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## Structural determination and bonding properties of gas-phase OPt<sub>2</sub><sup>-</sup> anion and its

## neutral

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**Table S1.** Cartesian coordinates of the low-lying isomers of  $OPt_2^{-/0}$ .

	А				В			
	Х	Y	Ζ		Х	Y	Ζ	
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	
0	0.96695900	2.49075900	0.00000000	0	0.00000000	-0.00000000	2.80943946	
		С						
	Х	Y	Z					
Pt	-1.29749100	0.06686500	0.00000000					
Pt	1.29749100	0.06602800	0.00000000					
0	0.00000000	-1.29570900	0.00000000					
	۸.					D/		
	V	A	7		V	B	7	
D.	X 0.12020700	Y	L	D,	X	Y 1.25410200		
Pt	-0.13820700	-1.22198200	0.00000000	Pt	-0.094/2600	-1.25419300	0.00000000	
Pt	0.00000000	1.229//100	0.00000000	Pt	0.00000000	1.00488200	0.00000000	
0	1.34752000	-0.07/594200		()	0.97358100	2 430 / 8000		
	1.0 .,02000	0.07574200	0.00000000	U	0.72550100	2.43070000	0.00000000	
	1.0 1,02000	C'	0.00000000	U	0.72550100	2.43070000	0.000000000	
	X	C' Y	Z	U	0.72556100	2.43070000	0.00000000	
Pt	X 0.00000000	C' Y -1.55192737	Z-	U	0.72556100	2.45076000		
Pt	X 0.00000000	C' Y -1.55192737	Z - 0.04425118	U	0.92550100	2.43078000		
Pt Pt	X 0.00000000 -0.00000000	C' Y -1.55192737	Z - 0.04425118	U	0.72338100	2.43078000		
Pt Pt	X 0.00000000 -0.00000000	C' Y -1.55192737	Z 0.04425118 - 0.04425118	0	0.72558100	2.43078000		
Pt Pt O	X 0.00000000 -0.00000000 0.00000000	C' Y -1.55192737 0.00000000	Z 0.04425118 0.04425118 0.86294776	0	0.72558100	2.43078000		



**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  $OPt_2$  (isosurface value = 0.015).