Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Effective modulation of intramolecular ferromagnetic interaction of diradicals by functionalization of cross-conjugated coupler

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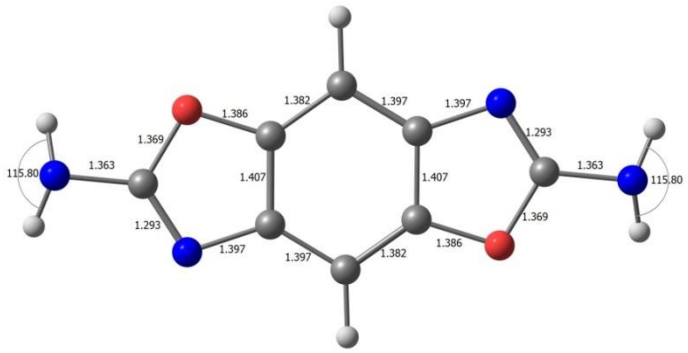
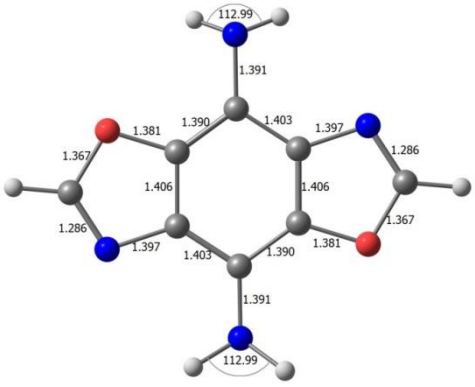
Table S1. List of couplers studied in this reference[1] and their corresponding LUMO energies calculated at B3LYP/6-311++G(d,p).

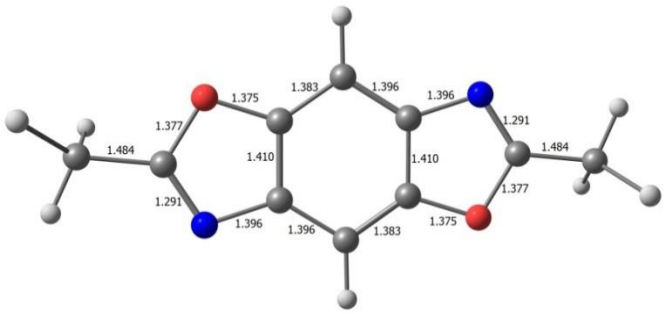
Coupler	LUMO energy (eV)
2,5-furan	-0.17
2,5-pyrrolle	-0.34
2,5-phenylene	-0.48
1,2,4-triazole	-0.50
2,5-thiophene	-0.70
2,5-pyridine	-1.14
2,5-phosphole	-1.45
1,3-azulene	-2.27



