Theoretical Calculation

All density functional theory (DFT) calculation was performed using the Gaussian 09 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.

The frontier orbital.

The Cartesian coordinates of all the optimized structures.

JL-1

C -2.41942025 1.23343959 -0.25245443

C -2.44200227 2.65699095 -0.11667296

C -1.32641451 3.48746697 -0.01842339

C -0.01498588 2.89075936 -0.00727893

C -0.01020496 1.48900193 -0.12093169

C -1.15730836 0.66184381 -0.19629961

C 1.29236487 3.48035506 0.15365526

C 2.41526000 2.66883504 0.00772754

C 2.40030343 1.25849124 -0.23592932

C 1.14535047 0.67350153 -0.19236202

C -0.69484519 -0.71614963 -0.18190857

C 0.69973817 -0.70850256 -0.18859595

C -3.65485513 0.46984340 -0.53954977

C 3.64128109 0.52108912 -0.55098947

C 1.50422437 -1.87464703 0.05419697

C 0.70008474 -3.04454102 0.40116060

C -0.65613357 -3.05055128 0.41709584

C -1.48007343 -1.88980343 0.08466609

C -2.86720870 -1.97206384 0.08970248

C 2.89176364 -1.94324588 0.02251124

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C 1.54679013 4.88953627 0.56862383

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C -6.22534048 -0.69251374 -1.09149692

C -5.97950283 0.65812919 -1.35180480

C -4.73200609 1.20036454 -1.07649128

C 4.70269821 1.28896425 -1.06512884

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C 2.72876605 6.99738040 0.27185262

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C -2.48311956 5.51846980 0.91242708

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C 7.57466240 -1.23924083 -1.48247629

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