Supplementary Material (ESI) for PCCP

Supporting Information

Comparative Calculation of EPR Spectral Parameters in $[Mo^{V}OX_4]^-$, $[Mo^{V}OX_5]^{2-}$, and $[Mo^{V}OX_4(H_2O)]^-$ complexes.

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Calculation of EPR spectral parameters.

The *g* matrix has been calculated by coupled perturbed method using well-known approach:[1,2,3,4]

$$g = g^{e} + \Delta g^{RMC} + \Delta g^{DC} + \Delta g^{OZ/SOC} \qquad (2)$$

The first term is the *g* value of the free electron ($g^e = 2.002319$) and is isotropic in nature. The second term represents a relativistic mass correction which was calculated from the kinetic energy integrals and the ground state spin density following equation 3:

$$\Delta g^{RMC} = -\frac{\alpha^2}{S}\sum_{ij} P_{ij}^{\alpha-\beta} < \varphi_i \mid \hat{T} \mid \varphi_j > \qquad (3)$$

In equation 3, α represents the fine structure constant, the total spin of the ground state is represented by *S*, $P_{ij}^{\alpha-\beta}$ is the SCF-based unrestricted spin density matrix, φ represents the Gaussian basis set, and $\hat{T}$ is the kinetic energy operator ($\hat{T} = -1/2\nabla^2$). The third term in equation 2, is a diamagnetic correction term that was calculated using the SCF spin density as (equation 4):

$$\Delta g^{DC} = \frac{1}{2S}\sum_{ij} P_{ij}^{\alpha-\beta} < \varphi_i \mid \sum_{A} \xi(r_A)[\vec{r}_A \vec{r} - \vec{r}_{A,r} \vec{r}] \mid \varphi_j > \qquad (4)$$

In equation 4, $\vec{r}_A$ represents the position vector of the electron with respect to nucleus *A*, while $\vec{r}$ represents the position vector relative to the gauge origin, and $\xi(r_A)$ is a spin-orbit coupling function, which is expressed as in equation 5:

$$\xi(r_{iA}) = \frac{\alpha^2}{2}\frac{Z_{eff}^{A}}{|r_i - R_A|^3} \qquad (5)$$

where, Z_{eff}^{A} is a semi-empirically estimated effective nuclear charge of atom A at position R_A. The operator described in the equation 5 has been parameterized by Koseki[5,6] which gives reasonable results for transition-

metal compounds. Although the operator $\xi(r_A)$ is less sophisticated as compared to recent approaches originated from Kaupp's group, it is expected to be reasonable (as shown *a posteriori* by the presented results) for the calculations of EPR spectral parameters in d^1 Mo^V complexes in which no d-d electron repulsion is present. The final term in equation 2, ($\Delta g^{OZ/SOC}$), which is the major perturbation to the overall Δg, arises as a cross term between the orbital Zeeman (this is a gauge including atomic orbital, GIAO method, equation 6) and spin-orbit coupling (equation 7) operators and was calculated as shown in equation 8:

$$\hat{H}^{OZ} = \beta \sum_i \vec{B}\,\vec{l}(i) \qquad (6)$$

$$\hat{H}^{SOC} = \sum_{A,i} \xi(r_{iA})\vec{l}_A(i)\vec{s}(i) \qquad (7)$$

$$\Delta g_{rs}{}^{OZ/SOC} = \frac{1}{\beta S}\frac{\partial^2 E}{\partial \vec{B}_r \partial \vec{\mu}_s} \qquad (8)$$

where, $\vec{l}(i)$ is the angular momentum operator of the i^{th} electron relative to the chosen gauge origin, $\vec{s}(i)$ is a spin operator for the i^{th} electron, $\vec{l}_A(i)$ is the angular momentum operator of the i^{th} electron relative to nucleus A, and $\vec{\mu}_s$ is the magnetic moment of the electron. Implementation of equation 2 into coupled perturbed SCF theory both at Hartree-Fock and Density Functional Theory levels has been described in the literature.[7]

The principal values of the A^{Mo} tensor was calculated as the sum of isotropic (Fermi contact term) and anisotropic (spin dipolar term) contributions:**Error! Bookmark not defined.**,[2]

$$A_{11} = A_F + A^{Mo}{}_1$$

$$A_{22} = A_F + A^{Mo}{}_2$$

$$A_{33} = A_F + A^{Mo}{}_3$$

The Fermi contact term is directly proportional to the spin density at the molybdenum nucleus and was estimated as:

$$A_F(Mo) = 8\pi/3\, g_e g_{Mo} \beta_e \beta_{Mo} \sum_{\mu,\lambda} P^{\alpha-\beta} \langle \chi_\mu | \delta(r_{Mo}) | \chi_\lambda \rangle$$

Where $P^{\alpha-\beta}$ is the spin density matrix; χ_μ and χ_λ are atomic basis functions; $r_{Mo} = r - R_{Mo}$ (R_{Mo} is the position of the molybdenum nucleus); β_e and β_{Mo} are Bohr and nuclear magnetons, respectively; g_{Mo} is the ratio of molybdenum magnetic moment (in units of β_{Mo}) and the total spin of molybdenum nucleus. The components of the symmetric and traceless anisotropic hyperfine coupling tensor A^{Mo} reflect the asymmetry of the spin density around the molybdenum nucleus which was estimated as:

$$A_{uv}(Mo) = g_e g_{Mo} \beta_e \beta_{Mo} \sum_{\mu,\lambda} P^{\alpha-\beta} \langle \chi_\mu | r^{-5}_{Mo} (r^2_{Mo} \delta_{uv} - 3 r_{Mo,u} r_{Mo,v}) | \chi_\lambda \rangle$$

The majority of the molecules discussed in here belong to C_{4v} point group, and in these case, diagonalization of A^{Mo} leads to $A^{Mo}_1 = A^{Mo}_2 \neq A^{Mo}_3$ ($A^{Mo}_1 + A^{Mo}_2 = -A^{Mo}_3$). In molecules with lower symmetry *e.g.* $[Mo^{V}OX_4(H_2O)]^-$, however, the hyperfine constants are unequial such that $A^{Mo}_1 \neq A^{Mo}_2 \neq A^{Mo}_3$ where $A^{Mo}_1 \approx A^{Mo}_2$.

Basis sets tested for the prediction of EPR parameters. In the present study, the relatively small (18s12p9d) DGauss full-electron DZVP basis set has been tailored for the accurate prediction of EPR *g*-tensors and *A* values by substituting original *p* and *d* basis functions in the DZVP basis set with either Stuttgart/Dresden effective core potentials or basis functions from the Ahlrich's basis set. These modified basis sets are presented in Supporting Information and Supporting Information Table 1 and can be described as follows: in all cases, sU stands for the use of the unrestricted *s* part of the DZVP basis set while all other modifications on the original DZVP basis set and SDD have been used or Ahlrich's basis set derived exponents that are used in all cases of addition. In the case of BS3 – BS10, one *p* function was removed and replaced with 2 SDD *p* functions, and, in the case of BS3, the *d* basis functions from the DZVP basis set were used, and in the BS4 – BS10, either one or two *d* functions were removed and replaced with SDD *d* functions. BS11 utilized both *d* and *p* parts of the DZVP basis set. In the case of BS12 – BS18, the *p* part of the DZVP basis set was used while either 1 or 2 *d*

functions were removed and replaced with either 2, 3, or 6 SDD *d* functions with contraction schemes as indicated in Supporting Information Table 1. In both BS19 and BS20, one *p* function was removed and replaced with 2 SDD *p* functions (as in BS3 – BS10). However, the original 4 *d* (contracted as 31) functions were removed and replaced with 6 *d* functions (contracted as 21111) from Ahlrich's basis set. BS20 also has an added *f* function from the Ahlrich's basis set library. In the majority of cases, the 6-311G(d) basis set[8] was used for fluorine, chlorine, bromine, oxygen, and nitrogen atoms. In selected cases, discussed in the results and discussion, a fully uncontracted DGauss DZVP basis set was also used for all atoms except molybdenum.

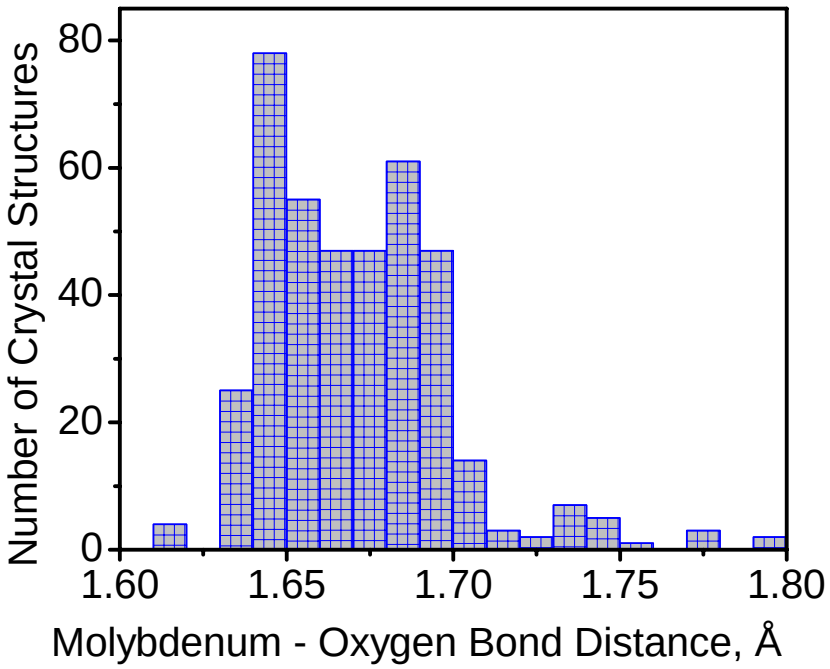

Figure S1. A histogram showing the number of crystal structures and Mo=O bond distances for structures with at least two bonded halogens and R < 5% as obtained from the Cambridge Structural Database.

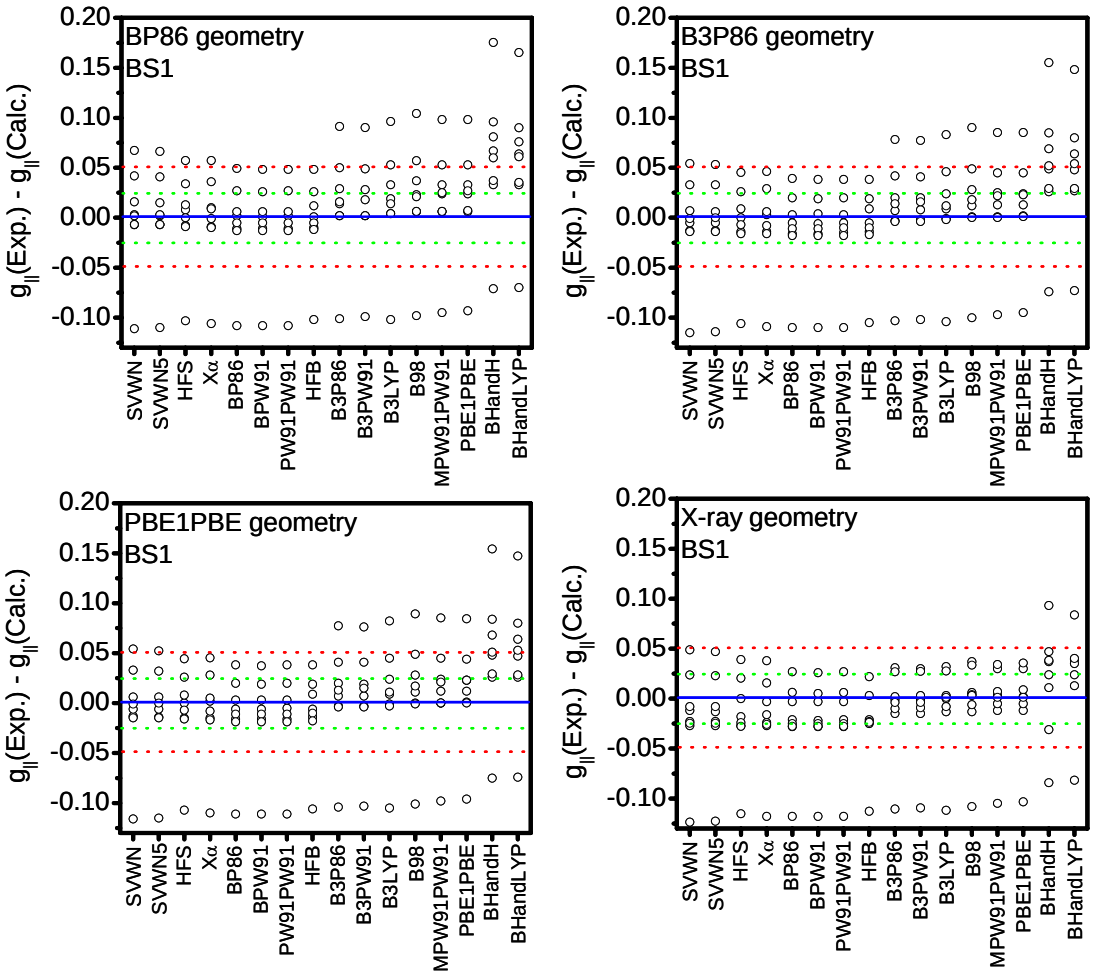

Figure S2. Deviations from experiment for the calculated g|| value (8 complexes) using BS1 and four different geometries. The complexes with the largest deviations are labeled.

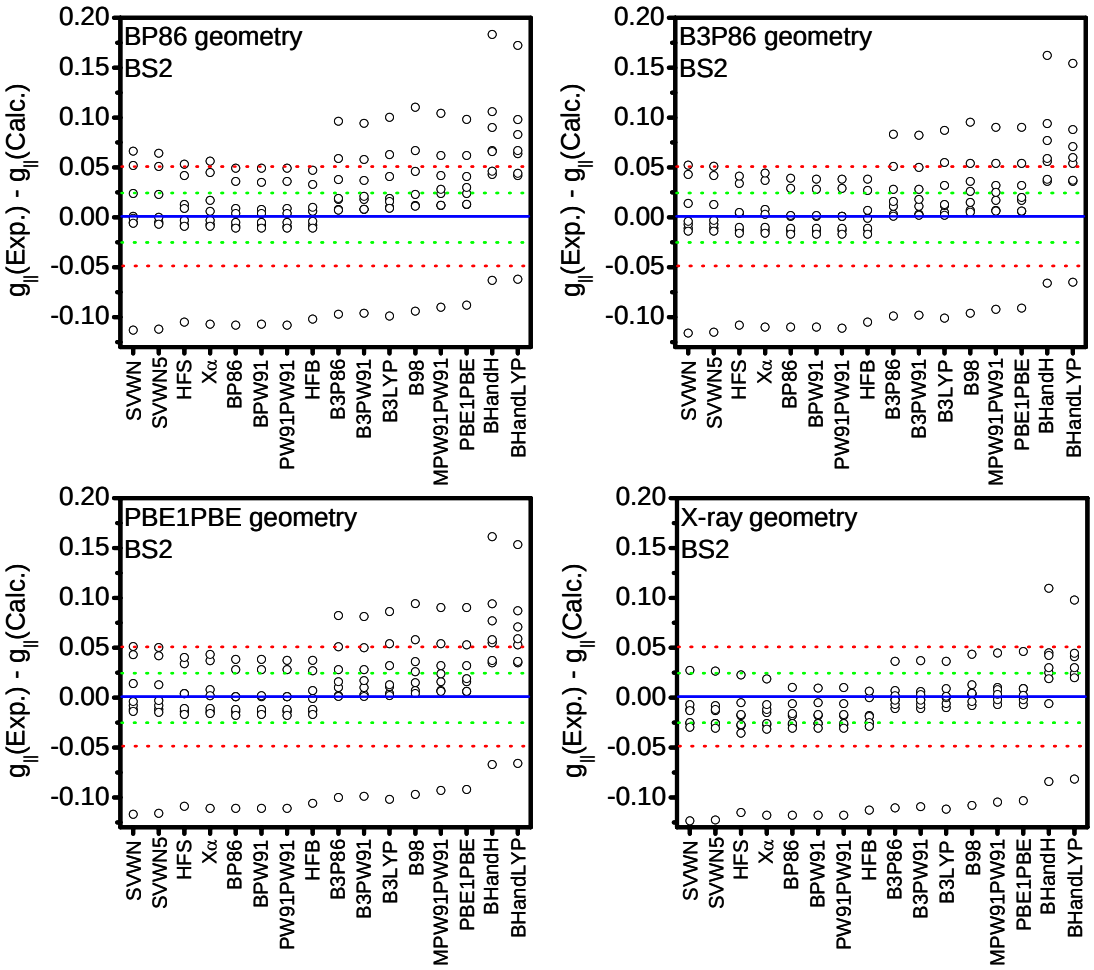

Figure S3. Deviations from experiment for the calculated g|| value (8 complexes) using BS2 and four different geometries. The complexes with the largest deviations are labeled.

