

Supporting information for: ALL FOR ONE AND ONE FOR ALL: ACCOMMODATING AN EXTRA ELECTRON IN C_{60}

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In this work we analyze the charge difference densities of the electronically stable states of the C_{60}^- anion. All calculations were performed using the geometry of the neutral C_{60} molecule with CC bond lengths of 1.458 Å and 1.401 Å taken from an electron diffraction measurement.¹ The densities for the C_{60}^- anion's states were obtained from our equation-of-motion electron-affinity coupled-cluster singles and doubles (EOM-EA-CCSD) calculations. For the neutral C_{60} , the CCSD density was used. All coupled cluster calculation were performed using CFOUR.²

We use a basis comprised of the cc-pVDZ³ basis set augmented with one diffuse s-type function on the atoms, taken from the corresponding augmented cc-pVDZ basis, and further augmented with 6 s-type, 6 p-type, and 6 d-type diffuse functions positioned at the center of the fullerene. We denote this basis set as DZ(+s)+6s6p6d. This basis set includes a total of 954 spherical Gaussian basis functions. The exponents of the centrally-centered diffuse function are given in Table S1.

In order to construct the density of the anionic states and the neutral C_{60} we had to prepare our own program which could construct the density from the MOLDEN output created in our

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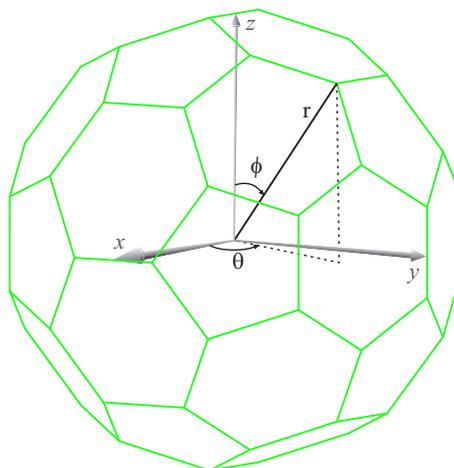


Figure S1: Orientation of C_{60} with respect to Cartesian coordinates and the definition of spherical coordinates used in this work.

Table S1: Even-tempered exponents of the diffuse basis functions placed at the center of the C_{60} molecule. The same exponents were used for the s-type, p-type, and d-type Gaussian type functions.

	s/p/d exponents
1	1.00000000
2	0.28571429
3	0.08163265
4	0.02332362
5	0.00666389
6	0.00190397

computations using the CFOUR package.² The necessity for a special program grew out of two major restrictions of any of the available programs. First most of them could not handle the very large output files created for C_{60} in such a large basis set and second we discuss in the manuscript, we desired to have a spherical representation of the density rather than on a rectangular grid which is also not readily supported. Since the value of the density at each grid point is independent of its value at other grid points, a straight forward parallelization resulted in a linear speed-up and we could easily converge the grid used. We also mention that we found it more convenient to work with a WFN format rather than directly with the MOLDEN output and, therefore, first transformed the output using the molden2aim package.⁴

References

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- (4) Molden2AIM v2.0.0. <http://people.smu.edu/wzou/>.