

Supporting Information for:
The Nature of Chemical Bond in Oxyanionic Crystals Based on QTAIM Topological Analysis of Electron Densities

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Table S1. Topological properties of electron density calculated at the BCPs for metal-oxygen and intra-anionic bonds in divalent metal nitrates

Crystal	Bonds	ρ_c (a.u.)	$\Delta\rho_c$ (a.u.)	H_c (a.u.)
Mg(NO ₃) ₂	N-O	0.448	-0.668	-0.809
	Mg-O	0.032	0.202	0.008
Ca(NO ₃) ₂	N-O	0.446	-0.643	-0.801
	Ca-O	0.024	0.103	0.003
Sr(NO ₃) ₂	N-O	0.444	-0.632	-0.795
	Sr-O	0.020	0.082	0.003
Ba(NO ₃) ₂	N-O	0.442	-0.622	-0.788
	Ba-O	0.019	0.068	0.002
Pb(NO ₃) ₂	N-O	0.442	-0.612	-0.787
	Pb-O	0.026	0.075	-0.0003
Zn(NO ₃) ₂	N-O	0.446	-0.651	-0.802
	Zn-O	0.053	0.213	-0.0037

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Table S2. Topological properties of electron density calculated at the BCPs for metal-oxygen and intra-anionic bonds in divalent metal sulfates

Crystal	Bonds	ρ_c (a.u.)	$\Delta\rho_c$ (a.u.)	H_c (a.u.)
MgSO ₄	S-O1	0.264	1.085	-0.2215
	S-O2	0.246	0.664	-0.2220
	Mg-O1	0.039	0.264	0.0091
	Mg-O2	0.029	0.173	0.0066
CaSO ₄	S-O1	0.256	0.853	-0.2253
	S-O2	0.255	0.863	-0.2225
	Ca-O1	0.025	0.114	0.0034
	Ca-O2	0.032	0.162	0.0042
SrSO ₄	S-O1	0.261	1.027	-0.2205
	S-O2	0.258	0.876	-0.2272
	S-O3	0.251	0.746	-0.2246
	Sr-O1	0.027	0.128	0.0037
	Sr-O2	0.022	0.096	0.0030
	Sr-O3	0.023	0.098	0.0028
BaSO ₄	S-O1	0.260	0.983	-0.2222
	S-O2	0.256	0.857	-0.2249
	S-O3	0.250	0.736	-0.2235
	Ba-O1	0.021	0.087	0.0027
	Ba-O2	0.024	0.093	0.0020
	Ba-O3	0.025	0.092	0.0015
PbSO ₄	S-O1	0.262	1.015	-0.2234
	S-O2	0.255	0.809	-0.2270
	S-O3	0.249	0.689	-0.2255
	Pb-O1	0.028	0.103	0.0012
	Pb-O2	0.035	0.120	-0.0008
	Pb-O3	0.032	0.105	-0.0005
ZnSO ₄	S-O1	0.254	0.809	-0.2251
	S-O2	0.242	0.597	-0.2201
	S-O3	0.259	0.977	-0.2207
	Zn-O1	0.036	0.117	-0.0015
	Zn-O2	0.055	0.229	-0.0038
	Zn-O3	0.072	0.373	-0.0047

Atomic numbering is in accordance with Fig. 1.

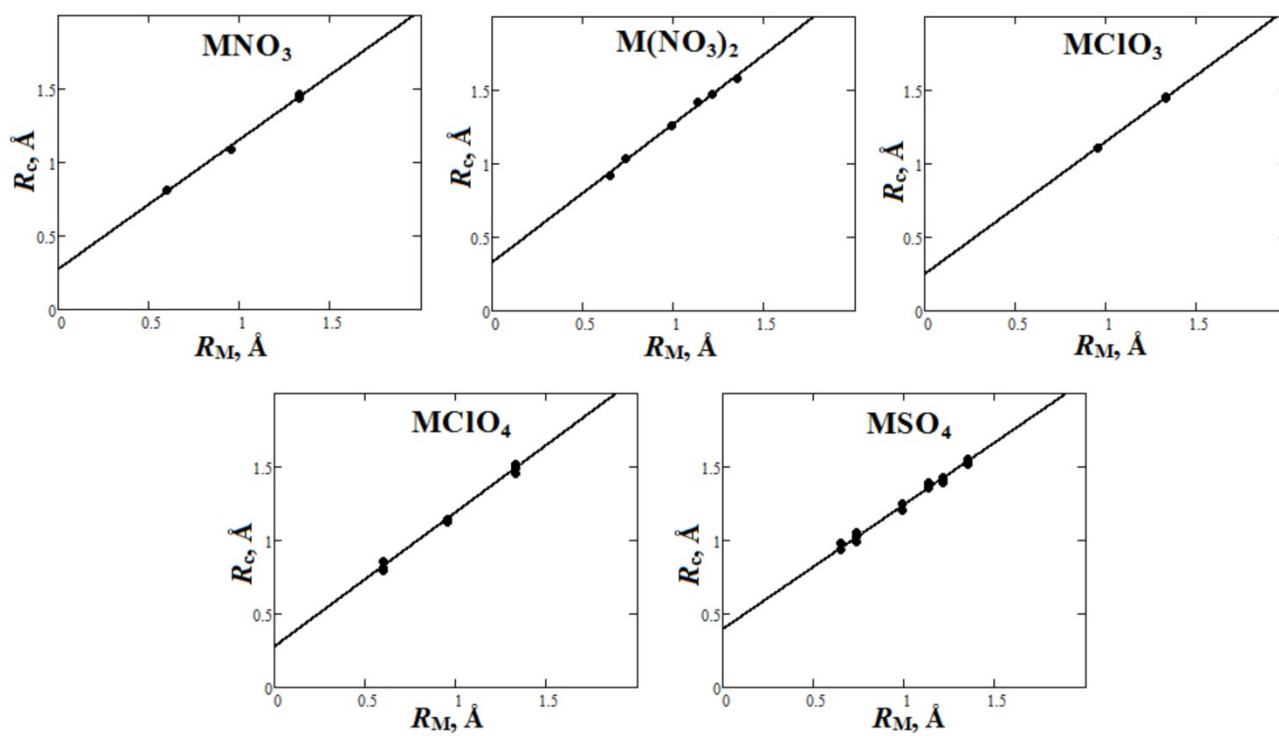


Figure S1 The scatterplots for the linear correlations in oxyanionic crystals with metal cations