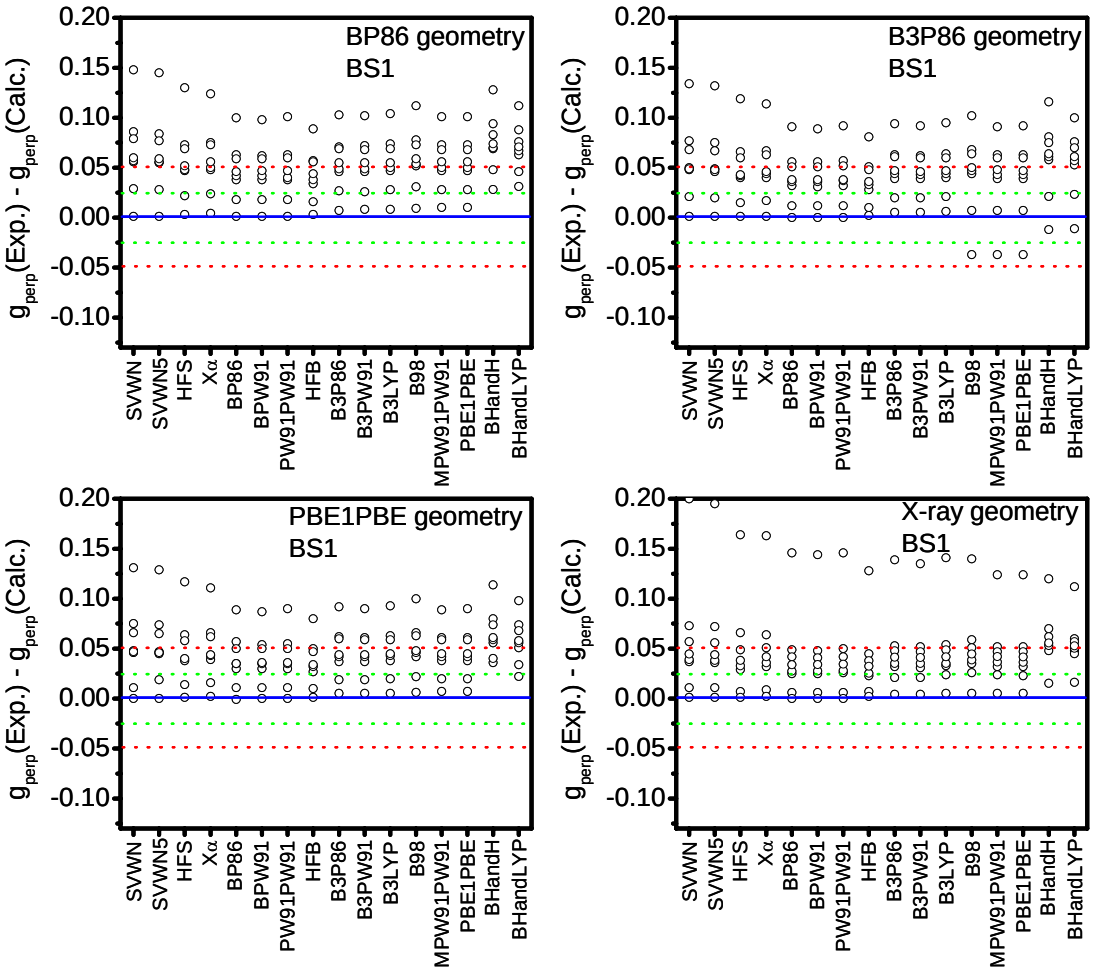

Figure S4. Deviations from experiment for the calculated $g^{\perp}$ value (8 complexes) using BS1 and four different geometries. The complexes with the largest deviations are labeled.

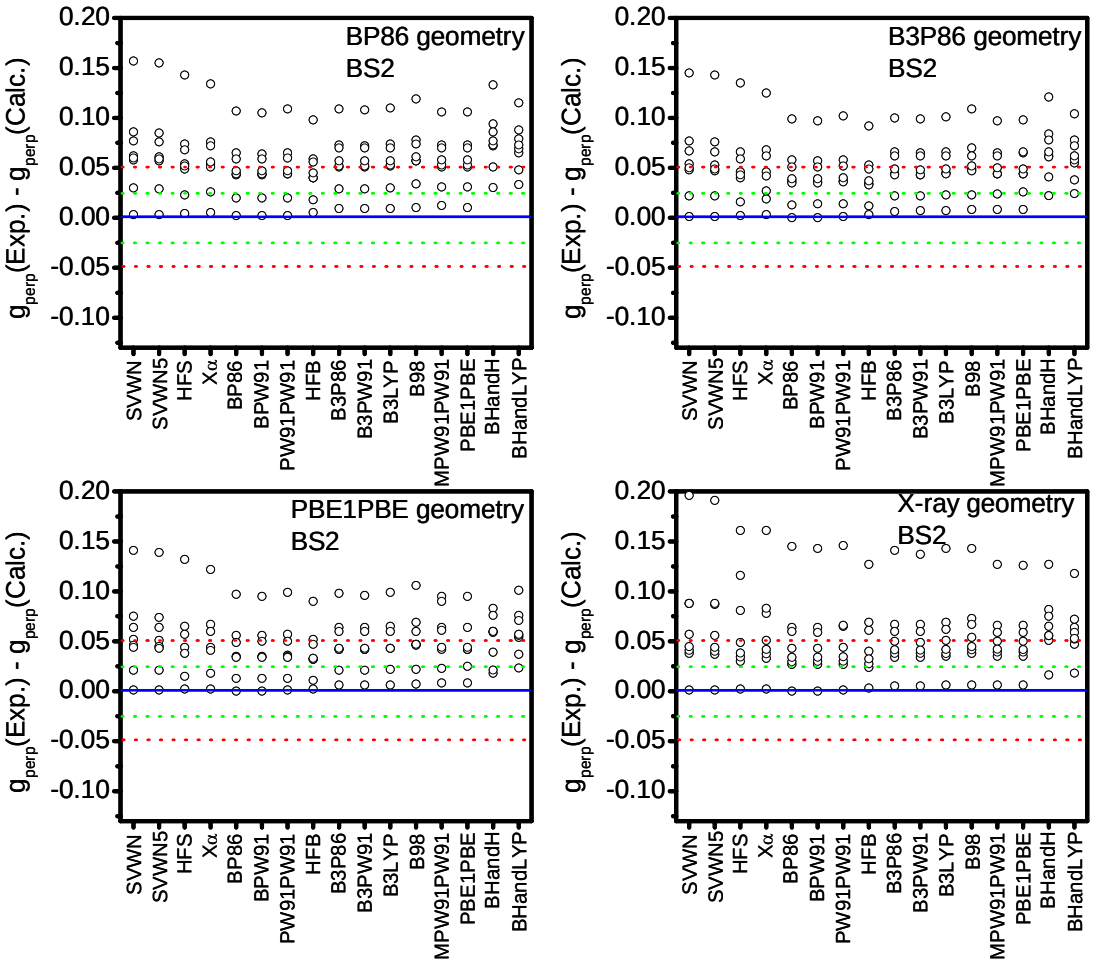

Figure S5. Deviations from experiment for the calculated $g^{\perp}$ value (8 complexes) using BS2 and four different geometries. The complexes with the largest deviations are labeled.

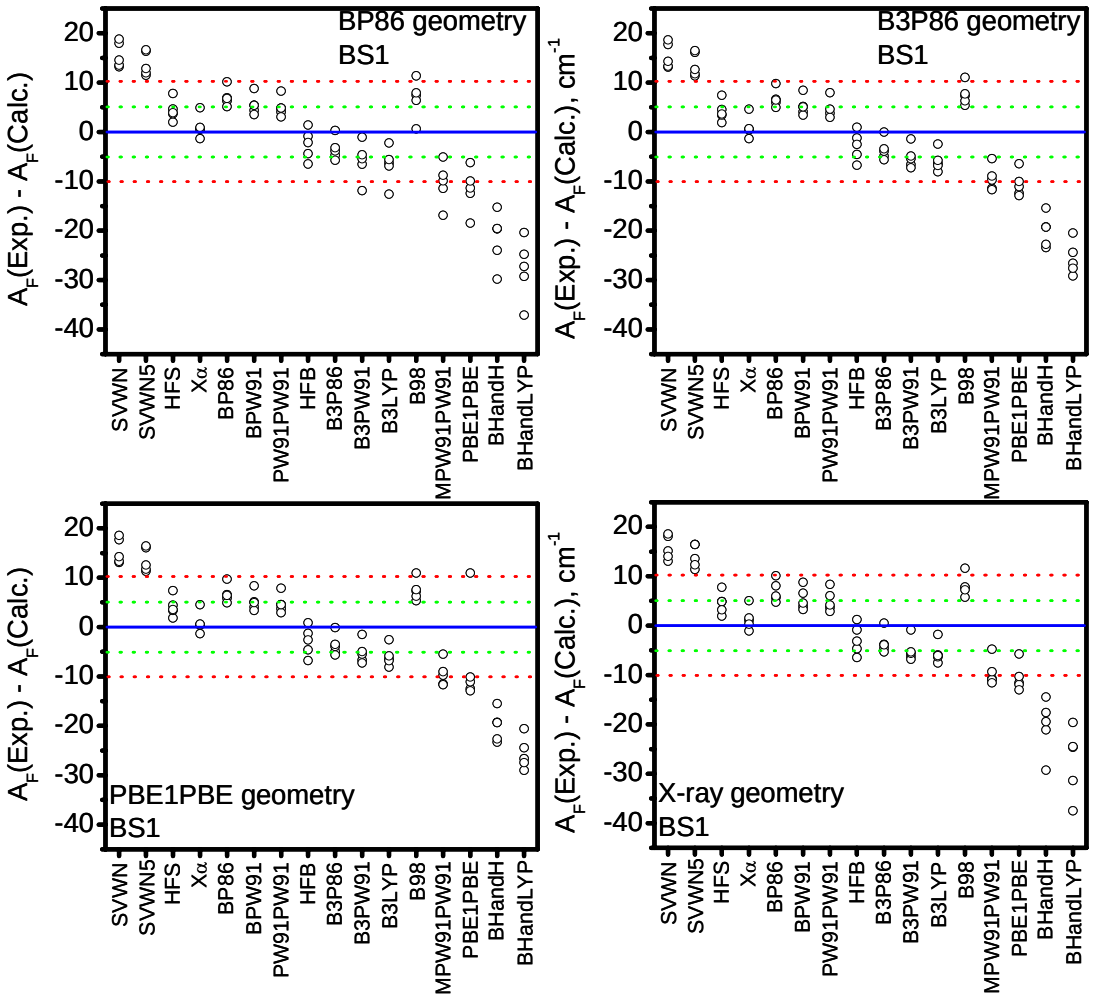

Figure S6. Deviations from experiment for the calculated *AF* value (6 complexes) using BS1 and four different geometries.

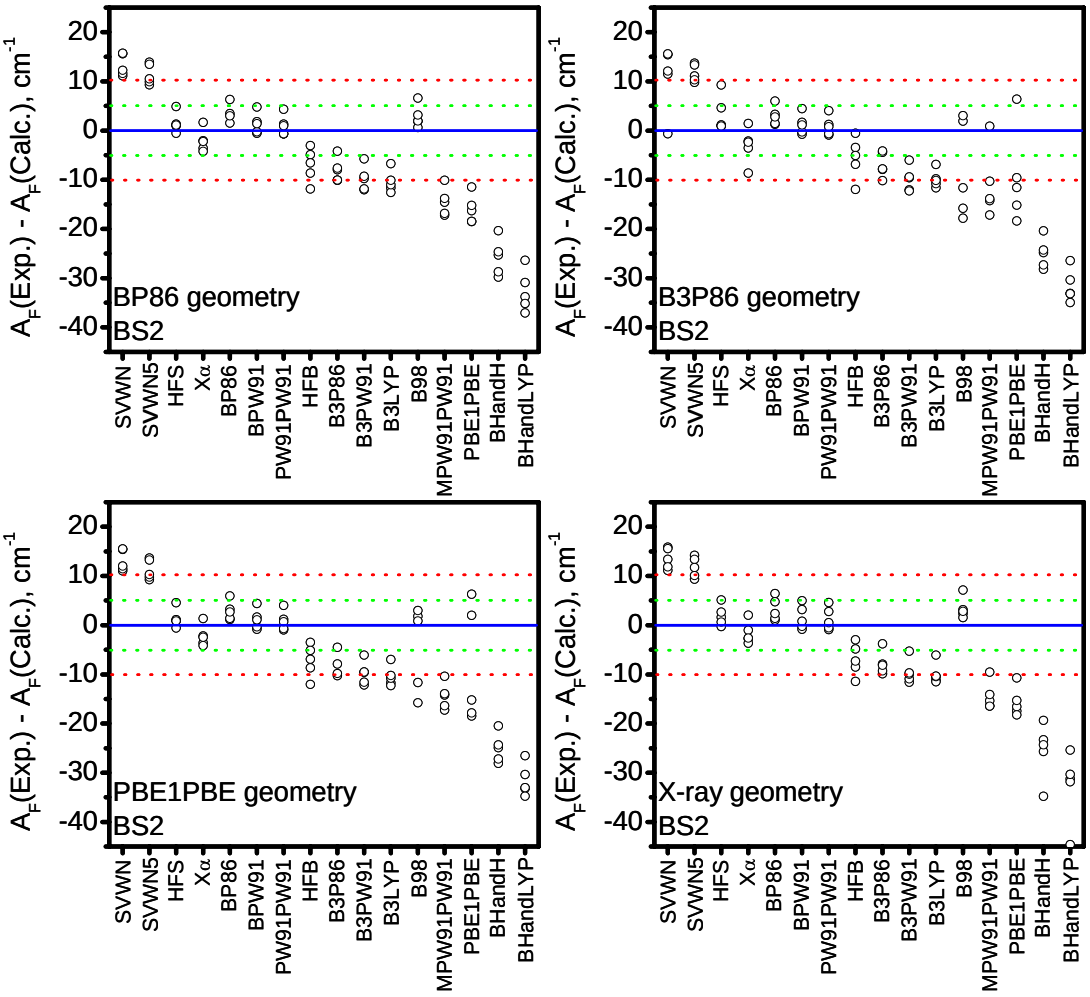

Figure S7. Deviations from experiment for the calculated *AF* value (6 complexes) using BS2 and four different geometries.

