalpy; *E*tot is the correction to the internal thermal energy; *k*B is the Boltzmann constant; *T* is the temperature; *G*corr is the thermal correction to Gibbs free energy (thermal Free Energies); *S*tot is the correction to the internal Entropy; *ε*0 is the total electronic energy. In our case, the isomerization process represents the reaction. The Sum of Electronic and Thermal Free Energies (*ε*0+*G*corr) are given below.

The Cartesian coordinates of all the optimized structures.

JL-1-M

**-2940.769731 a.u.**

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H -4.02305500 7.12649200 -0.97315200

H -3.69645300 8.85994800 -1.12613600

H -2.86613900 7.70210500 -2.18398600

H -1.55168100 -9.85299800 0.38318600

H -0.22905800 -8.86643600 -0.25359800

H -0.65865300 -8.78014100 1.46702300

H -3.69918200 -8.85732000 1.13246200

H -4.02492900 -7.12389200 0.97671100

H -2.86960700 -7.69829100 2.18959000

H -1.85334500 -7.95330800 -2.03006100

H -3.10778700 -9.00245500 -1.34037600

H -3.41424000 -7.27113600 -1.54696600

C -4.24924100 3.42248300 0.35280700

C -4.74947400 3.61814300 1.65735600

C -5.06041500 3.73623800 -0.75973700

C -6.04174700 4.12892300 1.82556700

C -6.34706800 4.24267000 -0.54663500

C -6.85975400 4.44581000 0.73818000

H -6.41751800 4.28170200 2.83578200

H -6.96496100 4.48395600 -1.40987500

C -4.24903500 -3.42206400 -0.35669700

C -4.74804000 -3.61542200 -1.66054900

C -5.06300500 -3.73454700 0.75595400

C -6.04255200 -4.12360800 -1.83017200

C -6.34945700 -4.23745500 0.54175600

C -6.86079700 -4.44134000 -0.74495100

H -6.41888400 -4.27202700 -2.84064200

H -6.96980200 -4.47467500 1.40459000

C 4.10490700 -1.59403200 0.13316200

C 4.85792100 -1.18733700 1.24056800

C 4.74199800 -2.39773800 -0.82483700

C 6.19391600 -1.56366400 1.38194000

H 4.39210700 -0.57822900 2.00955700

C 6.07621500 -2.76751200 -0.68065500

H 4.18317500 -2.73089700 -1.69593700

C 6.83800000 -2.36474200 0.42869200

H 6.72899000 -1.22623700 2.26273700

H 6.52697800 -3.38791300 -1.45087500

C 4.10518200 1.59325200 -0.13351500

C 4.74274800 2.39680400 0.82429800

C 4.85775500 1.18642600 -1.24117300

C 6.07699200 2.76631300 0.67969000

H 4.18427600 2.73005100 1.69559100

C 6.19377900 1.56248600 -1.38297000

H 4.39156600 0.57743300 -2.01002500

C 6.83833400 2.36341300 -0.42991300

H 6.52813300 3.38660800 1.44977500

H 6.72850000 1.22497400 -2.26394900

C -3.90872100 3.28959600 2.87094500

H -4.43496800 3.55422900 3.79348400

H -3.66711400 2.22107000 2.91447400

H -2.95429400 3.82877600 2.85830400

C -8.26383100 4.96574300 0.94299100

H -8.56109300 5.64698600 0.13819800

H -8.99458100 4.14575900 0.95910100

H -8.35830400 5.50223300 1.89321200

C -4.56066700 3.52650400 -2.17148700

H -4.36956300 2.46603000 -2.37531100

H -5.29424400 3.88214000 -2.90182900

H -3.61896400 4.05813800 -2.34898500

C -4.56453800 -3.52272400 2.16785300

H -4.37109700 -2.46230200 2.36963400

H -5.29975300 -3.87522400 2.89806800

H -3.62427000 -4.05620700 2.34744800

C -3.90770600 -3.28493900 -2.87391700

H -4.43327200 -3.55036000 -3.79662200

H -3.66801300 -2.21595900 -2.91734500

H -2.95234800 -3.82244500 -2.86124200

C -8.25791900 -4.98164600 -0.94540400

H -9.01486600 -4.29011700 -0.55366600

H -8.47502900 -5.14448600 -2.00587100