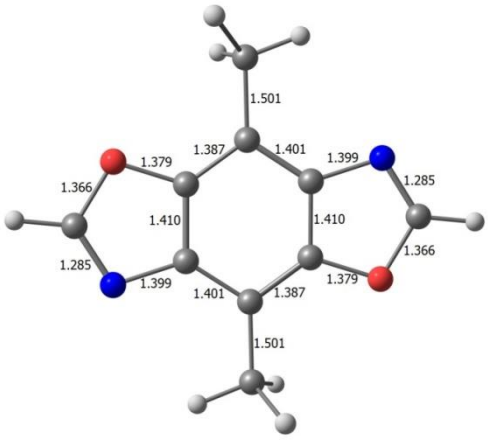
2,6-NH_2



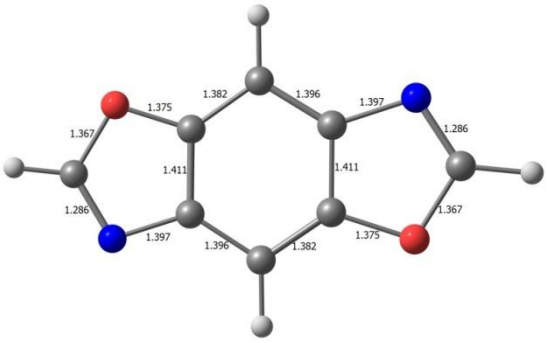
4,8-NH_2



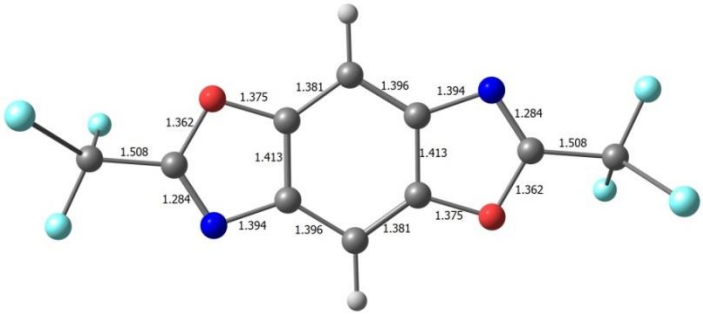
2,6-CH_3



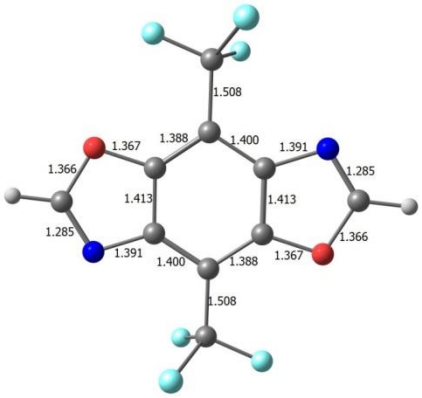
4,8- CH_3



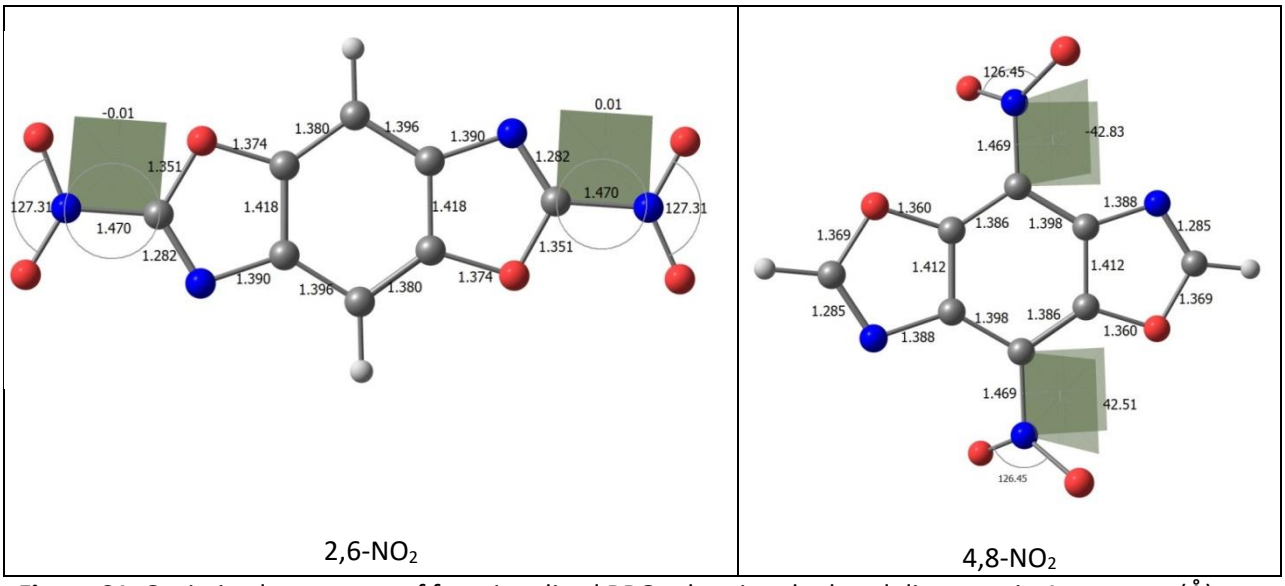
BBO (can also be referred to as 2,6-H or 4,8-H)