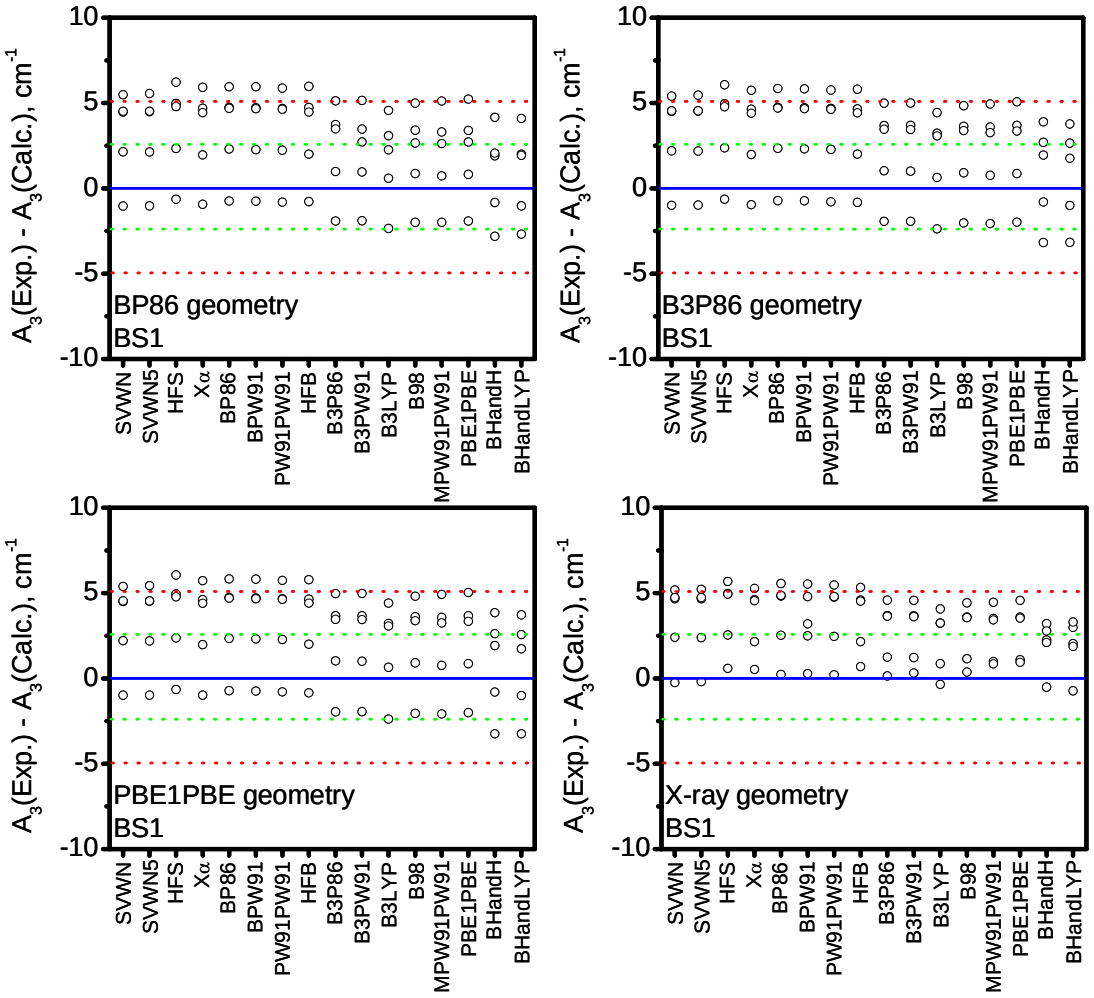

Figure S8. Deviations from experiment for the calculated *AMo3* value (5 complexes) using BS1 and four different geometries.

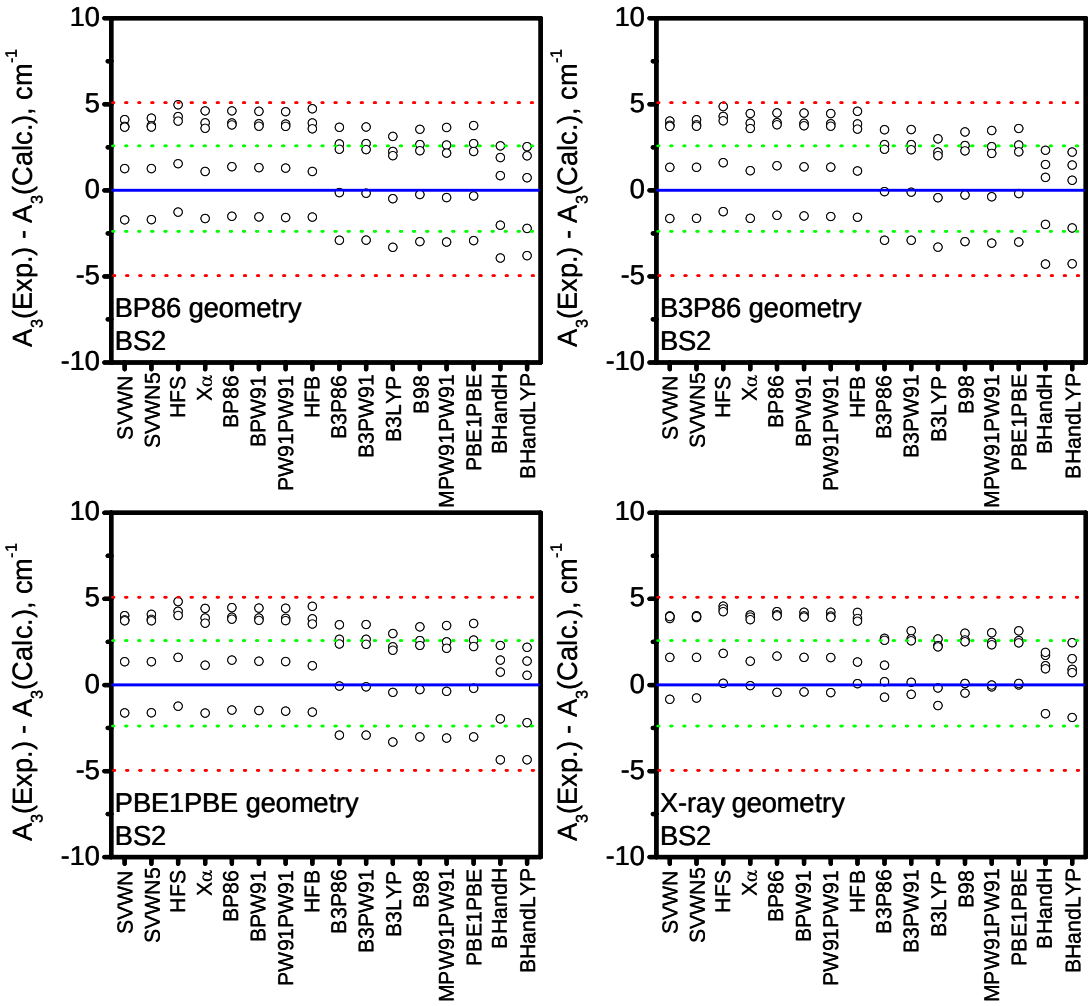

Figure S9. Deviations from experiment for the calculated *AMo3* value (5 complexes) using BS2 and four different geometries.

Table S1. DGauss full-electron DZVP basis set (18s12p9d) modifications used in Tables S2 – S5.

Basis set	*s*-part (contraction)	*p*-part (contraction)	*d*-part (contraction)	*f*-part (contraction)
BS1	Fully uncontracted original DZVP	Original DZVP contraction scheme	Fully uncontracted original DZVP	None
BS2	Fully uncontracted original DZVP	2*p* primitive functions are added with exponents taken from Ahlrich's library	Fully uncontracted original DZVP	1*f* polarization primitive function is added with exponents taken from Ahlrich's library
BS3	Fully uncontracted original DZVP	Original outer *p* function replaced with two diffuse primitives with exponents takes from Ahlrich's library	Original DZVP contraction scheme	None
BS4	Fully uncontracted original DZVP	Original outer *p* function replaced with two diffuse primitives with exponents takes from Ahlrich's library	Original outer 2*d* primitive Gaussians replaced with diffuse uncontracted 3*d* primitive Gaussians taken from Ahlrich's library	None
BS5	Fully uncontracted original DZVP	Original outer *p* function replaced with two diffuse primitives with exponents takes from Ahlrich's library	Original outer 2*d* primitive Gaussians replaced with diffuse 3*d* primitive Gaussians taken from Ahlrich's library contracted as 21	None
BS6	Fully uncontracted original DZVP	Original outer *p* function replaced with two diffuse primitives with exponents takes from Ahlrich's library	Original outer *d* primitive Gaussians replaced with diffuse uncontracted 3*d* primitive Gaussians taken from Ahlrich's library	None
BS7	Fully uncontracted original DZVP	Original outer *p* function replaced with two diffuse primitives with exponents takes from Ahlrich's library	Original outer *d* primitive Gaussians replaced with diffuse 3*d* primitive Gaussians taken from Ahlrich's library contracted as 21	None
BS8	Fully uncontracted original DZVP	Original outer *p* function replaced with two diffuse primitives with exponents takes from Ahlrich's library	Original outer *d* primitive Gaussians replaced with diffuse 6*d* primitive Gaussians taken from Ahlrich's library contracted as 411	None
BS9	Fully uncontracted	Original outer *p* function	Original outer *d* primitive	None

	original DZVP	replaced with two diffuse primitives with exponents takes from Ahlrich's library	Gaussians replaced with diffuse uncontracted 2*d* primitive Gaussians taken from Ahlrich's library	
BS10	Fully uncontracted original DZVP	Original outer *p* function replaced with two diffuse primitives with exponents takes from Ahlrich's library	Original outer 2*d* primitive Gaussians replaced with diffuse 6*d* primitive Gaussians taken from Ahlrich's library contracted as 411	None
BS11	Fully uncontracted original DZVP	Original DZVP contraction scheme	Original DZVP contraction scheme	None
BS12	Fully uncontracted original DZVP	Original DZVP contraction scheme	Original outer 2*d* primitive Gaussians replaced with diffuse uncontracted 3*d* primitive Gaussians taken from Ahlrich's library	None
BS13	Fully uncontracted original DZVP	Original DZVP contraction scheme	Original outer 2*d* primitive Gaussians replaced with diffuse 3*d* primitive Gaussians taken from Ahlrich's library contracted as 21	None
BS14	Fully uncontracted original DZVP	Original DZVP contraction scheme	Original outer *d* primitive Gaussians replaced with diffuse uncontracted 3*d* primitive Gaussians taken from Ahlrich's library	None
BS15	Fully uncontracted original DZVP	Original DZVP contraction scheme	Original outer *d* primitive Gaussians replaced with diffuse 3*d* primitive Gaussians taken from Ahlrich's library contracted as 21	None
BS16	Fully uncontracted original DZVP	Original DZVP contraction scheme	Original outer *d* primitive Gaussians replaced with diffuse 6*d* primitive Gaussians taken from Ahlrich's library contracted as 411	None
BS17	Fully uncontracted original DZVP	Original DZVP contraction scheme	Original outer *d* primitive Gaussians replaced with diffuse uncontracted 2*d* primitive Gaussians taken from Ahlrich's library	None

BS18	Fully uncontracted original DZVP	Original DZVP contraction scheme	Original outer 2*d* primitive Gaussians replaced with diffuse 6*d* primitive Gaussians taken from Ahlrich's library contracted as 411	None
BS19	Fully uncontracted original DZVP	Original outer *p* function replaced with two diffuse primitives with exponents takes from Ahlrich's library	Original outer 4*d* primitive Gaussians replaced with diffuse 6*d* primitive Gaussians taken from Ahlrich's library contracted as 21111	None
BS20	Fully uncontracted original DZVP	Original outer *p* function replaced with two diffuse primitives with exponents takes from Ahlrich's library	Original outer 4*d* primitive Gaussians replaced with diffuse 6*d* primitive Gaussians taken from Ahlrich's library contracted as 21111	1*f* polarization primitive function is added with exponents taken from Ahlrich's library

Table S2. Calculated and experimental $g_{||}$. Calculations were done using X-ray structures with different basis sets and RESC relativistic correction (B3P86).

Basis Set	$[MoOCl_4]^-$	$[MoNCl_4]^{2-}$	$[MoOF_5]^-$	$[MoOCl_5]^{2-}$	$[MoOBr_5]^{2-}$
Experiment	1.970[a]	1.906[b]	1.911[c]	1.963[c]	2.090[d]
BS1	1.983	1.910	1.875	1.973	2.088
BS2	1.979	1.909	1.867	1.970	2.088
BS3	2.005	1.909	1.899	1.996	2.108
BS4	1.983	1.903	1.890	1.978	2.088
BS5	1.979	1.889	1.875	1.974	2.088
BS6	1.982	1.896	1.883	1.976	2.088
BS7	1.980	1.888	1.875	1.974	2.087
BS8	1.986	1.899	1.887	1.978	2.088
BS9	1.987	1.989	1.889	1.979	2.089
BS10	1.978	1.905	1.894	1.974	2.082
BS11	2.001	1.909	1.899	1.997	2.107
BS12	1.983	1.903	1.890	1.979	2.088
BS13	1.980	1.889	1.875	1.974	2.087
BS14	1.983	1.896	1.883	1.976	2.087
BS15	1.980	1.888	1.875	1.974	2.087
BS16	1.987	1.898	1.887	1.978	2.088
BS17	1.988	1.899	1.888	1.979	2.089
BS18	1.979	1.905	1.893	1.975	2.082
BS19	1.976	1.883	1.868	1.971	2.084
BS20	1.975	1.883	1.868	1.970	2.083

[a]Inorg. Chem., 1970, 9, 397. [b]ZAAC 1982, 495, 148. [c]Chem Phys. Lett 1976, 42, 319. [d]Inorg. Chem., 1996, 35, 7758.

Table S3. Calculated and experimental $g_{\perp}$. Calculations were done using X-ray structures with different basis sets and RESC relativistic correction (B3P86).

