Supplementary Table.

Computed values of the ligand-field parameters of bisphenoidally distorted tetrahedral complexes.

The table consists of four parts. The top three parts contain the parameters of the symmetry-based or non-additive ligand field, the bottom part of those of the additive AOM. Within each symmetry-based set, the values given in the top pair of rows are those based upon the complete set of states of the partially filled shell and calculated from the 45 linear equations mentioned in the main text. The values of the second pair of rows are based on the Kohn-Sham orbital energy differences of the AOC computation, and those in the last pair are calculated from the AOM parameters of the lowest part of the table by using eq.(2). Note how the AOM parameterization represents a "data" reduction relative to the symmetry-based one.

		F	Cl	Br	I
Δ	V^{III}	-0.693(7)	-0.513(8)	-0.459(8)	-0.388(9)
	Cr^{IV}	-0.972(6)	-0.693(7)	-0.613(7)	
$[\Delta]_{AOC}$	V^{III}	-0.690	-0.499	-0.435	-0.380
	Cr^{IV}	-0.971	-0.686	-0.594	
$[\Delta]_{AOM}$	V^{III}	-0.690	-0.516	-0.464	-0.394
	Cr^{IV}	-0.969	-0.696	-0.618	
Δe	V^{III}	0.263(11)	0.111(12)	0.086(12)	0.054(11)
	Cr^{IV}	0.234(9)	0.092(11)	0.064(12)	
$[\Delta e]_{AOC}$	V^{III}	0.269	0.114	0.087	0.052
	Cr^{IV}	0.241	0.095	0.066	
$[\Delta e]_{AOM}$	V^{III}	0.251	0.123	0.101	0.077
	Cr^{IV}	0.221	0.104	0.082	
Δt_2	V^{III}	0.504(10)	0.349(11)	0.312(10)	0.269(11)
	Cr^{IV}	0.613(8)	0.420(10)	0.373(10)	
$[\Delta t_2]_{AOC}$	V^{III}	0.498	0.332	0.286	0.245
	Cr^{IV}	0.611	0.408	0.353	
$[\Delta t_2]_{AOM}$	V^{III}	0.517	0.338	0.297	0.246
	Cr^{IV}	0.626	0.409	0.355	
e_σ	V^{III}	1.108(18)	0.699(19)	0.610(19)	0.501(22)
	Cr^{IV}	1.292(15)	0.819(18)	0.706(19)	
e_π	V^{III}	0.427(13)	0.222(14)	0.186(14)	0.145(16)
	Cr^{IV}	0.402(11)	0.207(13)	0.168(14)	