Supplementary Material for

Bound electronic states of the smallest fullerene C_{20}^- anion

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Table S1: Total (a.u.) and relative (kcal/mol) energies, and the type of stationary points (minimum or saddle point) for the different ground-state structures of C_{20} obtained from a full geometry optimization using the different methods and basis sets.

Method/Basis Set	Symmetry	Total Energy	Relative Energy	Type
MP2/cc-pVDZ	D_{3d}	-759.340389	0.00	Minimum
MP2/cc-pVDZ	D_{2h}	-759.339025	0.86	Saddle
MP2/aug-cc-pVDZ	D_{3d}	-759.449050	0.00	Minimum
MP2/aug-cc-pVDZ	D_{2h}	-759.447680	0.86	Saddle
B3LYP/cc-pVDZ	D_{3d}	-761.501033	0.99	Minimum
B3LYP/cc-pVDZ	D_{2h}	-761.502525	0.00	Minimum
B3LYP/cc-pVDZ	C_{2h}	-761.500943	0.95	Minimum
B3LYP/cc-pVTZ	D_{3d}	-761.670692	0.00	Minimum
B3LYP/cc-pVTZ	D_{2h}	-761.670566	0.08	Saddle
B3LYP/cc-pVTZ	C_{2h}	-761.670525	0.11	Minimum

Table S2: Cartesian coordinates (Å) of the D_{3d} structure of C_{20} used in the EA-EOM-CCSD calculations. The structure was obtained from a full geometry optimization at the CCSD/cc-pVDZ level.

C	-1.1802534214	-0.6814196306	1.4538596246
C	1.1802534214	0.6814196306	-1.4538596246
C	0.7624932991	1.8317172442	-0.6591796852
C	-0.7624932991	-1.8317172442	0.6591796852
C	0.7624932991	-1.8317172442	0.6591796852
C	-0.7624932991	1.8317172442	-0.6591796852
C	0.0000000000	0.0000000000	-1.9512456115
C	0.0000000000	0.0000000000	1.9512456115
C	1.1802534214	-0.6814196306	1.4538596246
C	-1.1802534214	0.6814196306	-1.4538596246
C	-1.9675603144	-0.2555200549	-0.6591796826
C	1.9675603144	0.2555200549	0.6591796826
C	1.2050670155	1.5761971866	0.6591796804
C	-1.2050670155	-1.5761971866	-0.6591796804
C	0.0000000000	-1.3628392597	-1.4538596217
C	0.0000000000	1.3628392597	1.4538596217
C	-1.2050670155	1.5761971866	0.6591796804
C	1.2050670155	-1.5761971866	-0.6591796804
C	1.9675603144	-0.2555200549	-0.6591796826
C	-1.9675603144	0.2555200549	0.6591796826

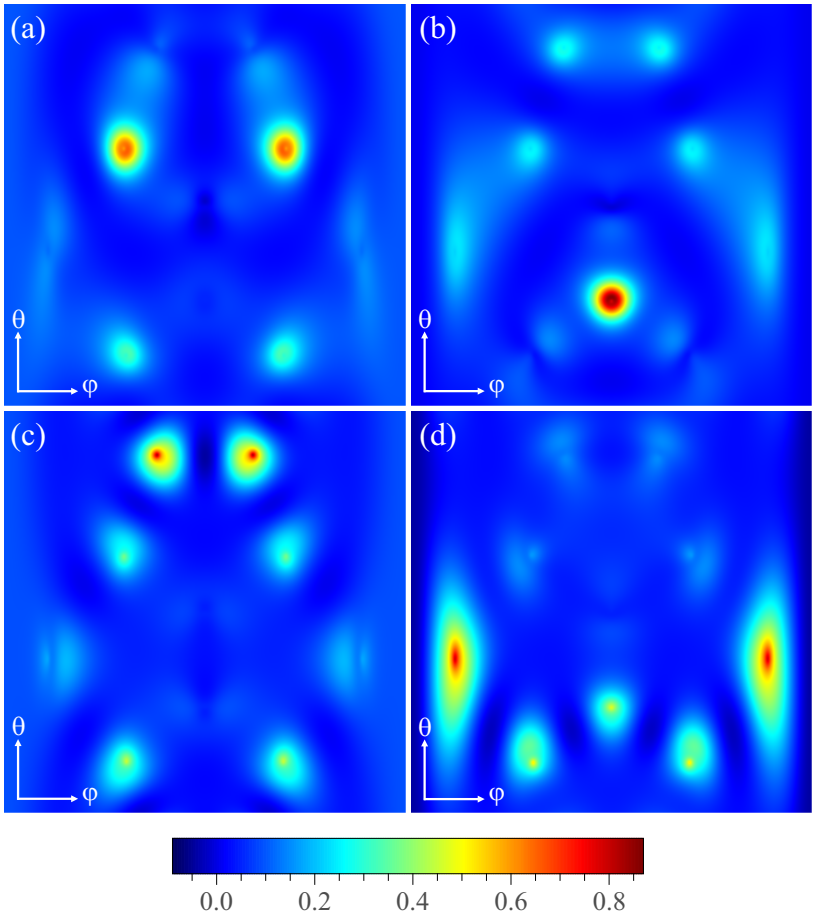

Figure S1: Angular distributaion of the excess electron density for the two components of the 1 ^2E_u [(a) and (b)] and 2 ^2E_u [(c) and (d)] states of C_{20}^-. The range of both the azimuthal (θ) and polar (φ) angles is from 0 to π. The corresponding distributation for $\pi \leq \theta \leq 2\pi$ is identical since the density is symmetric with respect to θ.