Basis Set	$[MoOCl_4]^-$	$[MoNCl_4]^{2-}$	$[MoOF_5]^-$	$[MoOCl_5]^{2-}$	$[MoOBr_5]^{2-}$
Experiment	1.934[a]	1.9843[b]	1.911[c]	1.94[c]	1.945[d]
BS1	1.898	1.98	1.858	1.892	1.806
BS2	1.896	1.979	1.851	1.89	1.804
BS3	1.934	1.981	1.847	1.906	1.913
BS4	1.938	1.982	1.839	1.905	1.914
BS5	1.937	1.979	1.817	1.893	1.902
BS6	1.929	1.981	1.831	1.9	1.908
BS7	1.933	1.979	1.818	1.893	1.901
BS8	1.929	1.982	1.837	1.904	1.912
BS9	1.936	1.981	1.837	1.903	1.911
BS10	1.936	1.983	1.849	1.912	1.92
BS11	1.941	1.981	1.848	1.907	1.914
BS12	1.938	1.982	1.84	1.906	1.914
BS13	1.937	1.98	1.818	1.894	1.902
BS14	1.929	1.981	1.832	1.9	1.908
BS15	1.934	1.979	1.82	1.893	1.902
BS16	1.929	1.982	1.838	1.904	1.912
BS17	1.936	1.982	1.838	1.904	1.911
BS18	1.936	1.984	1.85	1.912	1.92
BS19	1.934	1.978	1.809	1.889	1.898
BS20	1.937	1.978	1.813	1.89	1.899

[a]Inorg. Chem., 1970, 9, 397. [b]ZAAC 1982, 495, 148. [c]Chem Phys. Lett 1976, 42, 319. [d]Inorg. Chem., 1996, 35, 7758.

Table S4. Calculated and experimental Fermi contact terms (A_F, cm^{-1}). Calculations were done using X-ray structures with different basis sets and RESC relativistic correction (B3P86).

Basis Set	$[MoOCl_4]^-$	$[MoNCl_4]^{2-}$	$[MoOF_5]^-$	$[MoOCl_5]^{2-}$	$[MoOBr_5]^{2-}$
Experiment	48.97[a]		61.06[b]	46.63[b]	42.0[c]
BS1	49.292	71.896	65.619	51.900	47.794
BS2	53.578	75.086	70.904	55.883	51.940
BS3	47.046	71.563	60.409	47.079	42.820
BS4	52.618	74.433	67.139	52.596	48.222
BS5	51.727	73.493	65.961	51.857	47.504
BS6	49.053	70.581	63.200	49.099	44.703
BS7	51.838	73.794	65.781	52.102	47.755
BS8	50.023	72.288	64.149	50.168	45.763
BS9	49.162	71.176	63.522	49.343	44.895
BS10	55.594	76.644	70.371	55.324	50.924
BS11	46.995	71.769	60.527	47.096	42.848
BS12	52.631	74.606	67.207	52.601	48.247
BS13	51.740	73.661	66.030	51.866	47.531
BS14	49.066	70.740	63.283	49.121	44.737
BS15	51.852	73.957	65.851	52.118	47.786
BS16	50.044	72.445	64.231	50.175	45.790
BS17	49.181	71.333	63.610	49.351	44.924
BS18	55.612	76.818	70.428	55.319	50.944
BS19	55.008	77.102	69.781	55.270	50.825
BS20	55.746	77.651	70.3234	55.852	51.435

[a] Inorg. Chem., 1970, 9, 397. [b] Chem Phys. Lett., 1976, 32, 319. [c]Inorg. Chem., 1996, 35, 7758.

Table S5. Calculated and experimental anisotropic HFCs (A^{Mo}_3, cm^{-1}). Calculations were done using X-ray structures with different basis sets and RESC relativistic correction (B3P86).

Basis Set	$[MoOCl_4]^-$	$[MoNCl_4]^{2-}$	$[MoOF_5]^-$	$[MoOCl_5]^{2-}$	$[MoOBr_5]^{2-}$
Experiment	25.74[a]		31.87[b]	28.07[b]	24.0[c]
BS1	24.451	23.598	27.277	24.422	21.855
BS2	25.513	24.258	30.729	25.400	22.720
BS3	21.136	21.513	22.022	20.608	20.240
BS4	21.616	20.763	23.773	21.395	20.970
BS5	24.451	23.407	27.111	24.162	23.674
BS6	22.535	21.710	24.884	22.337	21.912
BS7	24.357	23.400	26.893	24.127	23.656
BS8	21.685	20.871	23.905	21.321	20.911
BS9	21.815	21.043	23.888	21.429	21.052
BS10	20.326	19.474	22.434	20.189	19.786
BS11	21.119	21.503	22.031	20.606	20.238
BS12	21.606	20.744	23.770	21.391	20.971
BS13	24.440	23.388	27.111	24.158	23.676
BS14	22.525	21.693	24.884	22.333	21.914
BS15	24.346	23.383	26.892	24.123	23.658
BS16	21.677	20.855	23.911	21.317	20.912
BS17	21.807	21.027	23.890	21.425	21.053
BS18	20.316	19.454	22.429	20.185	19.786
BS19	25.456	24.375	28.270	25.189	24.685
BS20	25.618	24.497	28.505	25.393	24.883

[a]Inorg. Chem., 1970, 9, 397. [b]Chem Phys. Lett 1976, 42, 319. [c]Inorg. Chem., 1996, 35, 7758

Table S6. Effect of relativistic calculations using both X-ray and optimized geometries (B3P86).

Complex	Mo=O, Å	Relativistic Method	Basis Set (Mo)	$g_{\|}$	$g_{\perp}$	A_F	A_3
$[MoOCl_4]^-$	1.61 X-ray[a]	no rel	BS1	1.989	1.929	25.761	24.543
		DKH2	BS1	1.980	1.928	53.067	24.591
		DKH0	BS1	1.979	1.928	54.697	24.551
		RESC	BS1	1.980	1.928	51.486	24.589
$[MoOF_4]^-$	1.697 Opt	no rel	BS1	1.860	1.887	31.011	27.117
		DKH2	BS1	1.853	1.886	66.117	27.204
		DKH0	BS1	1.853	1.886	68.505	27.161
		RESC	BS1	1.853	1.886	64.159	27.202
$[MoOBr_4]^-$	1.689 Opt	no rel	BS1	2.094	1.919	23.737	24.070
		DKH2	BS1	2.084	1.917	47.738	24.186
		DKH0	BS1	2.083	1.917	48.924	24.144
		RESC	BS1	2.084	1.917	46.298	24.184
$[MoNCl_4]^{2-}$	1.65 Opt	no rel	BS1	1.841	1.980	38.439	24.252
		DKH2	BS1	1.828	1.979	80.125	24.175
		DKH0	BS1	1.828	1.979	82.733	24.129
		RESC	BS1	1.828	1.979	77.741	24.174
$[MoOF_5]^{2-}$	1.738 Opt	no rel	BS1	1.861	1.816	31.865	26.704
		DKH2	BS1	1.854	1.817	67.931	26.879
		DKH0	BS1	1.854	1.818	70.385	26.840
		RESC	BS1	1.854	1.817	65.920	26.878
$[MoOBr_5]^{2-}$	1.707 Opt	no rel	BS1	2.090	1.885	24.687	23.756
		DKH2	BS1	2.071	1.884	49.403	23.948
		DKH0	BS1	2.075	1.885	50.572	23.908
		RESC	BS1	2.076	1.884	47.912	23.945
$[MoOCl_5]^{2-}$	1.712 Opt	no rel	BS1	1.969	1.876	26.303	24.284
		DKH2	BS1	1.955	1.877	53.837	24.417
		DKH0	BS1	1.955	1.877	55.427	24.382
		RESC	BS1	1.955	1.877	52.232	24.416

[a]CCDC reference number:

Table S7. Calculated and experimental EPR spectral parameters of complexes (using BP86 optimized geometries and BS1).

g(parr)	BS1																
BP86 Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
$MoOF_4$[a]	1.895	1.853	1.854	1.861	1.859	1.868	1.869	1.868	1.869	1.845	1.846	1.842	1.838	1.842	1.842	1.799	1.805
$MoOCl_4$[b]	1.968	1.975	1.975	1.976	1.977	1.979	1.979	1.979	1.978	1.966	1.966	1.964	1.962	1.962	1.962	1.935	1.935
$MoOBr_4$[c]		2.093	2.092	2.085	2.087	2.088	2.088	2.088	2.082	2.082	2.081	2.083	2.079	2.077	2.075	2.057	2.055
$MoOF_5$[d]	1.874	1.858	1.859	1.866	1.864	1.872	1.873	1.872	1.873	1.845	1.846	1.841	1.837	1.841	1.841	1.793	1.798
$MoOCl_5$[d]	1.963	1.96	1.961	1.963	1.964	1.968	1.968	1.968	1.968	1.949	1.945	1.944	1.94	1.939	1.939	1.896	1.899
$MoOBr_5$[e]	2.09	2.088	2.087	2.077	2.081	2.084	2.084	2.084	2.078	2.074	2.072	2.076	2.069	2.065	2.063	2.03	2.029
$MoOCl_4(H_2O)$[e]	1.9632	1.97	1.97	1.972	1.973	1.976	1.976	1.976	1.975	1.961	1.961	1.959	1.957	1.957	1.956	1.926	1.928
$MoOBr_4(H_2O)$[f]	1.98	2.091	2.09	2.083	2.086	2.088	2.088	2.088	2.082	2.081	2.079	2.082	2.078	2.075	2.073	2.051	2.05
$MoNCl_4$[g]	1.9063	1.839	1.84	1.849	1.849	1.857	1.858	1.858	1.858	1.815	1.816	1.81	1.802	1.808	1.808	1.731	1.741
mean deviation		0.000687	0.000437	-0.00094	-0.00169	-0.00656	-0.00694	-0.006688	-0.00519	0.01294	0.01356	0.01519	0.01956	0.0188125	0.019438	0.05981	0.056813
MAD		0.031888	0.031388	0.029013	0.029763	0.027638	0.02726	0.0275125	0.027013	0.03819	0.03831	0.04069	0.04406	0.0425625	0.042688	0.07756	0.074313
g(perpen)																	
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
$MoOF_4$[a]	1.925	1.869	1.87	1.878	1.877	1.887	1.887	1.887	1.891	1.879	1.879	1.878	1.873	1.878	1.878	1.856	1.862
$MoOCl_4$[b]	1.93	1.901	1.902	1.908	1.906	1.912	1.912	1.912	1.914	1.903	1.904	1.902	1.899	1.902	1.902	1.882	1.884
$MoOBr_4$[c]		1.912	1.912	1.916	1.912	1.92	1.92	1.919	1.919	1.909	1.909	1.909	1.905	1.907	1.907	1.887	1.889
$MoOF_5$[d]	1.911	1.763	1.766	1.781	1.787	1.811	1.813	1.81	1.822	1.808	1.809	1.807	1.799	1.81	1.81	1.783	1.799
$MoOCl_5$[d]	1.94	1.854	1.856	1.867	1.865	1.877	1.878	1.877	1.883	1.869	1.868	1.866	1.862	1.867	1.867	1.846	1.852
$MoOBr_5$[e]	1.945	1.866	1.868	1.876	1.872	1.886	1.886	1.885	1.889	1.876	1.877	1.876	1.872	1.877	1.877	1.862	1.869
$MoOCl_4(H_2O)$[e]	1.94	1.883	1.884	1.892	1.89	1.898	1.898	1.9	1.902	1.891	1.891	1.89	1.886	1.89	1.89	1.87	1.873
$MoOBr_4(H_2O)$[f]	1.947	1.887	1.888	1.895	1.891	1.901	1.9	1.9	1.903	1.892	1.892	1.892	1.888	1.891	1.891	1.873	1.876
$MoNCl_4$[g]	1.9843	1.983	1.983	1.981	1.98	1.983	1.983	1.983	1.981	1.977	1.976	1.976	1.975	1.974	1.974	1.956	1.953
mean deviation		0.064538	0.063163	0.055538	0.056788	0.045913	0.04566	0.0460375	0.042163	0.05341	0.05329	0.05441	0.05854	0.0541625	0.054163	0.07429	0.069288
MAD		0.064538	0.063163	0.055538	0.056788	0.045913	0.04566	0.0460375	0.042163	0.05341	0.05329	0.05441	0.05854	0.0541625	0.054163	0.07429	0.069288
A(Fermi)																	
BP86 Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
$MoOF_4$[a]		41.065	43.088	54.038	57.754	53.22	54.951	55.396	64.905	63.622	65.237	65.415	51.774	69.803	70.814	77.321	84.389
$MoOCl_4$[b]	49.8	31.818	33.438	42.021	44.884	39.648	41.015	41.531	48.383	49.471	50.87	52.014	38.42	54.868	56.02	65.044	70.14
$MoOBr_4$[c]	42	29.419	30.917	38.6	41.253	36.025	37.311	37.917	43.424	45.86	47.224	48.8	35.666	51.151	52.394	62.508	66.908
$MoOF_5$[d]	61.06	42.253	44.407	56.39	60.519	54.774	56.669	57.02	67.551	65.772	67.564	67.358	53.638	72.482	73.508	80.709	88.301
$MoOCl_5$[d]	46.6	33.368	35.121	44.617	47.924	41.464	43.068	43.548	50.999	52.321	58.481	59.19	45.953	63.469	65.051	76.389	83.693
$MoOBr_5$[e]	44	30.449	32.04	40.322	43.347	37.095	38.589	39.179	44.843	47.838	49.45	50.884	37.601	53.914	55.355	67.972	73.22
$MoOCl_4(H_2O)$[e]	46.63	32.096	33.76	42.738	45.725	39.832	41.266	41.755	48.785	49.797	51.275	52.246	38.713	55.402	56.584	66.177	71.40789
$MoOBr_4(H_2O)$[f]		29.457	30.987	38.993	41.745	35.862	37.204	37.786	43.341	45.78	47.214	48.637	35.498	51.246	52.522	63.262	67.701
$MoNCl_4$[g]		48.361	50.97	65.786	70.982	61.34	63.702	64.119	76.576	78.167	80.708	80.158	66.111	87.937	89.489	109.579	119.25
mean deviation		15.1145	13.40117	4.233667	1.073	6.875333	5.362	4.8566667	-2.31583	-3.49483	-5.79567	-6.7337	6.68317	-10.199333	-11.4703	-21.452	-27.26332
MAD		15.1145	13.40117	4.233667	1.514333	6.875333	5.362	4.8566667	2.788167	3.6045	5.79567	6.73367	6.68317	10.199333	11.47033	21.4515	27.26332
A3																	
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
$MoOF_4$[a]		26.432	26.403	25.95	26.347	26.002	26.044	26.11	26.186	27.159	27.181	27.643	27.363	27.354	27.236	28.86	29.019
$MoOCl_4$[b]	25.7	23.561	23.567	23.36	23.742	23.392	23.428	23.462	23.693	24.719	24.741	25.104	24.83	24.974	24.881	26.537	26.726
$MoOBr_4$[c]		23.01	23.027	22.885	23.264	22.796	22.829	22.869	23.115	24.244	24.265	24.607	24.384	24.526	24.439	26.244	26.377

$MoOF_5$[d]	31.87	26.381	26.321	25.655	25.952	25.909	25.918	25.995	25.894	26.741	26.72	27.303	26.881	26.752	26.636	27.704	27.776
$MoOCl_5$[d]	28.1	23.624	23.597	23.12	23.413	23.361	23.373	23.421	23.363	24.359	25.388	25.84	25.446	25.473	25.379	26.198	26.101
$MoOBr_5$[e]	22	23.043	23.031	22.64	22.94	22.743	22.756	22.81	22.779	23.918	23.898	24.351	23.993	23.991	23.907	24.812	24.688
$MoOCl_4(H_2O)$[e]	28.07	23.555	23.553	23.272	23.629	23.373	23.402	23.44	23.601	24.586	24.593	24.982	24.659	24.77	24.677	26.007	26.138
$MoOBr_4(H_2O)$[f]		22.967	22.978	22.774	23.132	22.749	22.775	22.821	23.006	24.1	24.109	24.473	24.196	24.318	24.231	25.708	25.789
$MoNCl_4$[g]		24.135	24.077	23.411	23.706	23.672	23.67	23.724	23.473	24.087	24.032	24.533	24.105	23.906	23.829	23.813	23.413
mean deviation		3.1152	3.1342	3.5386	3.2128	3.3924	3.3726	3.3224	3.282	2.2834	2.08	1.632	1.9862	1.956	2.052	0.8964	0.8622
MAD		3.5324	3.5466	3.7946	3.5888	3.6896	3.675	3.6464	3.5936	3.0506	2.8392	2.5724	2.7834	2.7524	2.8148	2.356	2.3478

[a] Inorg. Chem., 1983, 28, 2571. [b]Inorg. Chem., 1970, 9, 397. [c] Zh. Neorg. Khim., 1969, 14, 438. [d]Chem Phys. Lett 1976, 42, 319. [e]Inorg. Chem., 1996, 35, 7758. [f] Zh. Neorg. Khim, 1992, 37, 346. [g] ZAAC 1982, 495, 148.

