Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Matrial for: Accurate spin-orbit and spin-other-orbit contributions to the g-tensor for transition metal containing systems

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S.1 RhC test molecule

Table 1 Gaussian 09 calculations of the g-tensor, using several basis sets and the PBE functional. In Gaussian 09 only the Z_{eff} method was used, so they can only be compared to the non-relativistic calculations of ORCA using the same spin-orbit approximation. All values are expressed as $\Delta g = g_{ortho} - g_e$ in ppt.

	ORCA, Z_{eff}		G09, Z_{eff}	
	Δg_{ortho}	Δg_{para}	Δg_{ortho}	Δg_{para}
VDZ	111.73	0.21	108.1	0.21
VDZ, 2df	91.89	0.22	91.85	0.22
VDZ, 2df, p	96.27	0.22	95.76	0.22
VDZ, ppp, p	94.03	0.22	93.62	0.22
TZV	122.04	0.20	118.84	0.20
TZV, 2df	104.28	0.21	104.32	0.21
TZV, 2df, p	106.09	0.22	105.98	0.22
TZV, ppp, p	103.08	0.22	103.00	0.22
exp	51.78	1.58	51.78	1.58

Table 2 GIPAW results of g-tensor calculation in function of the box size (in Bohr). All values are expressed as $\Delta g = g_{ortho} - g_e$ in ppt.

Box Size	V_{eff}, PM	
	Δg_{ortho}	Δg_{para}
5	−8.76	−47.01
10	40.07	−0.23
15	43.15	−0.11
15	43.15	−0.11
20	48.67	−0.10
25	51.68	−0.10
30	53.22	−0.11
35	54.06	−0.11
exp	51.78	1.58

Molecule	d ($\mathring{A}$)	Molecule	d ($\mathring{A}$)
RhC	1.613	ZnAg	2.550
BO	1.204	YO	1.788
BS	1.609	PdH	1.529
AlO	1.618	CdH	1.781
GaO	1.744	CdF	2.014
ScO	1.668	CdAg	2.727
ZnH	1.595	InO	1.875
ZnF	1.799		

Table 3 Internuclear distances d of the diatomic spin-1/2 molecules as reported by P. Belanzoni, E. van Lenthe and E. J. Baerends, J. Chem. Phys., 2001, **114**, 4421-4433

S.2 Doublet Molecules

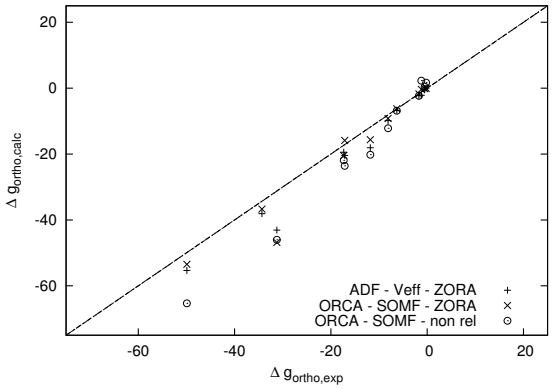

Figure 1 Correlation diagram between $\Delta g_{ortho,exp}$ and $\Delta g_{ortho,calc}$ (y-axis) for several doublet molecules. Results of SOMF (with and without ZORA) and ADF (two-component method) are presented. For all calculations a triple-ζ quality basis set with polarization functions (Ahlrichs 2df if possible) was used.

S.3 High Spin Molecules

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Molecule	d ($\mathring{A}$)	Molecule	d ($\mathring{A}$)
B_2	1.618	CrN	1.556
NH	1.053	Ge_2^+	2.461
NF	1.343	$GaAs^+$	2.744
NCl	1.643	YB^+	2.263
NBr	1.808	YAl^+	2.816
NI	2.007	ZrV	2.076
O_2	1.235	MoN	1.659
PH	1.453	NbO	1.714
SeO	1.677	$TiNb$	2.046
SO	1.518	$ZrNb$	2.245
$S2$	1.931	CrF	1.784
BC	1.496	$CrAg$	2.554
C_2^+	1.418	MnO	1.629
AlC	1.986	MnS	2.043
SiB	1.935	MnH	1.710
$SiAl$	2.459	MnF	1.833
Si_2^+	2.327	$MnCl$	2.241
VO	1.597	$MnBr$	2.395
TiV	1.835	$MnAg$	2.539
V_2^+	1.741		

Table 4 Internuclear distances d of the diatomic high spin molecules as used by S. Pathkovskii and T. Ziegler, J. Phys. Chem. A, 2001, **105**, 5490-5497