

Pb···S and Pb···O σ-hole interactions in the crystal structures of Pb(II) complexes: Experimental and theoretical study

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Supporting Information

	ρ	$\nabla^2\rho$	DI(Pb,S)	ε
BCP1	0.0175	0.0605	0.1110	0.0677
BCP2	0.0120	0.0418	0.0599	0.1147
BCP3	0.0163	0.0378	0.1764	0.1283
BCP4	0.0163	0.0378	0.1764	0.1283
BCP5	0.0122	0.0404	0.0779	0.0173
BCP6	0.0177	0.0431	0.1761	0.1013

Table S1. Values for selected AIM parameters calculated for BCPs 1-6.

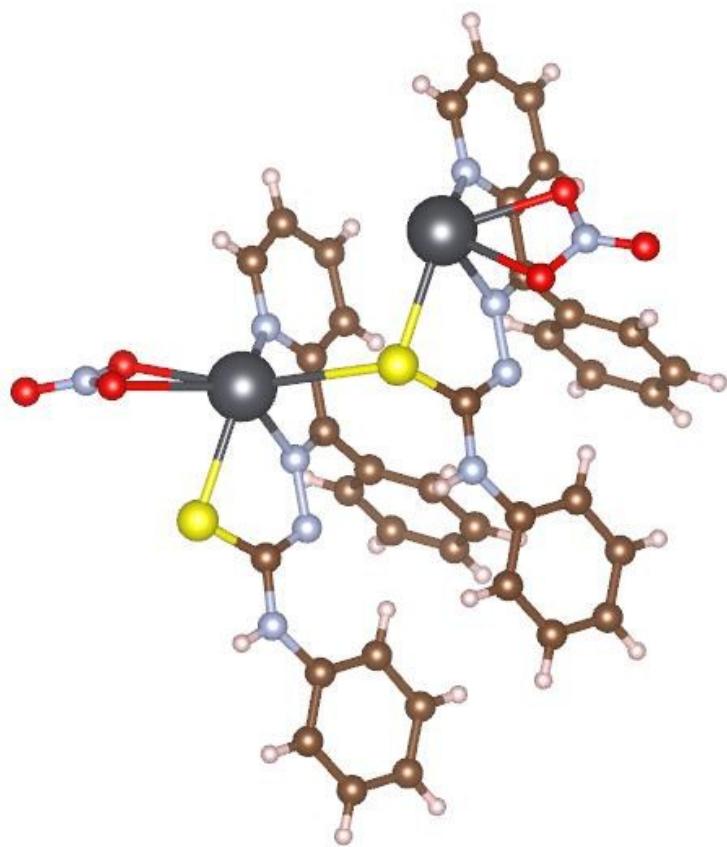


Figure S1. Dimer of **1** modified to preclude Pb...O short contact.