Table S8. Calculated and experimental EPR spectra parameters for test complexes using B3P86 optimized geometries and BS1.

g (parr)	BS1															
B3P86 Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
$MoOF_4$[a]	1.895	1.862	1.862	1.869	1.866	1.875	1.876	1.875	1.876	1.853	1.854	1.849	1.846	1.85	1.85	1.81	1.815
$MoOCl_4$[b]	1.968	1.981	1.981	1.982	1.982	1.984	1.984	1.983	1.982	1.971	1.97	1.969	1.967	1.967	1.966	1.942	1.941
$MoOBr_4$[c]		2.096	2.095	2.088	2.09	2.09	2.09	2.09	2.084	2.084	2.083	2.084	2.081	2.079	2.077	2.06	2.057
$MoOF_5$[d]	1.874	1.867	1.868	1.874	1.871	1.879	1.88	1.879	1.879	1.854	1.854	1.85	1.846	1.849	1.85	1.805	1.81
$MoOCl_5$[d]	1.963	1.968	1.968	1.97	1.971	1.974	1.974	1.973	1.973	1.956	1.955	1.954	1.951	1.95	1.95	1.914	1.915
$MoOBr_5$[e]	2.09	2.091	2.09	2.081	2.084	2.087	2.086	2.087	2.081	2.076	2.074	2.078	2.072	2.068	2.067	2.038	2.036
$MoOCl_4(H_2O)$[e]	1.9632	1.977	1.977	1.979	1.979	1.981	1.981	1.981	1.98	1.967	1.967	1.965	1.963	1.963	1.962	1.934	1.934
$MoOBr_4(H_2O)$[f]	1.98	2.095	2.094	2.086	2.089	2.09	2.09	2.09	2.085	2.083	2.082	2.084	2.08	2.077	2.075	2.054	2.053
$MoNCl_4$[g]	1.9063	1.852	1.853	1.861	1.86	1.867	1.868	1.868	1.868	1.828	1.829	1.823	1.816	1.821	1.821	1.751	1.758
mean deviation		-0.00669	-0.00669	-0.00781	-0.00781	-0.01219	-0.01244	-0.012063	-0.01056	0.00644	0.00681	0.00844	0.01231	0.0118125	0.012313	0.04894	0.047188
MAD		0.030263	0.029763	0.027888	0.028888	0.027762	0.02776	0.0273875	0.027138	0.03389	0.03376	0.03514	0.03731	0.0360625	0.036063	0.06744	0.065438
g (perpen)	BS1																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
$MoOF_4$[a]	1.925	1.877	1.879	1.885	1.885	1.893	1.894	1.893	1.897	1.886	1.886	1.885	1.881	1.886	1.886	1.867	1.872
$MoOCl_4$[b]	1.93	1.909	1.91	1.915	1.913	1.918	1.918	1.918	1.92	1.91	1.91	1.909	1.967	1.967	1.967	1.942	1.941
$MoOBr_4$[c]		1.921	1.921	1.924	1.921	1.927	1.927	1.927	1.927	1.917	1.917	1.917	1.914	1.915	1.915	1.898	1.899
$MoOF_5$[d]	1.911	1.777	1.779	1.792	1.797	1.82	1.822	1.819	1.83	1.817	1.819	1.816	1.809	1.82	1.819	1.795	1.811
$MoOCl_5$[d]	1.94	1.863	1.865	1.874	1.873	1.884	1.884	1.883	1.889	1.877	1.878	1.876	1.872	1.877	1.877	1.859	1.864
$MoOBr_5$[e]	1.945	1.877	1.878	1.885	1.882	1.894	1.894	1.893	1.897	1.884	1.885	1.885	1.881	1.885	1.885	1.87	1.875
$MoOCl_4(H_2O)$[e]	1.94	1.89	1.891	1.898	1.896	1.904	1.904	1.903	1.907	1.896	1.897	1.896	1.893	1.897	1.897	1.879	1.883
$MoOBr_4(H_2O)$[f]	1.947	1.898	1.899	1.904	1.901	1.909	1.909	1.909	1.911	1.9	1.901	1.9	1.897	1.899	1.9	1.883	1.886
$MoNCl_4$[g]	1.9843	1.983	1.983	1.983	1.983	1.984	1.984	1.984	1.982	1.979	1.979	1.978	1.977	1.977	1.977	1.963	1.961
mean deviation		0.056038	0.054788	0.048288	0.049038	0.039538	0.03916	0.0400375	0.036163	0.04666	0.04591	0.04716	0.04316	0.0392875	0.039288	0.05804	0.053663
MAD		0.056038	0.054788	0.048288	0.049038	0.039538	0.03916	0.0400375	0.036163	0.04666	0.04591	0.04716	0.05241	0.0485375	0.048538	0.06104	0.056413
A(Fermi)	BS1																
B3P86 Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
$MoOF_4$[a]		41.373	43.406	54.437	58.126	53.716	55.437	55.863	65.454	64.153	65.763	65.863	52.164	70.348	71.3	77.829	84.923
$MoOCl_4$[b]	49.8	32.058	33.686	42.359	45.202	40.003	41.36	41.85	48.829	49.817	51.201	52.257	38.756	55.185	56.261	65.202	70.281
$MoOBr_4$[c]	42	29.714	31.225	39.045	41.683	36.443	37.721	38.297	43.985	46.297	47.645	49.112	36.123	51.568	52.733	62.787	67.179
$MoOF_5$[d]	61.06	42.428	44.576	56.523	60.574	55.085	56.95	57.269	67.769	65.92	67.673	67.428	53.718	72.491	73.457	80.27	87.663
$MoOCl_5$[d]	46.6	33.474	35.221	44.711	47.934	41.637	43.204	43.652	51.151	52.23	53.838	54.661	41.238	58.263	59.48	70.016	75.75
$MoOBr_5$[e]	44	30.642	32.236	40.596	43.548	37.377	38.837	39.387	45.205	47.898	49.447	50.787	37.702	53.749	55.072	66.757	71.6
$MoOCl_4(H_2O)$[e]	46.63	32.314	33.98	42.992	45.951	40.148	41.569	42.021	49.138	50.042	51.492	52.381	38.939	55.553	56.653	65.917	71.004
$MoOBr_4(H_2O)$[f]		29.719	31.256	39.348	42.072	36.236	37.564	38.104	43.804	46.107	47.511	48.826	35.869	51.487	52.675	63.097	67.411
$MoNCl_4$[g]		48.414	51.001	65.645	70.671	61.476	63.79	64.183	76.516	77.762	80.202	79.679	65.695	87.099	88.547	106.245	115.1948
mean deviation		14.91	13.19433	3.977333	0.866333	6.566167	5.07483	4.6023333	-2.6645	-3.68567	-5.201	-6.0893	7.269	-9.4531667	-10.5943	-20.143	-25.5645
MAD		14.91	13.19433	3.977333	1.311	6.566167	5.07483	4.6023333	2.988167	3.68567	5.201	6.08933	7.269	9.4531667	10.59433	20.1432	25.5645
A3	BS1																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
$MoOF_4$[a]		26.485	26.459	26.03	26.44	26.068	26.113	26.177	26.284	27.201	27.227	27.685	27.405	27.396	27.276	28.87	29.042
$MoOCl_4$[b]	25.7	23.5	23.51	23.327	23.722	23.351	23.39	23.422	23.69	24.672	24.697	25.059	24.785	24.932	24.838	26.495	26.709
$MoOBr_4$[c]		22.94	22.961	22.841	22.232	22.744	22.779	22.818	23.098	24.182	24.206	24.547	24.318	24.469	24.379	26.184	26.338

$MoOF_5$[d]	31.87	26.466	26.413	25.794	26.119	26.02	26.035	26.107	26.065	26.878	26.867	27.435	27.025	26.921	26.802	27.974	28.101
$MoOCl_5$[d]	28.1	23.588	23.568	23.145	23.465	23.358	23.377	23.421	23.438	24.415	24.404	24.865	24.465	24.5	24.405	25.407	25.447
$MoOBr_5$[e]	22	22.989	22.982	22.643	22.964	22.718	22.735	22.787	22.825	23.94	23.931	24.368	24.029	24.066	23.979	25.178	25.169
$MoOCl_4(H_2O)$[e]	28.07	23.528	23.53	23.282	23.659	23.371	23.404	23.439	23.646	24.601	24.614	24.997	24.682	24.805	24.709	26.122	26.302
$MoOBr_4(H_2O)$[f]		22.916	22.931	22.756	23.13	22.719	22.749	22.791	23.019	24.083	24.096	24.455	24.185	24.318	24.228	25.789	25.915
$MoNCl_4$[g]		24.103	24.055	23.458	23.788	23.677	23.683	23.733	23.574	24.176	24.136	24.618	24.198	24.062	23.977	24.297	24.082
mean deviation		3.1338	3.1474	3.5098	3.1622	3.3844	3.3598	3.3128	3.2152	2.2468	2.2454	1.8032	2.1508	2.1032	2.2014	0.9128	0.8024
MAD		3.5294	3.5402	3.767	3.5478	3.6716	3.6538	3.6276	3.5452	3.0228	3.0178	2.7504	2.9624	2.9296	2.993	2.502	2.4736

[a] Inorg. Chem., 1983, 28, 2571. [b]Inorg. Chem., 1970, 9, 397. [c] Zh. Neorg. Khim, 1969, 14, 438. [d]Chem Phys. Lett 1976, 42, 319. [e]Inorg. Chem., 1996, 35, 7758. [f] Zh. Neorg. Khim, 1992, 37, 346. [g] ZAAC 1982, 495, 148.

Table S9. Calculated EPR spectra parameters for test complexes using PBE1PBE optimized geometries and BS1.

g parr	BS1																
PBE1PBE Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.895	1.862	1.863	1.869	1.867	1.875	1.876	1.875	1.876	1.854	1.854	1.85	1.846	1.85	1.851	1.811	1.815
MOCl4	1.968	1.981	1.982	1.983	1.983	1.984	1.984	1.984	1.982	1.971	1.971	1.969	1.968	1.968	1.967	1.942	1.942
MoOBr4		2.096	2.095	2.088	2.09	2.09	2.09	2.09	2.084	2.084	2.083	2.085	2.082	2.079	2.078	2.061	2.057
MoOF5	1.874	1.868	1.868	1.874	1.872	1.88	1.88	1.879	1.88	1.854	1.855	1.85	1.846	1.85	1.851	1.806	1.81
MoOCl5	1.963	1.969	1.969	1.97	1.971	1.974	1.974	1.974	1.973	1.956	1.956	1.954	1.952	1.951	1.951	1.915	1.916
MoOBr5	2.09	2.091	2.09	2.082	2.085	2.087	2.087	2.087	2.081	2.077	2.075	2.079	2.073	2.069	2.067	2.039	2.037
MoOCl4(H2O)	1.9632	1.978	1.978	1.979	1.98	1.982	1.982	1.982	1.981	1.967	1.967	1.966	1.964	1.963	1.963	1.934	1.935
MoOBr4(H2O)	1.98	2.096	2.095	2.087	2.09	2.091	2.091	2.091	2.086	2.084	2.083	2.085	2.081	2.078	2.076	2.055	2.054
MoNCl4	1.9063	1.852	1.854	1.862	1.861	1.868	1.869	1.868	1.868	1.829	1.83	1.824	1.817	1.821	1.822	1.752	1.759
mean deviation		-0.00719	-0.00744	-0.00831	-0.00869	-0.01269	-0.01294	-0.012563	-0.01094	0.00594	0.00606	0.00781	0.01156	0.0111875	0.011438	0.04819	0.046438
MAD		0.030513	0.030013	0.027888	0.028763	0.028012	0.02776	0.0278875	0.027513	0.03364	0.03351	0.03501	0.03701	0.0356875	0.035438	0.06694	0.064938
g perpen	BS1																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.925	1.879	1.88	1.887	1.886	1.895	1.895	1.895	1.898	1.888	1.888	1.887	1.883	1.887	1.887	1.869	1.874
MOCl4	1.93	1.919	1.911	1.916	1.914	1.919	1.919	1.919	1.92	1.911	1.911	1.91	1.908	1.91	1.91	1.894	1.896
MoOBr4		1.922	1.922	1.925	1.922	1.928	1.928	1.928	1.928	1.918	1.918	1.918	1.915	1.916	1.916	1.899	1.901
MoOF5	1.911	1.78	1.782	1.794	1.8	1.822	1.824	1.821	1.831	1.819	1.821	1.818	1.811	1.822	1.821	1.797	1.813
MoOCl5	1.94	1.865	1.866	1.876	1.874	1.883	1.886	1.885	1.89	1.878	1.879	1.877	1.874	1.879	1.879	1.86	1.866
MoOBr5	1.945	1.879	1.88	1.887	1.883	1.895	1.895	1.895	1.898	1.885	1.886	1.886	1.882	1.886	1.886	1.871	1.877
MoOCl4(H2O)	1.94	1.892	1.893	1.9	1.897	1.905	1.905	1.905	1.908	1.898	1.898	1.897	1.894	1.898	1.898	1.881	1.884
MoOBr4(H2O)	1.947	1.9	1.901	1.907	1.903	1.912	1.911	1.911	1.913	1.903	1.903	1.902	1.899	1.902	1.902	1.886	1.889
MoNCl4	1.9843	1.984	1.984	1.983	1.982	1.985	1.984	1.984	1.983	1.979	1.979	1.979	1.978	1.977	1.977	1.944	1.962
mean deviation		0.053038	0.053163	0.046538	0.047913	0.038288	0.03791	0.0384125	0.035163	0.04516	0.04466	0.04579	0.04916	0.0451625	0.045288	0.06504	0.057663
MAD		0.053038	0.053163	0.046538	0.047913	0.038463	0.03791	0.0384125	0.035163	0.04516	0.04466	0.04579	0.04916	0.0451625	0.045288	0.06504	0.057663
AF	BS1																
PBE1PBE Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		41.465	43.502	54.556	58.247	53.835	55.558	55.982	65.593	64.302	65.915	66.009	52.304	70.511	71.458	78.027	85.131
MOCl4	49.8	32.111	33.741	42.43	45.27	40.074	41.431	41.919	48.915	49.9	51.283	52.33	38.84	55.27	38.84	65.29	70.369
MoOBr4	42	29.77	31.283	39.123	41.758	36.518	37.798	38.367	44.078	46.385	47.732	49.188	36.217	51.658	52.813	62.881	67.274
MoOF5	61.06	42.488	44.637	56.586	60.63	55.163	57.026	57.342	67.841	65.995	67.746	67.501	53.797	72.558	73.519	80.315	87.688
MoOCl5	46.6	33.509	35.256	44.743	47.955	41.681	43.244	43.689	51.187	52.255	53.856	54.678	41.268	58.263	59.468	69.907	75.581
MoOBr5	44	30.679	32.273	40.638	43.578	37.424	38.88	39.426	45.254	47.924	49.466	50.8	37.744	53.749	55.058	66.638	71.424
MoOCl4(H2O)	46.63	32.369	34.037	43.057	46.011	40.22	41.639	42.089	49.217	50.119	51.567	52.452	39.02	55.626	56.717	65.968	71.039
MoOBr4(H2O)		29.774	31.311	39.409	42.128	36.299	37.626	38.161	43.877	46.164	47.565	48.874	35.931	51.532	52.71	63.095	67.387
MoNCl4		48.482	51.068	65.697	70.703	61.569	63.88	64.272	76.588	77.804	80.235	79.718	65.738	87.096	88.536	105.934	114.79
mean deviation		14.86067	13.14383	3.918833	0.814667	6.501667	5.012	4.543	-2.73367	-3.748	-5.26	-6.1432	7.20067	-9.5056667	-7.72083	-20.152	-25.5475
MAD		14.86067	13.14383	3.918833	1.266333	6.501667	5.012	4.543	3.028667	3.748	5.26	6.14317	7.20067	9.5056667	11.37417	20.1515	25.5475
Aaniso	BS1																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		26.489	26.465	26.039	26.542	26.075	26.121	26.185	26.296	27.208	27.234	27.692	27.411	27.404	27.283	28.873	29.047
MOCl4	25.7	23.493	23.504	23.326	23.723	23.348	23.387	23.419	23.694	24.669	24.695	25.056	24.782	24.931	24.836	26.493	26.71
MoOBr4		22.932	22.953	22.839	23.233	22.74	22.775	22.814	23.101	24.179	24.204	24.544	24.314	24.467	24.377	26.181	26.339