H -8.39785500 -5.93683200 -0.42429500

C 8.30397600 2.81474800 -0.56367200

C 8.30359400 -2.81637600 0.56198000

C 8.36143300 4.36020400 -0.62184800

H 7.93575800 4.81729500 0.27762800

H 9.40033100 4.70143400 -0.71047100

H 7.80376900 4.74024100 -1.48543300

C 9.11291600 2.32141300 0.65919300

H 10.15923500 2.64142200 0.58033600

H 8.71386900 2.71697200 1.59904200

H 9.09568900 1.22728900 0.72361100

C 8.97385100 2.26306800 -1.83632800

H 8.98651900 1.16711500 -1.84901200

H 8.46921400 2.60880000 -2.74561800

H 10.01346700 2.60638000 -1.88524600

C 8.97399100 -2.26482800 1.83441800

H 8.46957500 -2.61045200 2.74387200

H 10.01355200 -2.60835100 1.88300500

H 8.98688800 -1.16887700 1.84709300

C 8.36075400 -4.36184200 0.62014300

H 7.93469500 -4.81884800 -0.27919400

H 9.39961100 -4.70328400 0.70842900

H 7.80329300 -4.74176400 1.48391000

C 9.11223900 -2.32321000 -0.66114700

H 10.15851700 -2.64343700 -0.58263100

H 8.71280300 -2.71868500 -1.60086600

H 9.09522100 -1.22908200 -0.72555900

JL-2-M

-2433.595503 a.u.

C 2.44354600 1.99213500 -0.22167500

C 2.47505600 3.42752700 0.05016100

C 1.31959700 4.19809200 0.11633900

C 0.10124000 3.53411700 -0.10122700

C 0.05068100 2.19217500 -0.28732900

C 1.19230900 1.38319600 -0.32245800

C -1.06345900 4.28773300 0.12247200

C -2.27308600 3.60495900 0.06159700

C -2.34970500 2.17083000 -0.21033000

C -1.14803000 1.47030400 -0.31712400

C 0.67234900 0.01963600 -0.33769700

C -0.73060700 0.07192200 -0.33444100

C 3.69014000 1.22091300 -0.42424300

C -3.65110700 1.49468500 -0.40664000

C -1.56536600 -1.06682400 -0.10050700

C -0.79453400 -2.28879000 0.13201800

C 0.56276100 -2.33931400 0.12918700

C 1.42135100 -1.17802200 -0.10689200

C 2.80914700 -1.26620600 -0.04633500

C -2.95567900 -1.05148600 -0.03429700

C -0.54044500 5.64043300 0.46218100

C 3.83252700 -0.21593100 -0.32179900

C 5.14537800 -0.71751500 -0.51752100

C 6.27541000 0.03670200 -0.83794300

C 6.08750100 1.41213600 -0.98962900

C -4.73451500 2.31940900 -0.76154100

C -6.03049100 1.86396400 -0.95968500

C -6.31900100 0.50586000 -0.80921700

C -5.24653000 -0.33048500 -0.49522600

C -3.89920900 0.07213600 -0.30486200

C 7.63586600 -0.65992000 -1.01719100

C -7.72812100 -0.08776300 -0.98315900

C 0.90098700 5.58754300 0.45880700

C 1.63829800 6.72175300 0.75383000

C 0.98736600 7.93700000 1.05816800

C -0.40849900 7.97250600 1.05796900

C -1.17683900 6.83360400 0.76295700

C 1.80035200 9.17055400 1.37509200

C 3.35629500 -2.63164300 0.30637100

C -3.60146500 -2.37263000 0.32027200

C 3.72322700 -2.91324500 1.63999200

C 4.22558200 -4.17958900 1.95855200

C 4.37434200 -5.18150300 0.99558200

C 4.00705600 -4.88342300 -0.31945100

C 3.49830500 -3.63093900 -0.68148200

C -3.82159100 -3.35785800 -0.66730700

C -4.42129400 -4.56902200 -0.30374000

C -4.80504700 -4.83946000 1.01251300

C -4.57805500 -3.85203500 1.97523900

C -3.98342500 -2.62675600 1.65523600

C 3.11328500 -3.36750500 -2.12059500

C 3.57986600 -1.86911800 2.72434700

C 4.89084400 -6.55154000 1.36955800

C -3.75849400 -1.59685100 2.73935500

C -3.42356000 -3.12320100 -2.10788300

C -5.42151800 -6.16704200 1.38817700

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C 8.03015600 -1.36164200 0.30464400

