

Table S1. Contributions to the paramagnetic isotropic and the spin-orbit (Fermi contact) isotropic NMR shielding.

Compound	Paramagnetic Isotropic NMR Shielding contribution (ppm)			Fermi contact Isotropic NMR Shielding contribution (ppm)		
	Valence- Virtual	Valence- Valence	total	Valence- Virtual	Valence- Valence	total
$[\text{PtCl}_6]^{-2}$	0	0	0	0	0	0
$[\text{PtCl}_5\text{Br}]^{-2}$	-112.1	-54	-166.7	-76.7	-33.9	-110.7
trans- $[\text{PtCl}_4\text{Br}_2]^{-2}$	-216.8	-109.8	-326.4	-181.3	-76.8	-258
cis- $[\text{PtCl}_4\text{Br}_2]^{-2}$	-237.8	-106.5	344	-156.1	-66.7	-222.8
facial $[\text{PtCl}_3\text{Br}_3]^{-2}$ C_{3v}	-377.1	-154	-531	-263.8	-108.8	-372.6
meridian $[\text{PtCl}_3\text{Br}_3]^{-2}$	-358	-159.1	-516.7	-236.8	-108.8	-372.6
trans $[\text{PtCl}_2\text{Br}_4]^{-2}$	-490.4	-209.7	-699.5	-375.9	-150.3	-526.1
cis $[\text{PtCl}_2\text{Br}_4]^{-2}$	-511.2	-203.6	-714.3	-350.8	-138.5	-489.3
$[\text{PtClBr}_5]^{-2}$	-659	-250	-908.3	-467.5	-178.1	-645.6
$[\text{PtBr}_6]^{-2}$	-821.5	-292.8	-1113.5	-589.3	-216.1	-915.2