Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Table S1 – Experimental equilibrium bond lengths (Å) given by the cited references and T1 diagnostic values obtained during our coupled cluster calculations.

Molecules	r(O-C)	r(Y-Cu)	r(Cu-X)	T1
CuH[a]	-	-	1.46263	0.060
CuF[a]	-	-	1.74493	0.064
CuCl[a]	-	-	2.051183	0.047
CuBr[a]	-	-	2.17344	0.038
CuI[a]	-	-	2.338324	0.036
ArCuF[b]	-	2.219	1.753	0.042
ArCuCl[b]	-	2.2706	2.0501	0.037
ArCuBr[b]	-	2.2883	2.1728	0.032
KrCuF[c]	-	2.31801	1.7536	0.037
KrCuCl[c]	-	2.36286	2.0525	0.032
XeCuF[d]	-	2.4327	1.754	0.036
XeCuCl[d]	-	2.471	2.058	0.032
OCCuF[e]	1.1307	1.7639	1.7364	0.044
OCCuCl[e]	1.12755	1.79447	2.053419	0.041
OCCuBr[e]	1.12721	1.80238	2.17871	0.036
OCCuI[f]	1.1269	1.8154	2.3563	0.037

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e) N. R. Walker and M. C. L. Gerry, *Inorg. Chem*, 2001, **40**, 6158-6166.

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