Supporting Information: Description of Two-particle One-hole Electronic Resonances using Orbital Stabilization Methods

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Active Spaces

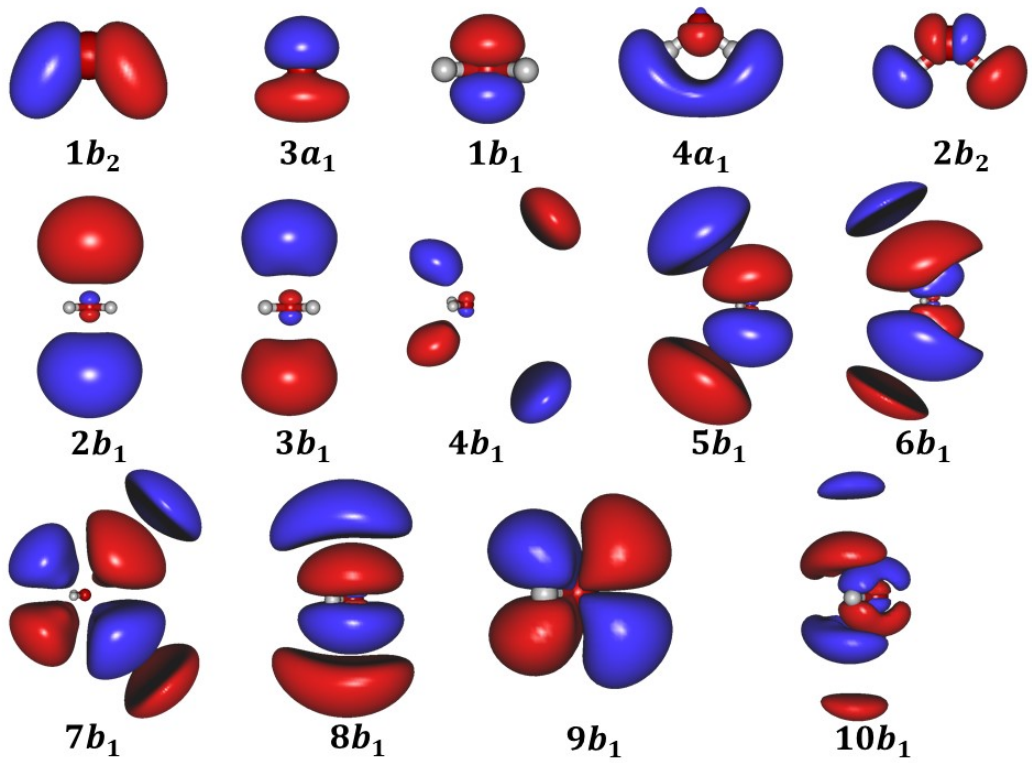

Figure S1: Active space for the RASSCF and MR-CISD calculations on the water anion. The first row contains the orbitals included in the active space (ACT) and the next two rows of diffuse orbitals are included in the auxiliary space (AUX).

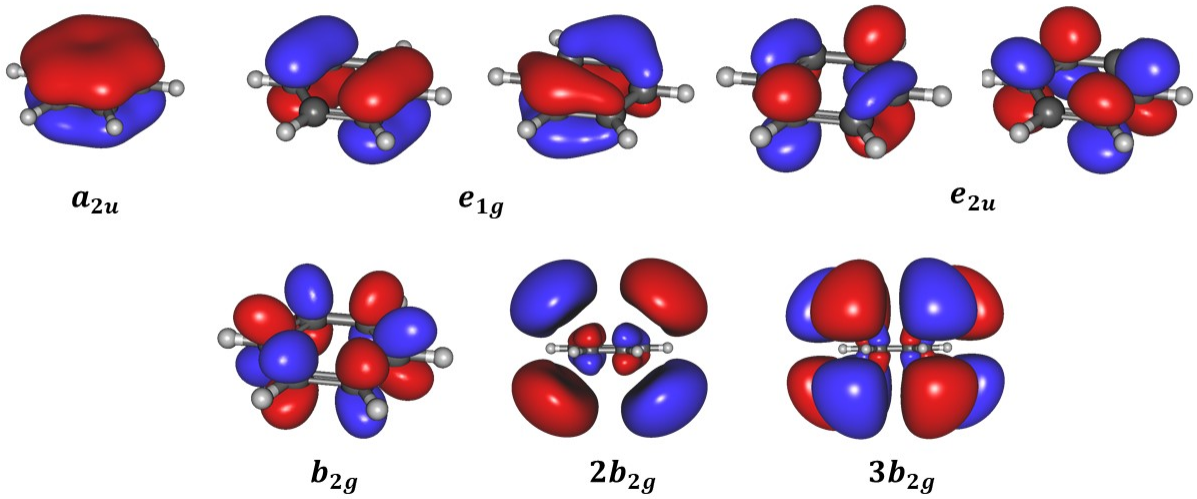

Figure S2: Active space for the RASSCF and MR-CISD calculations on the benzene anion. All the valence π and π^* orbitals are included in the active space (ACT) and the next two diffuse orbitals of the resonance symmetry are included in the auxiliary space (AUX).

Benzene $^2E_{2u}$ shape resonance

Table S1: Resonance position and widths for benzene $^2E_{2u}$ shape resonance obtained at the EOM-EA-CCSD/cc-pVTZ+[p] level. The energies are reported with respect to the neutral reference state.

GPA	$E_R(\Gamma)$/eV
	shape ($^2E_{2u}$)
(3,3,3)	1.64(0.000)
(4,4,4)	1.65(0.015)
(5,5,5)	1.65(0.016)

Cartesian Coordinates

Water Cartesian Coordinates (Angström)

O	0.000000	0.000000	0.118243
H	0.000000	0.758086	-0.472971
H	0.000000	-0.758086	-0.472971

Benzene Cartesian Coordinates (Angström)

H	0.000000	2.475082	0.000000
C	0.000000	1.393682	0.000000
C	1.206964	0.696841	0.000000
H	2.143484	1.237541	0.000000
C	1.206964	-0.696841	0.000000
H	2.143484	-1.237541	0.000000
C	0.000000	-1.393682	0.000000
H	0.000000	-2.475082	0.000000
C	-1.206964	-0.696841	0.000000
H	-2.143484	-1.237541	0.000000
C	-1.206964	0.696841	0.000000
H	-2.143484	1.237541	0.000000