2,6-CF_3

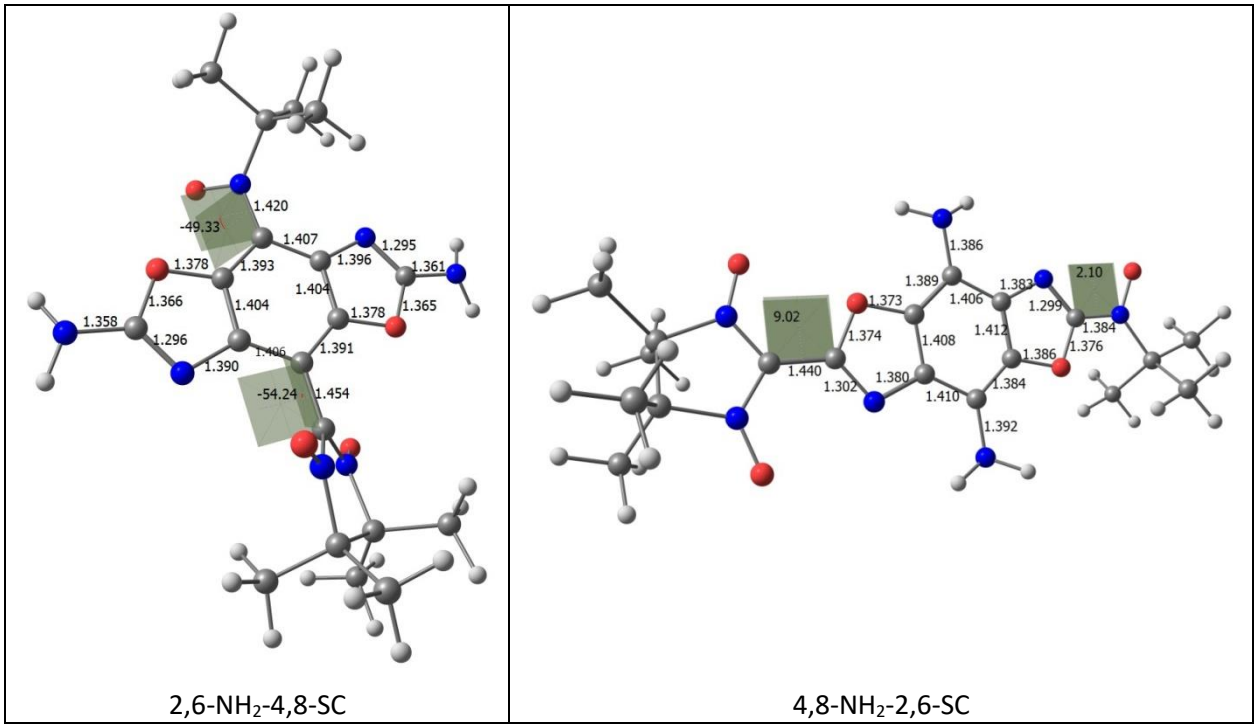


4,8-CF_3

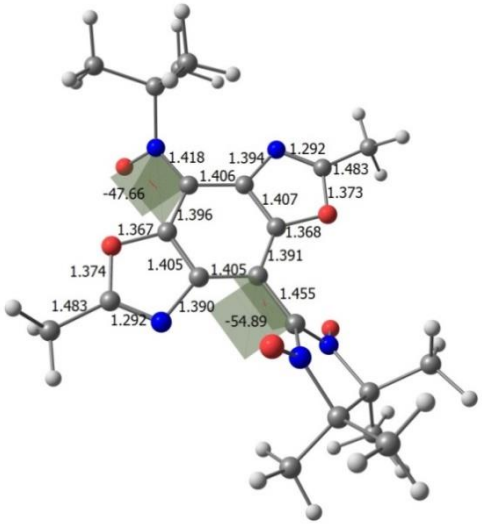


2,6-NO_2 4,8-NO_2

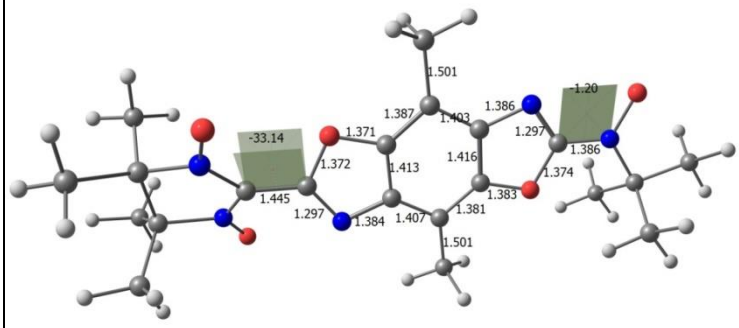
Figure S1. Optimized structures of functionalized BBOs showing the bond distances in Angstroms (Å). Bond angles for NH_2 and NO_2 are also shown as well as the dihedral angle for the case of BBO-NO_2. Structures in the left columns are for the 2,6-X and those in the right are for the 4,8-X (X=substituents).