MoOF5	31.87	26.477	26.425	25.814	26.142	26.036	26.051	26.123	26.09	26.899	26.89	27.455	27.047	26.947	26.828	28.011	28.145
MoOCl5	28.1	23.588	23.569	23.157	23.481	23.363	23.384	23.427	23.456	24.432	24.432	24.881	24.484	24.526	24.43	25.473	25.53
MoOBr5	22	22.985	22.98	22.651	22.977	22.72	22.738	22.789	22.841	23.953	23.946	24.38	24.045	24.088	24.001	25.242	25.249
MoOCl4(H2O)	28.07	23.523	23.526	23.284	23.665	23.37	23.405	23.439	23.655	24.605	24.619	25	24.687	24.812	24.716	26.141	26.327
MoOBr4(H2O)		22.929	22.945	22.781	23.16	22.738	22.769	22.81	23.051	24.108	24.123	24.479	24.211	24.348	24.258	25.831	25.964
MoNCl4		24.106	24.059	23.472	23.808	23.684	23.692	23.742	23.595	24.196	24.157	24.637	24.218	24.09	24.004	24.366	24.175
mean deviation		3.1348	3.1472	3.5016	3.1504	3.3806	3.355	3.3086	3.2008	2.2364	2.2316	1.7936	2.139	2.0872	2.1858	0.876	0.7558
MAD		3.5288	3.5392	3.762	3.5412	3.6686	3.6502	3.6242	3.5372	3.0176	3.01	2.7456	2.957	2.9224	2.9862	2.49	2.4594

Table S10. Calculated EPR spectra parameters for test complexes using X-ray geometries and BS1.

g parr	BS1																
X-ray Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.895	1.846	1.848	1.856	1.857	1.868	1.869	1.868	1.873	1.864	1.865	1.863	1.858	1.865	1.865	1.848	1.856
MOCl4	1.968	1.995	1.995	1.995	1.995	1.996	1.996	1.996	1.993	1.983	1.983	1.981	1.981	1.98	1.98	1.957	1.955
MoOBr4		2.104	2.103	2.097	2.099	2.097	2.097	2.097	2.091	2.092	2.091	2.093	2.09	2.088	2.087	2.075	2.071
MoOF5	1.874	1.886	1.887	1.892	1.89	1.895	1.896	1.895	1.895	1.875	1.875	1.871	1.868	1.871	1.872	1.837	1.839
MoOCl5	1.963	1.986	1.986	1.987	1.987	1.988	1.988	1.988	1.986	1.973	1.972	1.971	1.969	1.968	1.968	1.939	1.939
MoOBr5	2.09	2.098	2.098	2.09	2.093	2.093	2.093	2.093	2.087	2.088	2.087	2.09	2.086	2.083	2.081	2.121	1.835
MoOCl4(H2O)	1.9632	1.939	1.940	1.943	1.947	1.957	1.958	1.9571	1.960	1.936	1.936	1.935	1.93	1.929	1.928	1.87	1.879
MoOBr4(H2O)	1.98	2.104	2.103	2.095	2.098	2.098	2.098	2.0979	2.093	2.091	2.089	2.092	2.088	2.085	2.0833	2.064	2.061
MoNCl4	1.9063	1.931	1.931	1.934	1.932	1.934	1.934	1.934	1.93	1.91	1.91	1.905	1.903	1.905	1.905	1.868	1.866
mean deviation		-0.0182	-0.01853	-0.01906	-0.01998	-0.02367	-0.02404	-0.023691	-0.02218	-0.01004	-0.00971	-0.0086	-0.0054	-0.0057941	-0.00529	0.01694	0.051051
MAD		0.036361	0.036036	0.033938	0.033414	0.03199	0.03183	0.0319579	0.0292	0.02503	0.02479	0.02461	0.02636	0.0246403	0.024782	0.04572	0.071453
g perpen	BS1																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.925	1.914	1.914	1.918	1.916	1.919	1.919	1.919	1.918	1.904	1.904	1.901	1.899	1.901	1.902	1.877	1.877
MOCl4	1.93	1.893	1.894	1.901	1.898	1.905	1.905	1.904	1.907	1.898	1.899	1.897	1.895	1.898	1.898	1.882	1.885
MoOBr4		1.888	1.889	1.896	1.893	1.901	1.901	1.9	1.903	1.892	1.892	1.891	1.888	1.891	1.891	1.872	1.875
MoOF5	1.911	1.838	1.839	1.845	1.847	1.862	1.863	1.861	1.866	1.858	1.859	1.857	1.852	1.859	1.859	1.841	1.851
MoOCl5	1.94	1.883	1.884	1.891	1.889	1.898	1.899	1.898	1.902	1.892	1.893	1.891	1.889	1.893	1.893	1.878	1.883
MoOBr5	1.945	1.745	1.75	1.781	1.782	1.799	1.801	1.799	1.817	1.806	1.81	1.804	1.805	1.821	1.821	1.825	1.833
MoOCl4(H2O)	1.94	1.901	1.902	1.907	1.904	1.913	1.912	1.912	1.914	1.905	1.905	1.905	1.901	1.903	1.904	1.887	1.89
MoOBr4(H2O)	1.947	1.902	1.903	1.909	1.905	1.913	1.913	1.913	1.915	1.905	1.906	1.905	1.902	1.905	1.905	1.891	1.894
MoNCl4	1.9843	1.983	1.983	1.983	1.982	1.984	1.984	1.984	1.982	1.98	1.98	1.979	1.979	1.979	1.979	1.969	1.968
mean deviation		0.057905	0.056721	0.048443	0.049874	0.041206	0.04076	0.0416033	0.037648	0.04677	0.04584	0.04791	0.04998	0.0453639	0.045191	0.05904	0.055199
MAD		0.057905	0.056721	0.048443	0.049874	0.041206	0.04076	0.0416033	0.037648	0.04677	0.04584	0.04791	0.04998	0.0453639	0.045191	0.05904	0.055199
AF	BS1																
X-ray Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		39.989	41.929	52.539	55.923	52.933	54.498	54.762	64.207	62.51	63.973	63.766	49.65	68.291	68.963	74.292	81.483
MOCl4	49.8	31.706	33.318	42	44.75	39.695	41.014	41.459	48.565	49.292	50.633	51.582	38.143	54.552	55.516	64.26	69.378
MoOBr4	42	28.578	30.047	37.86	40.405	35.329	36.53	37.025	42.972	44.453	45.7	46.868	34.01	49.406	50.404	59.399	63.879
MoOF5	61.06	42.512	44.611	56.172	59.982	55.398	57.155	57.413	67.508	65.619	67.25	66.998	53.343	71.783	72.604	78.64	85.684
MoOCl5	46.6	33.524	35.247	44.624	47.672	41.836	43.319	43.711	51.253	51.9	53.387	54.114	40.821	57.512	58.517	67.691	77.99
MoOBr5	44	28.835	30.416	39.135	42.422	35.944	37.416	37.918	44.866	47.794	49.61	50.302	36.166	55.544	56.992	73.22	81.498
MoOCl4(H2O)	46.63	32.618	34.294	43.431	46.335	40.645	42.044	42.449	49.776	50.509	51.931	52.688	39.344	55.966	56.943	66.051	71.136
MoOBr4(H2O)		29.945	31.492	39.768	42.448	36.622	37.929	38.417	44.391	46.449	47.822	48.963	36.189	51.775	52.845	63.101	67.426
MoNCl4		45.19	47.569	61.053	65.542	57.772	59.775	60.069	76.907	71.896	73.952	73.481	59.075	79.908	80.88	94.635	102.933
mean deviation		15.38617	13.69283	4.478	1.420667	6.873833	5.43533	5.0191667	-2.475	-3.24617	-4.73683	-5.4103	8.04383	-9.1121667	-10.1477	-19.862	-26.57917
MAD		15.38617	13.69283	4.478	1.778	6.873833	5.43533	5.0191667	2.886667	3.4155	4.73683	5.41033	8.04383	9.1121667	10.14767	19.8618	26.57917
Aaniso	BS1																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		26.74	26.719	26.337	26.752	26.352	26.396	26.438	26.628	27.304	27.328	27.787	27.481	27.454	27.323	28.749	28.952
MOCl4	25.7	23.29	23.303	23.152	23.542	23.167	23.206	23.236	23.543	24.451	24.475	24.838	24.545	24.702	24.602	26.206	26.431

MoOBr4		22.47	22.478	22.295	22.645	22.245	22.264	22.304	22.538	23.537	23.545	23.922	23.64	23.766	23.665	25.357	25.497
MoOF5	31.87	26.681	26.652	26.192	26.593	26.307	26.343	26.4	26.534	27.277	27.294	27.802	27.445	27.411	27.288	28.657	28.879
MoOCl5	28.1	23.43	23.425	23.123	23.492	23.271	23.304	23.34	23.514	24.422	24.433	24.859	24.494	24.596	24.494	25.856	26.061
MoOBr5	22	22.252	22.184	21.403	21.475	21.767	21.72	21.785	21.302	21.855	21.688	22.35	21.623	21.141	21.051	19.21	18.703
MoOCl4(H2O)	28.07	23.326	23.333	23.119	23.51	23.207	24.865	23.275	23.541	24.427	24.444	24.83	24.498	24.638	24.538	25.965	26.189
MoOBr4(H2O)		22.679	22.696	22.543	22.92	22.511	22.541	22.582	22.849	23.853	23.867	24.234	23.937	24.088	23.993	25.551	25.71
MoNCl4		23.393	23.358	22.872	23.216	23.039	23.046	23.091	23.094	23.598	23.571	24.05	23.628	23.548	23.443	24.089	24.049
mean deviation		3.3522	3.3686	3.7502	3.4256	3.6042	3.2604	3.5408	3.4612	2.6616	2.6812	2.2122	2.627	2.6504	2.7534	1.9692	1.8954
MAD		3.453	3.4422	3.7502	3.4256	3.6042	3.2604	3.5408	3.4612	2.6616	2.6812	2.3522	2.627	2.6504	2.7534	2.1716	2.1878

Table S11. Calculated EPR spectra parameters for test complexes using BP86 optimized geometries and BS2.

