For table S1 please see the excel sheet provided. All energies are in eV unless otherwise indicated.

For detailed geometries please see the mol2 files which contain all optimized points of every molecule.

The optimizations were performed with ωb97xd/def2-tzvpp model chemistry with an ultrafine quadrature grid as described in the main paper. The processes were restricted to stay within their appropriate point group by using the “symmetry=on” keyword in gaussian. In order to print out all molecular orbitals and to make sure that there was no case of spin contamination we additionally used the keywords “guess=(mix, always)” and “pop=full.” We never saw any case of significant spin contamination, however we continued to use the previous keywords in all cases.

In order to make sure that the optimization would complete even if the normal SCF procedure failed we utilized the keyword “scf=xqc” which makes Gaussian use a quadratically convergent form of the SCF if it is not converged by the conventional algorithm.

In order to obtain the energies in the log files we did a frequency analysis after the optimization to make sure that the geometries were at a minimum in the case of the ground state molecules and at a saddle point transition state like structure for the planar and linear cases. The energies for the orbitals were than taken from the file and were converted to eV from hartrees using the conversion factor of 27.21138602 eV/hartree. This is different than the current 27.211386246 eV/hartree due to Gaussian09 using the 2006 version of various constants. Due to the redefinition of the kilogram (finally!), and other base units, in May of 2019 the value we used and the value that is currently accepted as the constant is different by 113 parts per 500,000,000 million or 0.226 parts per million. We do not expect this to make any difference in our conclusions about the systems studied in the paper.