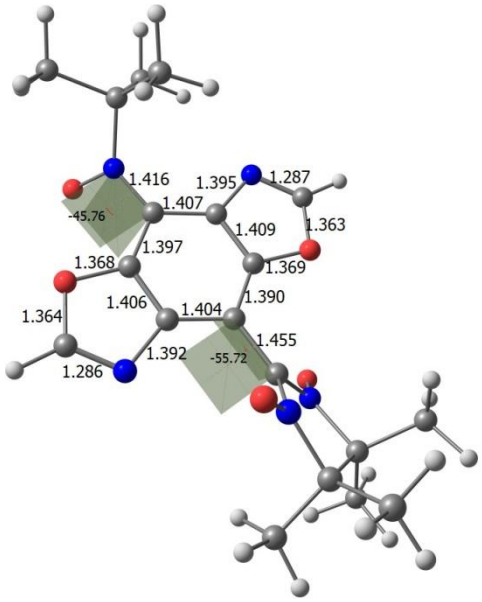
2,6-NH_2-4,8-SC 4,8-NH_2-2,6-SC



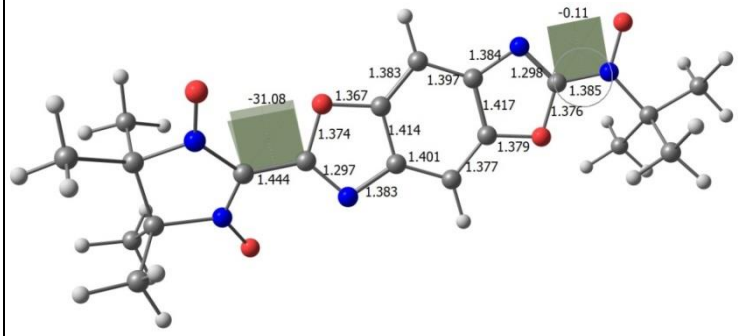
2,6-CH_3-4,8-SC



4,8-CH_3-2,6-SC



2,6-H-4,8-SC



4,8-H-2,6-SC

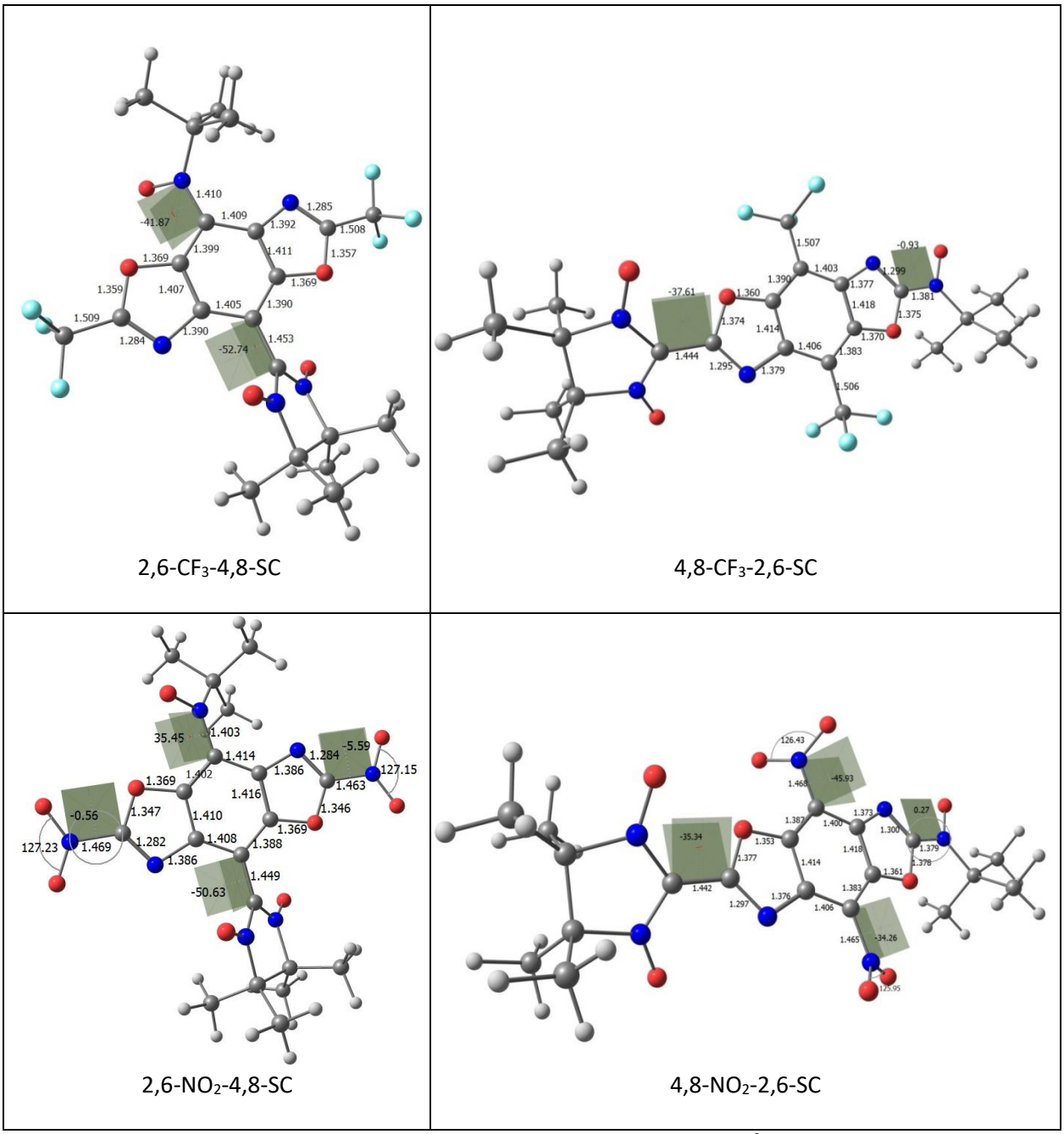


Figure S2. Geometries of diradicalized BBOs showing the bond distances (Å) within the coupler. Dihedral angles (degrees) between the BBO plane and the plane of SCs are also given which are measured according to the sequence C–C–N–O for NO and C–C–C–N for NN.

1. K. C. Ko, D. Cho and J. Y. Lee, *The Journal of Physical Chemistry A*, 2013, **117**, 3561-3568.