C 8.75108200 0.33727300 -1.38486000

C 7.53877900 -1.71362500 -2.14609100

C -8.76836400 0.99035700 -1.34214500

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H 1.15727800 10.02367800 1.61248700

H 4.50653300 -4.38747500 2.98954800

H 4.11980300 -5.64551100 -1.08863200

H -4.59380500 -5.32000600 -1.07275000

H -4.87001400 -4.03887900 3.00720300

H 2.02812400 -3.25314700 -2.23218300

H 3.42974400 -4.19336500 -2.76555500

H 3.56864200 -2.44547100 -2.49895800

H 4.18737500 -0.98158700 2.51151400

H 3.89315600 -2.26792100 3.69424300

H 2.54261800 -1.52690400 2.81709300

H 4.07166700 -7.21769800 1.67256200

H 5.59281200 -6.50055100 2.20895900

H 5.40295300 -7.03074600 0.52817500

H -4.09552100 -1.97238700 3.71057900

H -4.30028500 -0.66695800 2.52995500

H -2.69851200 -1.33172700 2.82718600

H -3.80828600 -2.16851300 -2.48365300

H -3.80528700 -3.92162500 -2.75206400

H -2.33327300 -3.09258900 -2.22418700

H -5.96510000 -6.60952500 0.54645500

H -6.12011600 -6.06268000 2.22547600

H -4.65416400 -6.89061500 1.69516000

H 4.72121800 3.02839600 -0.94667200

H 8.99545700 -1.87052500 0.19176100

H 7.29022500 -2.11048100 0.60530800

H 8.12272200 -0.63559200 1.12062500

H 9.70163100 -0.19626100 -1.49709100

H 8.54575100 0.84820000 -2.33263800

H 8.88977300 1.09858200 -0.60862000

H 6.79669100 -2.48621800 -1.92054700

H 8.50639800 -2.21150900 -2.28460500

H 7.25866500 -1.24536400 -3.09672700

H -9.75633600 0.52894400 -1.45072700

H -8.53059400 1.48758400 -2.28962300

H -8.84631900 1.75746400 -0.56314400

H -9.16758800 -1.19810900 0.22950300

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H -8.20072400 -0.03457600 1.15732600

H -7.40651500 -0.69235400 -3.06654300

H -8.71735000 -1.56687000 -2.25011000

H -7.03051500 -1.96781000 -1.89672500

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C -2.44351700 1.99217800 -0.22154400

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C -1.19229100 1.38321400 -0.32236400

C 1.06354300 4.28770800 0.12252900

C 2.27315600 3.60491300 0.06163600

C 2.34974500 2.17078400 -0.21029000

C 1.14805400 1.47027900 -0.31706500

C -0.67234900 0.01964400 -0.33761500

C 0.73060500 0.07190400 -0.33439300

C -3.69012700 1.22097900 -0.42408900

C 3.65112700 1.49462200 -0.40665400

C 1.56534600 -1.06684800 -0.10041900

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C -0.56279500 -2.33928800 0.12938800

C -1.42136500 -1.17799900 -0.10676600

C -2.80915900 -1.26616200 -0.04625100

C 2.95565900 -1.05153100 -0.03426000

C 0.54055800 5.64042000 0.46223500

C -3.83251000 -0.21587600 -0.32177600

C -5.14533000 -0.71746700 -0.51767800

C -6.27536800 0.03676200 -0.83804500

C -6.08749700 1.41223500 -0.98945100

C 4.73453300 2.31932400 -0.76160500

C 6.03048600 1.86384600 -0.95983800

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C 3.89919800 0.07206700 -0.30492500

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C 7.72805800 -0.08793300 -0.98352200

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C -1.80015600 9.17061200 1.37508300

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C 3.60144300 -2.37265100 0.32040100

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C -4.22585000 -4.17950100 1.95852500

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C -4.00714400 -4.88334600 -0.31945900

C -3.49828800 -3.63088800 -0.68144400

C 3.82145600 -3.35799700 -0.66708600

C 4.42115500 -4.56913800 -0.30343500

C 4.80501900 -4.83943800 1.01281200

C 4.57814100 -3.85189800 1.97544700

C 3.98351600 -2.62664000 1.65536200

C -3.11311100 -3.36748000 -2.12051900

C -3.58010400 -1.86905000 2.72436700

C -4.89118900 -6.55141100 1.36947200

C 3.75870400 -1.59660700 2.73938300

C 3.42333100 -3.12348700 -2.10766200

C 5.42148900 -6.16699300 1.38857900

C -4.82973500 1.96269300 -0.78577000

C -8.03006900 -1.36191600 0.30419600

C -8.75103900 0.33736400 -1.38492800

C -7.53865500 -1.71332800 -2.14660700

C 8.76830700 0.99017800 -1.34251900

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C 7.71480700 -1.14206700 -2.11608400

