

Supporting Information

Table A. Theoretical phosphorus shielding tensors for $M[N(^iPr_2PSe)_2]_2$ ($M = Pd, Pt; Se, Te$)

M^{II}		σ_{iso} ppm	σ_{11} ppm	σ_{22} ppm	σ_{33} ppm	Ω ppm
Pd	SC	222	178	218	269	91
		210	143	228	258	115
	SO	261	239	246	299	60
		244	203	252	278	75
Pt	SC	233	189	234	278	89
		217	151	247	253	102
	SO	277	248	269	315	67
		255	220	255	291	71
Se	SC	214	167	217	257	90
		210	170	209	252	82
	SO	273	239	265	313	74
		270	240	266	305	65
Te	SC	239	202	240	275	73
		237	194	239	278	84
	SO	275	249	268	307	58
		273	243	264	313	70

Table B. Theoretical selenium shielding tensors for the anion of $M[N(^i\text{Pr}_2\text{PSe})_2]_2$ ($M = \text{Pd, Pt; Se, Te}$)

M^{II}		σ_{iso} ppm	σ_{11} ppm	σ_{22} ppm	σ_{33} ppm	Ω ppm
Pd	SC	1526	1140	1468	1968	828
		1534	1187	1602	1812	625
	SO	1698	1331	1606	2159	828
		1716	1395	1767	1985	590
Pt	SC	1607	1250	1540	2032	782
		1604	1265	1631	1916	651
	SO	1986	1467	1717	2174	707
		1793	1487	1815	2077	590
Se	SC	1404	1031	1395	1788	757
		1471	1026	1450	1937	911
	SO	1628	1254	1665	1965	711
		1688	1265	1712	2086	821
Te	SC	1597	1409	1557	1824	415
		1657	1352	1676	1942	590
	SO	1763	1542	1751	1996	454
		1825	1517	1866	2092	575

Table C. Theoretical traceless shielding tensors for nucleus M of $M[N(^i\text{Pr}_2\text{PSe})_2]_2$ (M = ^{105}Pd , ^{195}Pt ; ^{77}Se , ^{125}Te)

M^{II}		σ_{iso} ppm	σ_{11} ppm	σ_{22} ppm	σ_{33} ppm	Ω ppm	κ ppm
Pd	SC	498	-1336	1309	1521	2837	-0.86
	SO	1004	-909	1842	2079	2988	-0.84
Pt	SC	3097	1726	3692	3872	2146	-0.83
	SO	5700	3941	6453	6705	2764	-0.82
Se	SC	1289	1065	1338	1463	398	-0.37
	SO	1378	1307	1353	1475	168	0.45
Te	SC	2063	1554	2255	2382	828	-0.69
	SO	2567	2127	2342	3234	1107	0.61