Table S2. Relative energies (eV) of frontier orbitals with respect to the HOMO for $PtCl_6^{2-}$ and $PtBr_6^{2-}$ complexes. Eigenvalues have been shifted in order to set the HOMO to 0eV.

$PtCl_6^{2-}$ MO label	Occupation number	Pt 5d character (%)	$PtCl_6^{2-}$ MO eigenvalue (eV)
$9t_{1u}$	0.	43.2	9.80
$9a_{1g}$	0.	40.	9.37
$8a_{1g}$	0.	50.2	6.30
$5e_g$	0.	35.6	2.04
$1t_{1g}$(HOMO)	6.	0.	0.
$4t_{2g}$	6.	26.6	-0.25
$2t_{2u}$	6.	0.	-0.59
$8t_{1u}$	6	0.	-0.62

$PtBr_6^{2-}$ MO label	Occupation number	Pt 5d character (%)	$PtBr_6^{2-}$ MO eigenvalues (eV)
$10a_{1g}$	0.	50	7.84
$11t_{1u}$	0.	16.9	7.20
$9a_{1g}$	0.	33.4	5.48
$7e_g$	0.	29.6	1.47
$2t_{1g}$ (HOMO)	6.	0.	0.0
$6t_{2g}$	6.	22.3	-0.59
$10t_{1u}$	6.	0.	-0.62
$4t_{2u}$	6	0.	-0.63