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H 3.19635900 4.13125100 0.27727800

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H -1.03547200 -3.29341300 0.32873100

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H -6.90472400 2.06725700 -1.27000200

H 4.54825700 3.37442000 -0.92125700

H 6.79839400 2.57799700 -1.23542600

H 5.45920300 -1.38510900 -0.39877700

H -2.72583300 6.68401000 0.75392600

H 0.91452900 8.90607500 1.29236000

H 2.26225800 6.89665400 0.77381600

H -2.43727800 9.45864800 0.52906400

H -2.46414100 9.00340300 2.23262100

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H -4.50690700 -4.38737200 2.98949500

H -4.11987500 -5.64542800 -1.08864800

H 4.59357700 -5.32021800 -1.07237100

H 4.87017900 -4.03863300 3.00741000

H -2.02793000 -3.25317800 -2.23197000

H -3.42953400 -4.19333200 -2.76550600

H -3.56837100 -2.44542500 -2.49895000

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H -3.89338200 -2.26786200 3.69426300

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H -4.07216200 -7.21736700 1.67332500

H -5.59383500 -6.50029100 2.20830000

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H 4.09579900 -1.97204300 3.71062200

H 4.30050900 -0.66675900 2.52982500

H 2.69873800 -1.33143500 2.82727200

H 3.80810200 -2.16887300 -2.48357300

H 3.80496200 -3.92201400 -2.75177400

H 2.33303900 -3.09281600 -2.22390000

H 5.96441500 -6.60990500 0.54666200

H 6.12067700 -6.06243900 2.22536400

H 4.65420500 -6.89029200 1.69637600

H -4.72126600 3.02851100 -0.94626500

H -8.99534200 -1.87082600 0.19118500

H -7.29010100 -2.11078300 0.60470200

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H -9.70156500 -0.19617700 -1.49731400

H -8.54569500 0.84853100 -2.33257400

H -8.88977100 1.09847400 -0.60850300

H -6.79656000 -2.48595300 -1.92121100

H -8.50625900 -2.21120800 -2.28524600

H -7.25853600 -1.24486000 -3.09713900

H 9.75624700 0.52873600 -1.45126000

H 8.53044600 1.48751100 -2.28991800

H 8.84638200 1.75720200 -0.56344900

H 9.16756000 -1.19841200 0.22899200

H 7.48279700 -1.56572000 0.63271500

H 8.20082900 -0.03486300 1.15692800

H 7.40628400 -0.69242700 -3.06691300

H 8.71714600 -1.56702000 -2.25060700

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JL-2-TS

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C -0.15186800 3.55666500 -0.00239100

C -0.08055600 2.20537800 0.00533000

C -1.21457500 1.38383300 0.02905200

C 0.99978000 4.35526100 -0.00956200

C 2.21975300 3.69090400 -0.01808400

C 2.32687300 2.23073700 -0.05726900

C 1.13293500 1.50486500 -0.01329600

C -0.67123400 0.03065000 0.01925700

C 0.73075000 0.10302400 0.00116000

C -3.71908900 1.17633900 0.18011500

C 3.64801900 1.55846500 -0.15069200

C 1.58043600 -1.04351700 0.03539000

C 0.82952000 -2.29884800 0.02055100

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C -3.83604100 -0.25948700 0.02268600

C -5.16585200 -0.77444700 0.02622000

C -6.32859200 -0.04555000 0.24939500

C -6.16572900 1.31967200 0.51420400

C 4.76002100 2.38341300 -0.40707900

C 6.07829700 1.95136200 -0.42932300

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C 3.90802000 0.13665900 0.00013900

C -7.72892100 -0.68091600 0.24191300

C 7.79989400 0.04247700 -0.13365600

C -0.98480400 5.66824200 -0.03001300

C -1.73977900 6.82853500 -0.04778000

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C -4.90458500 1.88531800 0.47059000

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C -8.37784200 -0.50151300 1.63534500

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C 7.96711100 -1.03235700 -1.23446100

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