g parr	BS2																
BP86 Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.895	1.843	1.844	1.853	1.85	1.859	1.86	1.859	1.862	1.836	1.837	1.832	1.828	1.833	1.833	1.789	1.797
MOCl4	1.968	1.973	1.973	1.976	1.975	1.977	1.976	1.977	1.976	1.96	1.96	1.958	1.956	1.956	1.955	1.925	1.926
MoOBr4		2.093	2.092	2.086	2.088	2.087	2.087	2.087	2.081	2.077	2.076	2.078	2.075	2.071	2.07	2.049	2.046
MoOF5	1.874	1.85	1.851	1.861	1.857	1.865	1.866	1.865	1.868	1.836	1.837	1.833	1.828	1.832	1.833	1.784	1.791
MoOCl5	1.963	1.962	1.963	1.966	1.966	1.968	1.968	1.968	1.967	1.945	1.945	1.944	1.94	1.939	1.939	1.896	1.899
MoOBr5	2.09	2.091	2.09	2.081	2.084	2.086	2.086	2.086	2.08	2.071	2.069	2.074	2.067	2.062	2.06	2.024	2.023
MoOCl4(H2O)	1.9632	1.969	1.97	1.972	1.972	1.974	1.974	1.974	1.974	1.956	1.955	1.954	1.952	1.951	1.95	1.917	1.919
MoOBr4(H2O)	1.98	2.093	2.092	2.085	2.087	2.088	2.087	2.088	2.082	2.077	2.076	2.079	2.074	2.07	2.068	2.043	2.042
MoNCl4	1.9063	1.84	1.842	1.853	1.85	1.857	1.857	1.857	1.859	1.81	1.812	1.806	1.796	1.802	1.808	1.723	1.734
	mean dev	0.002312	0.001812	-0.00094	-0.00019	-0.00431	-0.00431	-0.004312	-0.00356	0.01856	0.01856	0.01994	0.02481	0.0243125	0.024188	0.06731	0.063563
	MAD	0.033513	0.032763	0.030263	0.031263	0.028888	0.02839	0.0288875	0.027638	0.04281	0.04256	0.04469	0.04831	0.0468125	0.046188	0.08306	0.079063
g perpen	BS2																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.925	1.863	1.864	1.871	1.871	1.882	1.882	1.881	1.885	1.874	1.874	1.873	1.868	1.874	1.874	1.853	1.86
MOCl4	1.93	1.9	1.901	1.907	1.904	1.91	1.91	1.91	1.912	1.901	1.901	1.9	1.896	1.899	1.899	1.879	1.882
MoOBr4		1.911	1.912	1.915	1.912	1.919	1.918	1.918	1.918	1.906	1.906	1.907	1.903	1.904	1.904	1.884	1.887
MoOF5	1.911	1.754	1.756	1.768	1.777	1.804	1.806	1.802	1.813	1.802	1.803	1.801	1.792	1.805	1.805	1.778	1.796
MoOCl5	1.94	1.854	1.855	1.866	1.864	1.875	1.876	1.875	1.881	1.867	1.868	1.866	1.862	1.867	1.867	1.846	1.852
MoOBr5	1.945	1.868	1.869	1.877	1.873	1.886	1.886	1.885	1.889	1.875	1.875	1.875	1.871	1.875	1.875	1.859	1.866
MoOCl4(H2O)	1.94	1.882	1.883	1.891	1.889	1.896	1.896	1.896	1.9	1.888	1.888	1.887	1.883	1.887	1.887	1.867	1.871
MoOBr4(H2O)	1.947	1.887	1.888	1.895	1.891	1.9	1.9	1.9	1.902	1.89	1.89	1.89	1.886	1.889	1.889	1.87	1.874
MoNCl4	1.9843	1.981	1.981	1.98	1.979	1.982	1.982	1.982	1.979	1.975	1.975	1.975	1.974	1.972	1.974	1.954	1.951
	mean dev	0.066663	0.065663	0.058413	0.059288	0.048413	0.04804	0.0489125	0.045163	0.05629	0.05604	0.05691	0.06129	0.0567875	0.056538	0.07704	0.071287
	MAD	0.066663	0.065663	0.058413	0.059288	0.048413	0.04804	0.0489125	0.045163	0.05629	0.05604	0.05691	0.06129	0.0567875	0.056538	0.07704	0.071287
AF	BS2																
BP86 Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		44.42	46.584	58.26	62.312	58.297	60.17	60.506	70.808	69.252	71.009	71.007	57.422	75.887	77.142	83.314	91.332
MOCl4	49.8	34.169	35.885	44.892	48.113	43.503	45.044	45.47	52.858	53.975	55.539	56.516	43.168	59.89	61.272	70.138	76.203
MoOBr4	42	31.543	33.129	41.185	44.177	39.588	41.033	41.55	47.57	50.039	51.556	52.983	40.136	55.819	57.3	67.221	72.592
MoOF5	61.06	45.347	47.615	60.067	64.637	59.551	61.584	61.767	72.91	71.161	73.078	72.685	59.166	78.294	79.578	86.364	94.861
MoOCl5	46.6	35.462	37.3	47.148	50.834	45.083	46.86	47.241	55.236	56.641	58.481	59.189	45.953	63.469	65.051	76.389	83.693
MoOBr5	44	32.397	34.07	42.691	46.077	40.534	42.191	42.681	48.898	51.966	53.739	55.007	42.03	58.582	60.287	72.73	79.13
MoOCl4(H2O)	46.63	34.366	36.122	45.494	48.85	43.616	45.228	45.624	53.189	54.267	55.915	56.716	43.451	60.411	61.837	71.29	77.522
MoOBr4(H2O)		31.503	33.115	41.468	44.569	39.358	40.862	41.349	47.416	49.929	51.519	52.782	39.962	55.903	57.43	68	73.456
MoNCl4		50.153	52.82	67.74	73.407	64.82	67.368	67.661	80.591	82.249	84.95	84.255	70.269	92.516	89.489	113.516	124.586
	mean dev	12.801	10.99483	1.4355	-2.09967	3.035833	1.35833	0.9595	-6.76183	-7.99317	-9.703	-10.501	2.69767	-14.395833	-15.8725	-25.674	-32.3185
	MAD	12.801	10.99483	1.618167	2.662	3.035833	1.61967	1.4088333	6.761833	7.99317	9.703	10.501	2.69767	14.395833	15.8725	25.6737	32.3185
Aaniso	BS2																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		27.89	27.85	27.322	27.74	27.432	27.479	27.517	27.539	28.644	28.661	29.099	28.819	28.825	28.707	30.337	30.462
MOCl4	25.7	24.437	24.437	24.158	24.601	24.323	24.39	24.405	24.6	25.834	25.866	26.193	25.947	26.125	26.028	27.73	27.91

MoOBr4		23.772	23.784	23.586	24.024	23.626	23.685	23.707	23.939	25.271	25.301	25.609	25.413	25.59	25.5	27.359	27.482
MoOF5	31.87	27.759	27.685	26.897	27.256	27.263	27.276	27.309	27.131	28.215	28.187	28.743	28.328	28.223	28.11	29.293	29.338
MoOCl5	28.1	24.379	24.348	23.819	24.178	24.192	24.232	24.262	24.193	25.404	25.388	25.84	25.446	25.473	25.379	26.198	26.101
MoOBr5	22	23.72	23.706	23.275	23.638	23.507	23.541	23.577	23.556	24.899	24.884	25.312	24.979	25.007	24.922	25.934	25.792
MoOCl4(H2O)	28.07	24.396	24.388	24.044	24.467	24.278	24.337	24.356	24.49	25.686	25.703	26.057	25.764	25.908	25.811	27.214	27.335
MoOBr4(H2O)		25.343	23.698	23.443	23.864	23.548	23.6	23.625	23.806	25.108	25.123	25.457	25.209	25.363	25.274	26.83	26.9
MoNCl4		24.763	24.7	23.964	24.307	24.372	24.392	24.441	24.162	24.92	24.867	25.366	24.944	24.756	23.829	24.685	24.281
	mean dev	2.2098	2.2352	2.7094	2.32	2.4354	2.3928	2.3662	2.354	1.1404	1.1424	0.719	1.0552	1.0008	1.098	-0.1258	-0.1472
	MAD	2.8978	2.9176	3.2194	2.9752	3.0382	3.0092	2.997	2.9764	2.3536	2.3624	2.241	2.3456	2.3736	2.398	2.2598	2.2536

Table S12. Calculated EPR spectra parameters for test complexes using B3P86 optimized geometries and BS2.

g parr	BS2															
B3P86 Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.895	1.852	1.853	1.861	1.858	1.866	1.867	1.866	1.868	1.844	1.845	1.84	1.841	1.841	1.841	1.801	1.807
MOCl4	1.968	1.979	1.979	1.981	1.981	1.981	1.981	1.981	1.98	1.965	1.965	1.963	1.961	1.961	1.962	1.932	1.932
MoOBr4		2.096	2.095	2.089	2.09	2.089	2.089	2.09	2.084	2.079	2.078	2.081	2.077	2.073	2.072	2.051	2.049
MoOF5	1.874	1.86	1.861	1.87	1.866	1.873	1.873	1.873	1.875	1.846	1.846	1.842	1.838	1.842	1.842	1.797	1.803
MoOCl5	1.963	1.97	1.97	1.973	1.973	1.974	1.974	1.974	1.974	1.952	1.952	1.951	1.948	1.946	1.946	1.907	1.909
MoOBr5	2.09	2.094	2.093	2.085	2.087	2.088	2.088	2.089	2.083	2.074	2.072	2.077	2.064	2.065	2.07	2.031	2.03
MoOCl4(H2O)	1.9632	1.977	1.977	1.979	1.979	1.98	1.98	1.98	1.98	1.962	1.961	1.961	1.958	1.957	1.957	1.925	1.926
MoOBr4(H2O)	1.98	2.096	2.095	2.088	2.09	2.09	2.09	2.091	2.085	2.079	2.078	2.081	2.076	2.072	2.071	2.046	2.045
MoNCl4	1.9063	1.854	1.855	1.865	1.862	1.867	1.868	1.868	1.868	1.823	1.824	1.819	1.811	1.816	1.816	1.744	1.752
	mean dev	-0.00531	-0.00544	-0.00781	-0.00706	-0.00994	-0.01019	-0.010313	-0.00919	0.01181	0.01206	0.01319	0.01781	0.0174375	0.016813	0.05706	0.054438
	MAD	0.032638	0.032013	0.028888	0.030138	0.027763	0.02751	0.0276375	0.027262	0.03656	0.03656	0.03844	0.04181	0.0404375	0.039563	0.07356	0.070688
g perpen	BS2																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.925	1.871	1.872	1.879	1.879	1.888	1.889	1.888	1.891	1.881	1.882	1.88	1.876	1.881	1.881	1.863	1.87
MOCl4	1.93	1.908	1.908	1.914	1.911	1.917	1.916	1.916	1.918	1.908	1.908	1.907	1.907	1.906	1.904	1.889	1.892
MoOBr4		1.92	1.92	1.924	1.92	1.926	1.926	1.926	1.925	1.915	1.915	1.915	1.911	1.912	1.913	1.895	1.897
MoOF5	1.911	1.766	1.768	1.776	1.786	1.812	1.814	1.809	1.819	1.811	1.812	1.81	1.802	1.814	1.813	1.79	1.807
MoOCl5	1.94	1.863	1.864	1.874	1.872	1.882	1.883	1.882	1.887	1.874	1.875	1.874	1.87	1.875	1.875	1.856	1.862
MoOBr5	1.945	1.878	1.879	1.886	1.883	1.894	1.894	1.893	1.896	1.883	1.883	1.883	1.883	1.883	1.879	1.867	1.873
MoOCl4(H2O)	1.94	1.892	1.893	1.9	1.898	1.905	1.905	1.904	1.907	1.897	1.897	1.896	1.893	1.896	1.896	1.879	1.882
MoOBr4(H2O)	1.947	1.897	1.898	1.904	1.92	1.908	1.908	1.907	1.91	1.898	1.899	1.898	1.895	1.897	1.898	1.881	1.885
MoNCl4	1.9843	1.983	1.983	1.982	1.981	1.984	1.984	1.983	1.981	1.978	1.977	1.977	1.976	1.976	1.976	1.962	1.96
	mean dev	0.058038	0.057163	0.050913	0.049038	0.041538	0.04116	0.0425375	0.039163	0.04904	0.04866	0.04966	0.05254	0.0492875	0.050038	0.06691	0.061413
	MAD	0.058038	0.057163	0.050913	0.049038	0.041538	0.04116	0.0425375	0.039163	0.04904	0.04866	0.04966	0.05254	0.0492875	0.050038	0.06691	0.061413
AF	BS2																
B3P86 Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		44.734	46.907	58.65	62.675	58.793	60.653	60.968	71.339	69.773	71.521	71.446	57.803	76.411	77.602	83.799	91.839
MOCl4	49.8	34.374	36.095	45.167	48.364	43.802	45.329	45.73	53.218	54.246	55.789	56.689	61.413	60.116	43.421	70.197	76.227
MoOBr4	42	31.803	33.398	41.568	44.54	39.947	41.379	41.867	48.04	50.397	51.893	53.223	40.501	56.14	57.534	67.396	72.739
MoOF5	61.06	45.475	47.731	60.08	64.588	59.801	61.795	61.937	72.996	71.243	73.113	72.686	59.153	78.22	79.435	85.878	94.178
MoOCl5	46.6	47.25	35.513	37.34	55.246	45.166	46.9	47.25	47.143	50.737	58.87	56.426	64.439	45.72	58.193	74.788	81.549
MoOBr5	44	32.522	34.191	42.844	46.147	40.705	42.32	42.773	49.086	51.874	53.573	54.771	59.797	58.224	53.573	71.291	77.194
MoOCl4(H2O)	46.63	34.555	36.312	45.703	49.021	43.883	45.477	45.842	53.475	54.436	56.049	56.79	43.594	60.468	61.802	70.928	76.991
MoOBr4(H2O)		31.738	33.356	41.783	44.848	39.682	41.168	41.621	47.815	50.183	51.738	52.915	40.245	56.055	57.483	67.744	73.043
MoNCl4		50.123	52.763	67.467	72.953	64.838	67.331	67.602	80.352	81.695	84.284	83.634	69.687	91.499	93.179	110.063	120.318
	mean dev	10.68517	11.14167	2.898	-2.96933	2.797667	1.14833	0.7818333	-5.64467	-7.1405	-9.86617	-10.083	-6.4678	-11.466333	-10.6447	-25.065	-31.46467
	MAD	10.90183	11.14167	2.898	3.448	2.797667	1.49333	1.2908333	5.644667	7.1405	9.86617	10.0825	8.61517	11.759667	12.771	25.0647	31.46467
Aaniso	BS2																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		27.945	27.909	27.402	27.835	27.5	27.55	27.584	27.638	28.689	28.708	29.143	28.862	28.869	28.749	30.348	30.488
MOCl4	25.7	24.358	24.361	24.102	24.562	24.265	24.336	24.348	24.577	25.773	25.809	26.133	25.972	26.071	25.889	27.679	27.886

MoOBr4		23.683	23.698	23.519	23.972	23.556	23.619	23.638	23.903	25.195	25.228	25.534	25.335	25.52	25.428	27.289	27.438
MoOF5	31.87	27.84	27.77	27.01	27.412	27.369	27.389	27.411	27.286	28.354	28.334	28.873	28.474	28.391	28.275	29.545	29.644
MoOCl5	28.1	24.314	24.289	23.809	24.2	24.163	24.211	24.237	24.241	25.442	25.44	25.872	25.5	25.572	25.475	26.598	26.635
MoOBr5	22	23.632	23.623	23.237	23.627	23.45	23.492	23.522	23.57	24.901	24.899	25.308	24.98	25.068	24.999	26.289	26.272
MoOCl4(H2O)	28.07	24.349	24.345	24.03	24.476	24.258	24.323	24.338	24.519	25.686	25.71	26.057	25.774	25.931	25.831	27.316	27.491
MoOBr4(H2O)		23.612	23.631	23.401	23.842	23.501	23.558	23.579	23.802	25.076	25.097	25.425	25.185	25.351	25.259	26.898	27.081
MoNCl4		24.695	24.641	23.973	24.357	24.346	24.377	24.42	24.236	24.991	24.955	25.431	25.022	24.901	24.813	25.173	24.972
	mean																
	dev	2.2494	2.2704	2.7104	2.2926	2.447	2.3978	2.3768	2.3094	1.1168	1.1096	0.6994	1.008	0.9414	1.0542	-0.3374	-0.4376
	MAD	2.9022	2.9196	3.2052	2.9434	3.027	2.9946	2.9856	2.9374	2.3064	2.3128	2.1958	2.3088	2.317	2.3294	2.1698	2.1456

Table S13. Calculated EPR spectra parameters for test complexes using PBE1PBE optimized geometries and BS2.

