

## Supplementary Information

Table A. Theoretical phosphorus chemical shift tensors for  $M[N(^1\text{Pr}_2\text{PSe})_2]_2$  ( $M = \text{Zn}, \text{Cd}, \text{Hg}$ )

$M^{\text{II}}$	$\delta_{\text{iso}}$ ppm	$\delta_{11}$ ppm	$\delta_{22}$ ppm	$\delta_{33}$ ppm
Zn	98.7	137.8	103.1	55.3
	97.3	136.3	99.2	56.3
	95.3	132.6	97.3	56.0
	95.2	131.5	98.1	55.9
Cd	100.5	140.2	100.1	61.4
	96.8	137.7	94.3	58.6
	93.2	135.4	86.0	58.2
	88.6	128.3	89.0	48.4
Hg	96.5	138.3	90.9	60.2
	93.0	132.2	94.2	52.4
	92.4	131.0	91.0	55.1
	91.8	131.1	88.6	55.7

Table B. Theoretical selenium chemical shift tensors for  $M[N(^i\text{Pr}_2\text{PSe})_2]_2$  ( $M = \text{Zn}, \text{Cd}, \text{Hg}$ )

$M^{\text{II}}$	$\delta_{\text{iso}}$ ppm	$\delta_{11}$ ppm	$\delta_{22}$ ppm	$\delta_{33}$ ppm
Zn	-291	138	-444	-566
	-292	136	-434	-578
	-292	153	-445	-584
	-293	135	-443	-572
Cd	-320	161	-424	-696
	-337	153	-452	-712
	-341	133	-455	-702
	-348	117	-460	-703
Hg	-235	183	-375	-515
	-243	183	-372	-540
	-246	188	-393	-535
	-249	175	-393	-530

Table C. Theoretical cadmium and mercury magnetic shielding tensors for  $M[N(^1\text{Pr}_2\text{PSe})_2]_2$  ( $M = \text{Cd}, \text{Hg}$ )

$M^{II}$	$\sigma_{\text{iso}}$ ppm	$\sigma_{11}$ ppm	$\sigma_{22}$ ppm	$\sigma_{33}$ ppm
Cd	2809	2798	2801	2828
Hg	5463	5417	5438	5534

Table D. Traceless phosphorus chemical shift tensors for  $M[N(^1Pr_2PSe)_2]_2$  ( $M = Zn, Cd, Hg$ )

$M^{II}$		$\delta_{iso}$ ppm	$\delta_{11}$ ppm	$\delta_{22}$ ppm	$\delta_{33}$ ppm	
Zn	Expt	0	20.3	5.7	-25.9	
		0	20.4	6.6	-27.0	
		0	24.0	5.7	-29.7	
		0	22.1	5.9	-27.9	
	Calc	0	39.1	4.4	-43.4	
		0	39.0	1.9	-41.0	
		0	37.3	2.0	-39.3	
		0	36.3	2.9	-39.3	
	Cd	Expt	0	20.3	4.4	24.7
			0	20.8	4.7	-25.4
0			22.2	3.9	-26.2	
0			21.9	5.0	-26.9	
Calc		0	39.7	-0.4	-39.1	
		0	40.9	-2.5	-38.2	
		0	42.2	-7.2	-35.0	
		0	39.7	0.4	-40.2	
Hg		Expt	0	21.2	4.1	-25.2
			0	21.2	4.1	-25.3
	0		23.5	3.3	-26.9	
	0		22.6	4.9	-27.6	
	Calc	0	41.8	-5.6	-36.3	
		0	39.2	1.2	-40.6	
		0	38.6	-1.4	-37.3	
		0	39.3	-3.2	-36.1	

Table E. Traceless selenium chemical shift tensors for  $M[N(^i\text{Pr}_2\text{PSe})_2]_2$  ( $M = \text{Zn}, \text{Cd}, \text{Hg}$ )

$M^{II}$		$\delta_{\text{iso}}$ ppm	$\delta_{11}$ ppm	$\delta_{22}$ ppm	$\delta_{33}$ ppm	
Zn	Expt	0	420	-174	-247	
		0	420	-151	-269	
		0	403	-155	-247	
		0	439	-159	-279	
	Calc	0	429	-153	-275	
		0	428	-142	-286	
		0	445	-153	-292	
		0	428	-150	-279	
	Cd	Expt	0	438	-114	-324
			0	436	-98	-338
			0	444	-101	-344
			0	444	-101	-344
		Calc	0	481	-104	-376
			0	490	-115	-375
0			474	-114	-361	
0			465	-112	-355	
Hg		Expt	0	405	-122	-283
			0	407	-118	-290
	0		404	-121	-284	
	0		426	-130	-295	
	Calc	0	418	-140	-280	
		0	426	-129	-297	
		0	434	-147	-289	
		0	424	-144	-281	

Table F. Traceless cadmium and mercury chemical shift tensors for  $M[N(^i\text{Pr}_2\text{PSe})_2]_2$  ( $M = \text{Cd}, \text{Hg}$ )

$M^{II}$		$\delta_{\text{iso}}$ ppm	$\delta_{11}$ ppm	$\delta_{22}$ ppm	$\delta_{33}$ ppm
Cd	Expt	0	54	34	-89
	Calc	0	11	8	-19
Hg	Expt	0	296	226	-522
	Calc	0	46	25	-71