

Table S1: Merz-Kollman partial charges for Pt(phen)(imid)₂

Metal		His		Phen	
<i>Atom name</i>	<i>Charge</i>	<i>Atom name</i>	<i>Charge</i>	<i>Atom name</i>	<i>Charge</i>
Pt	0.560	N ϵ	0.324	N1	0.025
		C ϵ	-0.140	C2	0.001
		N δ	-0.350	C3	0.134
		C δ	-0.448	C4	-0.262
		C γ	0.293	C5	-0.017
		C β	-0.423	C6	0.077
		H ϵ	0.248	C7	-0.219
		H δ N	0.425	H2	0.190
		H δ C	0.267	H4	0.217
		H β 1	0.160	H5	0.192
		H β 2	0.162	H7	0.216