

Structural determination and bonding properties of gas-phase OPt_2^- anion and its neutral

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Table S1. Cartesian coordinates of the low-lying isomers of $\text{OPt}_2^{-/0}$.

A			B				
	X	Y	Z		X	Y	Z
Pt	-0.09917500	-1.28855500	0.00000000	Pt	0.00000000	-0.00000000	-
							1.32713118
Pt	0.00000000	1.03309300	0.00000000	Pt	0.00000000	0.00000000	1.03898355
O	0.96695900	2.49075900	0.00000000	O	0.00000000	-0.00000000	2.80943946
C							
	X	Y	Z		X	Y	Z
Pt	-1.29749100	0.06686500	0.00000000				
Pt	1.29749100	0.06602800	0.00000000				
O	0.00000000	-1.29570900	0.00000000				
A'			B'				
	X	Y	Z		X	Y	Z
Pt	-0.13820700	-1.22198200	0.00000000	Pt	-0.09472600	-1.25419300	0.00000000
Pt	0.00000000	1.22977100	0.00000000	Pt	0.00000000	1.00488200	0.00000000
O	1.34752000	-0.07594200	0.00000000	O	0.92358100	2.43078000	0.00000000
C'							
	X	Y	Z		X	Y	Z
Pt	0.00000000	-1.55192737	-				
			0.04425118				
Pt	-0.00000000	1.55192737	-				
			0.04425118				
O	0.00000000	0.00000000	0.86294776				

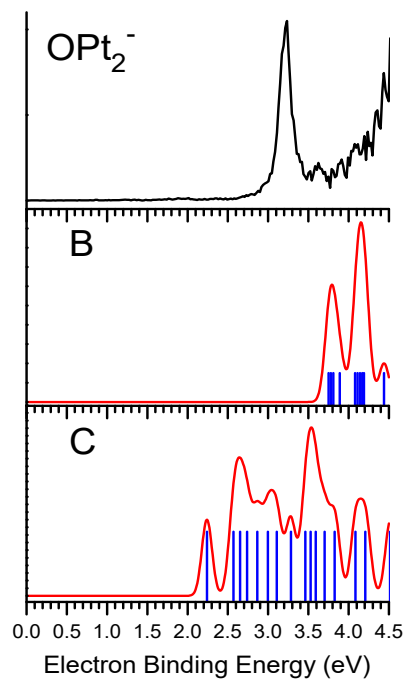


Figure S1. Theoretical simulated 266nm spectra of the low-lying isomers based on the generalized Koopmans' theorem. The blue vertical lines are the theoretical simulated spectral lines, which are correlated with the singly occupied molecular orbital (SOMO) and its lower molecular orbitals of GM. All peaks in the simulated spectra are broadened with unit-area Gaussian functions of 0.15 eV full width at half maximum by shifted to align with the ones at the PBE0 level.

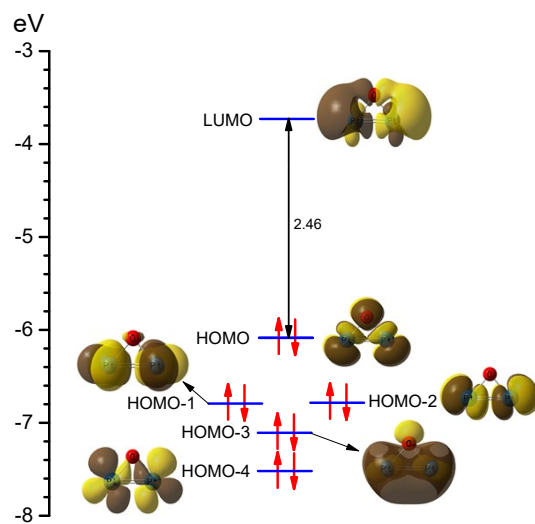


Figure S2. Molecular orbitals of neutral OPT₂ (isosurface value = 0.015).