

# A Bayesian Method for Selecting Data Points for Thermodynamic Modeling of Off-Stoichiometric Metal Oxides

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**Table SI-1:** 1<sup>st</sup> order Redlich-Kister expansion of excess terms for a three sublattice CEF model with two conditions on each sublattice.

L1 L2	$\gamma_{Sr}^A \gamma_{Ba}^A \gamma_{Fe}^B \gamma_{Fe}^{+3} \gamma_O^O (L_1^\circ + (\gamma_{Sr}^A - \gamma_{Ba}^A) L_2')$
L3 L4	$\gamma_{Sr}^A \gamma_{Ba}^A \gamma_{Fe}^B \gamma_{Fe}^{+3} \gamma_{Va}^O (L_3^\circ + (\gamma_{Sr}^A - \gamma_{Ba}^A) L_4')$
L5 L6	$\gamma_{Sr}^A \gamma_{Ba}^A \gamma_{Fe}^B \gamma_{Fe}^{+4} \gamma_O^O (L_5^\circ + (\gamma_{Sr}^A - \gamma_{Ba}^A) L_6')$
L7 L8	$\gamma_{Sr}^A \gamma_{Ba}^A \gamma_{Fe}^B \gamma_{Fe}^{+4} \gamma_{Va}^O (L_7^\circ + (\gamma_{Sr}^A - \gamma_{Ba}^A) L_8')$
L9 L10	$\gamma_{Fe}^B \gamma_{Fe}^{+3} \gamma_{Fe}^B \gamma_{Fe}^{+4} \gamma_{Sr}^A \gamma_O^O (L_9^\circ + (\gamma_{Fe}^B \gamma_{Fe}^{+3} - \gamma_{Fe}^B \gamma_{Fe}^{+4}) L_{10}')$
L11 L12	$\gamma_{Fe}^B \gamma_{Fe}^{+3} \gamma_{Fe}^B \gamma_{Fe}^{+4} \gamma_{Ba}^A \gamma_O^O (L_{11}^\circ + (\gamma_{Fe}^B \gamma_{Fe}^{+3} - \gamma_{Fe}^B \gamma_{Fe}^{+4}) L_{12}')$
L13 L14	$\gamma_{Fe}^B \gamma_{Fe}^{+3} \gamma_{Fe}^B \gamma_{Fe}^{+4} \gamma_{Sr}^A \gamma_{Va}^O (L_{13}^\circ + (\gamma_{Fe}^B \gamma_{Fe}^{+3} - \gamma_{Fe}^B \gamma_{Fe}^{+4}) L_{14}')$
L15 L16	$\gamma_{Fe}^B \gamma_{Fe}^{+3} \gamma_{Fe}^B \gamma_{Fe}^{+4} \gamma_{Ba}^A \gamma_{Va}^O (L_{15}^\circ + (\gamma_{Fe}^B \gamma_{Fe}^{+3} - \gamma_{Fe}^B \gamma_{Fe}^{+4}) L_{16}')$
L17 L18	$\gamma_O^O \gamma_{Va}^O \gamma_{Sr}^A \gamma_{Fe}^B \gamma_{Fe}^{+3} (L_{17}^\circ + (\gamma_O^O - \gamma_{Va}^O) L_{18}')$
L19 L20	$\gamma_O^O \gamma_{Va}^O \gamma_{Ba}^A \gamma_{Fe}^B \gamma_{Fe}^{+3} (L_{19}^\circ + (\gamma_O^O - \gamma_{Va}^O) L_{20}')$
L21 L22	$\gamma_O^O \gamma_{Va}^O \gamma_{Sr}^A \gamma_{Fe}^B \gamma_{Fe}^{+4} (L_{21}^\circ + (\gamma_O^O - \gamma_{Va}^O) L_{22}')$
L23 L24	$\gamma_O^O \gamma_{Va}^O \gamma_{Ba}^A \gamma_{Fe}^B \gamma_{Fe}^{+4} (L_{23}^\circ + (\gamma_O^O - \gamma_{Va}^O) L_{24}')$

**Table SI-2:** Table of optimized CEF parameters from Cross fit algorithm for Bayesian iterations 31 – 38 and the ground truth (all data) model

	litr 31	litr 32	litr 33	litr 34	litr 35	litr 36	litr 37	litr 38	Ground Truth
<b>A17</b>	1.004E-04	1.004E-04	1.000E-04	1.004E-04	1.004E-04	1.004E-04	1.000E-04	1.004E-04	1.000E-04
<b>A18</b>	1.002E-04	1.002E-04	1.000E-04	1.002E-04	1.003E-04	1.003E-04	1.000E-04	1.003E-04	1.000E-04
<b>B17</b>	1.250E-04	1.264E-04	8.504E-05	1.246E-04	1.292E-04	1.297E-04	8.351E-05	1.333E-04	8.047E-05
<b>B18</b>	1.132E-04	1.134E-04	8.971E-05	1.124E-04	1.155E-04	1.158E-04	8.866E-05	1.177E-04	8.658E-05
<b>C17</b>	-9.624E-05	-1.395E-04	-7.038E-05	-1.173E-04	-1.395E-04	-1.523E-04	-8.207E-05	-1.375E-04	-8.637E-05
<b>C18</b>	-6.937E-05	-1.014E-04	-2.526E-05	-8.477E-05	-9.770E-05	-1.067E-04	-3.428E-05	-1.009E-04	-3.607E-05
<b>gDiffA1</b>	9.348E-05	9.343E-05	9.337E-05	9.337E-05	9.341E-05	9.341E-05	9.339E-05	9.330E-05	9.282E-05
<b>gDiffA2</b>	9.930E-05	9.929E-05	9.930E-05	9.934E-05	9.934E-05	9.934E-05	9.935E-05	9.934E-05	9.918E-05
<b>gDiffB1</b>	-7.135E-04	-7.189E-04	-7.246E-04	-7.214E-04	-7.173E-04	-7.166E-04	-7.192E-04	-7.279E-04	-7.980E-04
<b>gDiffB2</b>	-1.205E-05	-1.221E-05	-1.004E-05	-5.107E-06	-4.628E-06	-4.656E-06	-3.957E-06	-4.637E-06	-1.934E-05
<b>gDiffC1</b>	1.309E-04	1.316E-04	1.324E-04	1.320E-04	1.315E-04	1.314E-04	1.317E-04	1.329E-04	1.433E-04
<b>gDiffC2</b>	3.551E-05	3.560E-05	3.544E-05	3.462E-05	3.432E-05	3.415E-05	3.433E-05	3.449E-05	3.602E-05

Excess Terms

Endmember Terms