Supplementary Materials

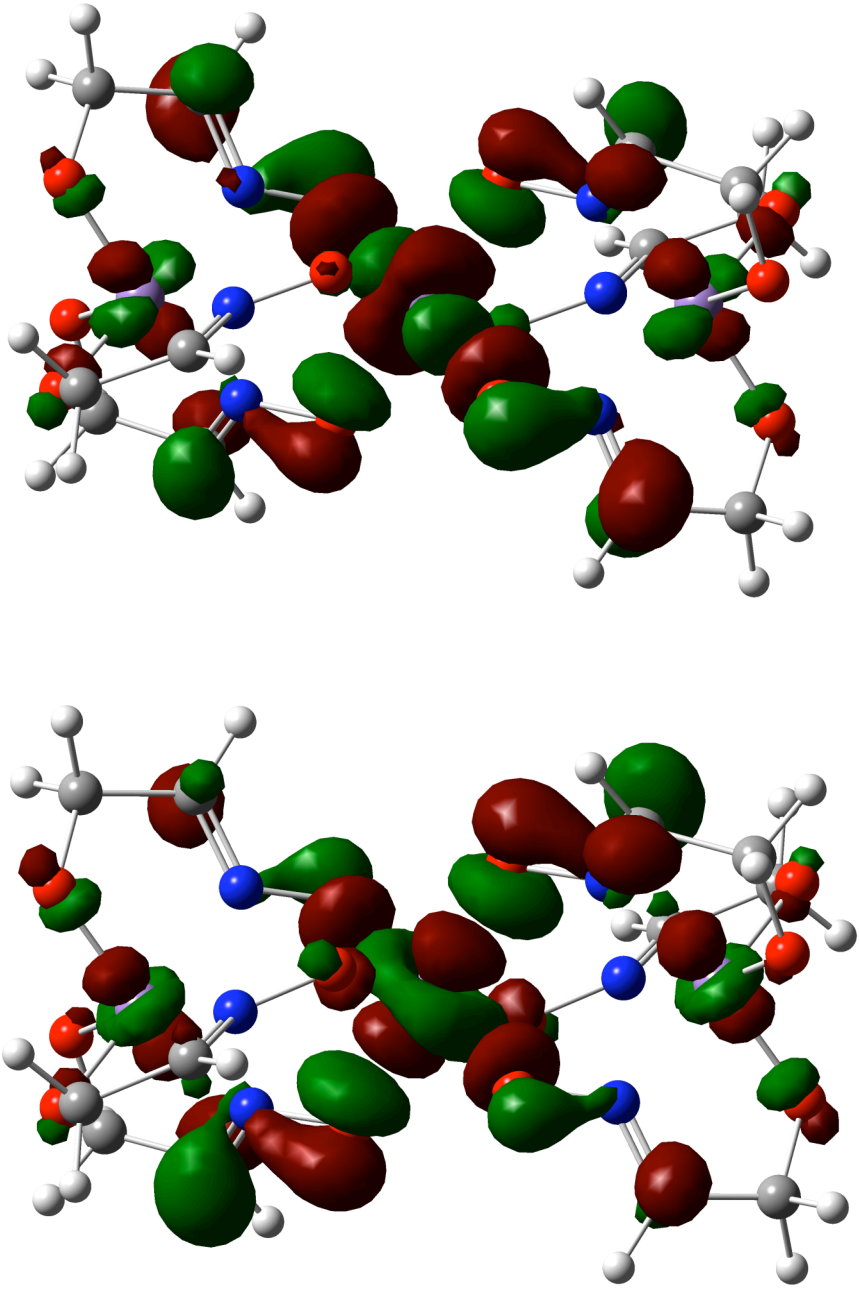

Fig. S1: The two-fold degenerate LUMO of the complex (at the BPE/TZVP level). The contour isosurface value for the orbital plots is 0.03.

Computational Details

Density functional theory (DFT) calculations have been performed using the *Gaussian 03* program.[1, 2] Optimized molecular geometries were calculated using the BPE[3, 4] exchange-correlation functional.

The triple-zeta TZVP[5] basis set and tight SCF convergence criteria were used for calculations. Wave function stability calculations were performed to confirm that the calculated wave functions corresponded to the ground state. Harmonic frequency calculations were performed to ensure that the stationary points were true energy minima.

The analysis of molecular orbitals (MOs) in terms of atomic orbital contributions were carried out using the *AOMix* program[6, 7] and the Mulliken population analysis.[8] Atomic charges were calculated by natural population analysis (NPA)[9] as implemented in Gaussian 03. Two-center Mayer bond orders were obtained using the *AOMix-L* program.[6, 10]

References

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