g parr	BS2															
PBE1PBE Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.895	1.852	1.853	1.861	1.858	1.867	1.867	1.867	1.868	1.844	1.845	1.841	1.837	1.841	1.842	1.801	1.808
MOCl4	1.968	1.98	1.98	1.982	1.982	1.982	1.982	1.982	1.981	1.966	1.965	1.964	1.961	1.961	1.962	1.933	1.933
MoOBr4		2.097	2.096	2.089	2.091	2.09	2.089	2.09	2.084	2.08	2.079	2.081	2.077	2.074	2.072	2.057	2.049
MoOF5	1.874	1.86	1.861	1.87	1.866	1.873	1.873	1.873	1.875	1.846	1.846	1.842	1.838	1.842	1.842	1.797	1.803
MoOCl5	1.963	1.971	1.971	1.974	1.974	1.975	1.975	1.975	1.975	1.953	1.953	1.952	1.948	1.947	1.947	1.908	1.91
MoOBr5	2.09	2.094	2.093	2.086	2.088	2.089	2.088	2.089	2.083	2.074	2.073	2.077	2.064	2.066	2.071	2.032	2.031
MoOCl4(H2O)	1.9632	1.977	1.978	1.98	1.979	1.981	1.98	1.981	1.98	1.962	1.962	1.961	1.959	1.957	1.957	1.926	1.927
MoOBr4(H2O)	1.98	2.097	2.096	2.089	2.091	2.091	2.091	2.091	2.086	2.08	2.079	2.082	2.077	2.073	2.072	2.047	2.046
MoNCl4	1.9063	1.855	1.856	1.866	1.863	1.868	1.868	1.869	1.869	1.824	1.825	1.82	1.812	1.816	1.816	1.745	1.753
	mean dev	-0.00581	-0.00606	-0.00856	-0.00769	-0.01081	-0.01056	-0.010938	-0.00969	0.01131	0.01144	0.01256	0.01794	0.0170625	0.016313	0.05631	0.053563
	MAD	0.032888	0.032388	0.029138	0.030263	0.027888	0.02789	0.0277625	0.027512	0.03631	0.03619	0.03806	0.04219	0.0403125	0.039313	0.07306	0.070063
g perpen	BS2																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.925	1.873	1.874	1.881	1.881	1.89	1.89	1.889	1.893	1.883	1.883	1.882	1.878	1.883	1.883	1.865	1.871
MOCl4	1.93	1.909	1.909	1.915	1.912	1.917	1.917	1.917	1.919	1.909	1.909	1.908	1.908	1.907	1.905	1.891	1.893
MoOBr4		1.921	1.922	1.925	1.921	1.927	1.927	1.927	1.926	1.916	1.916	1.916	1.912	1.914	1.914	1.897	1.899
MoOF5	1.911	1.77	1.772	1.779	1.789	1.814	1.816	1.812	1.821	1.813	1.815	1.812	1.805	1.816	1.816	1.893	1.81
MoOCl5	1.94	1.865	1.866	1.875	1.873	1.884	1.884	1.883	1.888	1.876	1.876	1.875	1.871	1.876	1.876	1.857	1.864
MoOBr5	1.945	1.881	1.881	1.888	1.885	1.896	1.895	1.895	1.898	1.885	1.885	1.885	1.885	1.884	1.881	1.869	1.874
MoOCl4(H2O)	1.94	1.894	1.895	1.902	1.899	1.906	1.906	1.905	1.908	1.898	1.898	1.897	1.894	1.85	1.898	1.881	1.884
MoOBr4(H2O)	1.947	1.903	1.904	1.909	1.906	1.913	1.913	1.913	1.914	1.904	1.904	1.904	1.9	1.903	1.903	1.887	1.89
MoNCl4	1.9843	1.983	1.983	1.982	1.982	1.984	1.984	1.983	1.982	1.978	1.978	1.978	1.977	1.976	1.976	1.963	1.961
	mean dev	0.055538	0.054788	0.048913	0.049413	0.039788	0.03966	0.0406625	0.037413	0.04704	0.04679	0.04766	0.05054	0.0534125	0.048038	0.05204	0.059413
	MAD	0.055538	0.054788	0.048913	0.049413	0.039788	0.03966	0.0406625	0.037413	0.04704	0.04679	0.04766	0.05054	0.0534125	0.048038	0.05204	0.059413
AF	BS2																
PBE1PBE Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		44.816	46.993	58.754	62.78	58.9	60.762	61.075	71.461	69.905	71.654	71.573	57.923	76.553	77.739	83.966	92.013
MOCl4	49.8	34.423	36.146	45.23	48.424	43.867	45.393	45.791	53.294	54.321	55.863	56.755	61.477	60.192	43.495	70.275	76.304
MoOBr4	42	31.955	33.451	41.638	44.606	40.014	41.445	41.93	48.121	50.476	51.97	53.39	40.583	56.219	57.602	67.48	72.821
MoOF5	61.06	45.547	47.805	60.158	64.663	59.885	61.88	62.02	73.078	71.334	73.203	72.781	59.25	78.308	79.521	85.968	94.252
MoOCl5	46.6	35.543	37.369	47.165	50.747	45.201	46.93	47.278	55.268	56.439	58.198	58.876	45.735	62.96	64.41	74.665	81.358
MoOBr5	44	32.559	34.228	42.883	46.173	40.749	42.359	42.808	49.127	51.896	53.587	54.781	59.774	58.218	41.999	71.169	77.007
MoOCl4(H2O)	46.63	34.607	36.364	45.762	49.074	43.949	45.54	45.904	53.543	54.506	56.116	56.853	43.663	60.531	61.854	70.969	77.014
MoOBr4(H2O)		31.787	33.406	41.835	44.893	39.736	41.22	41.669	47.874	50.228	51.778	52.952	40.294	56.083	57.499	67.724	72.996
MoNCl4		50.183	52.821	67.506	72.97	64.92	67.411	67.68	80.407	81.723	84.302	83.66	69.713	91.478	93.148	109.744	119.896
	mean dev	12.576	10.78783	1.209	-2.26617	2.7375	1.0905	0.7265	-7.05683	-8.147	-9.80783	-10.558	-3.3987	-14.389667	-9.7985	-25.073	-31.44433
	MAD	12.576	10.78783	1.397333	2.724833	2.7375	1.47383	1.2725	7.056833	8.147	9.80783	10.5577	5.75167	14.389667	12.56717	25.0727	31.44433
Aaniso	BS2																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		27.948	27.913	27.409	27.844	27.506	27.556	27.59	27.647	28.693	28.713	29.147	28.867	28.873	28.753	30.349	30.49
MOCl4	25.7	24.348	24.352	24.098	24.561	24.259	24.331	24.343	24.578	25.768	25.805	26.128	25.969	26.068	25.885	27.675	27.887

MoOBr4		23.672	23.687	23.513	23.969	23.549	23.612	23.631	23.902	25.189	25.223	25.528	25.329	25.516	25.423	27.284	27.437
MoOF5	31.87	27.848	27.779	27.025	27.431	27.381	27.402	27.424	27.306	28.373	28.355	28.891	28.495	28.415	28.299	29.579	29.684
MoOCl5	28.1	24.31	24.287	23.816	24.213	24.165	24.215	24.24	24.256	25.456	25.457	25.885	25.517	25.596	25.499	26.66	26.715
MoOBr5	22	23.624	23.616	23.24	23.635	23.448	23.491	23.52	23.581	24.911	24.91	25.316	25.011	25.087	25.011	26.348	26.349
MoOCl4(H2O)	28.07	24.341	24.338	24.029	24.479	24.255	24.321	24.335	24.524	25.688	25.713	26.058	25.777	25.936	25.837	27.332	27.514
MoOBr4(H2O)		23.629	23.64	23.42	23.866	23.516	23.573	23.594	23.829	25.098	25.121	25.445	25.209	25.379	25.286	26.937	27.065
MoNCl4		24.694	24.641	23.983	24.374	24.351	24.383	24.425	24.255	25.009	24.975	25.447	25.042	24.928	24.84	25.243	25.068
	mean																
	dev	2.2538	2.2736	2.7064	2.2842	2.4464	2.396	2.3756	2.299	1.1088	1.1	0.6924	0.9942	0.9276	1.0418	-0.3708	-0.4818
	MAD	2.9034	2.92	3.2024	2.9382	3.0256	2.9924	2.9836	2.9314	2.3004	2.306	2.19	2.3062	2.3096	2.3202	2.1584	2.1326

Table S14. Calculated EPR spectra parameters for test complexes using X-ray geometries and BS2.

g parr	BS2																
X-ray Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.895	1.907	1.908	1.913	1.91	1.913	1.913	1.913	1.913	1.897	1.897	1.894	1.892	1.895	1.895	1.87	1.871
MOCl4	1.968	1.994	1.994	1.996	1.995	1.995	1.994	1.995	1.993	1.979	1.979	1.978	1.976	1.975	1.975	1.949	1.948
MoOBr4		2.106	2.105	2.099	2.1	2.098	2.097	2.098	2.092	2.09	2.089	2.09	2.088	2.085	2.084	2.069	2.065
MoOF5	1.874	1.881	1.882	1.891	1.886	1.89	1.891	1.891	1.893	1.867	1.868	1.865	1.861	1.864	1.865	1.829	1.833
MoOCl5	1.963	1.988	1.989	1.99	1.989	1.989	1.989	1.989	1.988	1.97	1.97	1.969	1.967	1.965	1.965	1.933	1.933
MoOBr5	2.09	2.103	2.102	2.095	2.097	2.096	2.095	2.096	2.09	2.088	2.087	2.09	2.086	2.082	2.081	2.096	2.921
MoOCl4(H2O)	1.9632	1.938	1.936	1.941	1.945	1.954	1.954	1.952	1.957	1.928	1.928	1.928	1.92	1.918	1.917	1.855	1.867
MoOBr4(H2O)	1.98	2.104	2.102	2.097	2.099	2.098	2.098	2.099	2.092	2.09	2.089	2.091	2.087	2.086	2.084	2.05	2.05
MoNCl4	1.9063	1.936	1.937	1.942	1.938	1.937	1.937	1.937	1.935	1.909	1.909	1.905	1.902	1.903	1.904	1.864	1.862
	mean dev	-0.02612	-0.02647	-0.02789	-0.02722	-0.02891	-0.02886	-0.029067	-0.02777	-0.01097	-0.01075	-0.01	-0.0065	-0.0059566	-0.00572	0.02259	-0.08194
	MAD	0.032944	0.033098	0.033602	0.031924	0.031493	0.03126	0.0315818	0.02936	0.02234	0.02225	0.02195	0.02346	0.0224778	0.022353	0.04512	0.146212
g perpen	BS2																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4	1.925	1.837	1.838	1.844	1.847	1.861	1.861	1.86	1.864	1.858	1.858	1.856	1.852	1.859	1.859	1.843	1.853
MOCl4	1.93	1.892	1.893	1.9	1.897	1.903	1.903	1.903	1.906	1.896	1.896	1.895	1.892	1.895	1.895	1.879	1.883
MoOBr4		1.889	1.89	1.897	1.893	1.9	1.9	1.9	1.902	1.89	1.89	1.889	1.885	1.889	1.889	1.87	1.873
MoOF5	1.911	1.823	1.823	1.795	1.828	1.851	1.852	1.845	1.842	1.851	1.851	1.849	1.844	1.852	1.852	1.836	1.847
MoOCl5	1.94	1.883	1.884	1.891	1.889	1.897	1.897	1.896	1.9	1.89	1.891	1.889	1.886	1.89	1.89	1.875	1.881
MoOBr5	1.945	1.749	1.754	1.784	1.784	1.8	1.802	1.799	1.818	1.804	1.808	1.802	1.802	1.818	1.819	1.818	1.827
MoOCl4(H2O)	1.94	1.9	1.9	1.907	1.903	1.911	1.911	1.91	1.912	1.902	1.903	1.902	1.899	1.9	1.9	1.885	1.889
MoOBr4(H2O)	1.947	1.903	1.904	1.909	1.906	1.913	1.913	1.913	1.916	1.905	1.907	1.907	1.902	1.905	1.905	1.892	1.895
MoNCl4	1.9843	1.983	1.983	1.982	1.982	1.984	1.984	1.983	1.981	1.979	1.979	1.978	1.978	1.978	1.978	1.968	1.966
	mean dev	0.069249	0.068063	0.064001	0.060968	0.050339	0.05004	0.0517496	0.04803	0.0546	0.05394	0.05573	0.05846	0.0530862	0.052905	0.06596	0.060428
	MAD	0.069249	0.068063	0.064001	0.060968	0.050339	0.05004	0.0517496	0.04803	0.0546	0.05394	0.05573	0.05846	0.0530862	0.052905	0.06596	0.060428
AF	BS2																
X-ray Geom	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		43.263	45.326	56.48	60.243	57.848	59.524	59.661	69.753	67.94	69.513	69.178	55.061	74.106	75.007	80.043	88.148
MOCl4	49.8	33.934	35.633	44.674	47.771	43.36	44.837	45.191	52.776	53.578	55.069	55.884	42.65	59.32	60.498	69.136	75.185
MoOBr4	42	30.509	32.051	40.145	43.017	38.596	39.934	40.339	46.721	48.285	49.664	50.724	38.135	53.676	54.895	63.761	69.149
MoOF5	61.06	45.5	47.69	59.478	63.813	60.014	61.889	61.963	72.474	70.904	72.634	72.221	58.678	77.466	78.514	84.348	92.322
MoOCl5	46.6	35.466	37.259	46.879	50.285	45.198	46.835	47.13	55.085	55.883	57.511	58.125	45.057	61.963	63.187	72.243	78.41
MoOBr5	44	30.619	32.258	41.342	45.031	39.209	40.842	41.239	48.851	51.94	53.962	54.444	40.871	60.467	62.229	78.795	88.617
MoOCl4(H2O)	46.63	34.776	36.536	46.004	49.263	44.256	45.819	46.136	53.933	54.765	56.34	56.97	43.837	60.719	61.916	70.921	76.957
MoOBr4(H2O)		31.865	33.487	42.044	45.059	39.925	41.379	41.777	48.196	50.368	51.88	52.905	40.392	56.157	57.455	67.584	72.861
MoNCl4		46.411	48.808	62.12	67.07	60.449	62.606	62.752	74.757	75.086	77.256	76.677	62.463	83.483	84.656	97.791	107.255
	mean dev	13.21433	11.44383	1.928	-1.515	3.242833	1.65567	1.3486667	-6.625	-7.54417	-9.18167	-9.713	3.477	-13.920167	-15.1915	-24.852	-31.75833
	MAD	13.21433	11.44383	2.021	2.191333	3.242833	2.01033	1.8263333	6.625	7.54417	9.18167	9.713	3.477	13.920167	15.1915	24.8523	31.75833
Aaniso	BS2																
	Exp	SVWN	SVWN5	HFS	Xalpha	BP86	BPW91	PW91PW91	HFB	B3P86	B3PW91	B3LYP	B98	MPW1PW91	PBE1PBE	BHandH	BHandLYP
MoOF4		28.222	28.183	27.661	28.133	27.788	27.826	27.822	27.931	28.804	28.813	29.258	28.948	28.925	28.796	30.246	30.416
MOCl4	25.7	24.095	24.101	23.866	24.326	24.031	24.102	24.109	24.375	25.513	25.548	25.873	25.613	25.805	25.699	27.366	27.587

MoOBr4		23.141	23.142	22.883	23.301	22.985	23.033	23.047	23.257	24.495	24.511	24.852	24.602	24.764	24.659	26.43	26.569
MoOF5	31.87	28.011	27.957	27.29	27.814	27.613	27.653	27.652	27.663	30.729	28.73	29.204	28.865	28.847	28.724	30.158	30.35
MoOCl5	28.1	24.092	24.081	23.687	24.156	24.016	24.081	24.095	24.248	25.4	25.422	25.813	25.486	25.624	25.52	26.985	27.197
MoOBr5	22	22.836	22.759	21.907	22.04	22.431	22.404	22.445	21.929	22.72	22.549	23.198	22.471	22.006	21.909	20.106	19.55
MoOCl4(H2O)	28.07	24.099	24.1	23.813	24.277	24.05	24.119	24.13	24.365	25.477	25.505	25.853	25.559	25.732	25.628	27.132	27.357
MoOBr4(H2O)		23.334	23.346	23.129	23.578	23.247	23.304	23.322	23.581	24.812	24.835	25.168	24.907	25.09	24.993	26.641	26.799
MoNCl4		23.752	23.706	23.11	23.545	23.496	23.537	23.559	23.518	24.258	24.238	24.691	24.3	24.248	24.138	24.854	24.849
	mean dev	2.5214	2.5484	3.0354	2.6254	2.7198	2.6762	2.6618	2.632	1.1802	1.5972	1.1598	1.5492	1.5452	1.652	0.7986	0.7398
	MAD	2.8558	2.852	3.0354	2.6414	2.8922	2.8378	2.8398	2.632	1.4682	1.8168	1.7082	1.7376	1.5896	1.652	1.465	1.4946

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