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Supporting information for article:

Crystal structures of alkali metal (Group 1) citrate salts

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Individual CIFs containing the DFT-optimized structures of the previously-reported Group 1b citrates are concatenated into one file, hw5048sup1.cif. The DFT-optimized structures of the new compounds are included in the references of Table 1.

$C_6H_5O_7$	CIF datablock
Li_1H_2	LIHCIT_DFT
$Li_1H_2(H_2O)_1$	PIGPUQ_P1_DFT
$Li_3(H_2O)_4$	FUQFUS_DFT
$Li_3(H_2O)_5$	CADJIA_DFT
Na_1H_2	NAHCIT_DFT
$Na_3(H_2O)_2$	Ramm048_UMOGAE_DFT
$Na_3(H_2O)_{5.5}$	FATTID_DFT
K_2H_1	ZZZQRO01_DFT
$K_3(H_2O)_1$	ZZZHVI01_DFT
Rb_1H_2	RBHCIT03_DFT
H_3	CITRAC10_DFT
$H_3(H_2O)_1$	CITARC_DFT

Table S1 A MS Excel spreadsheet Group1_distance_angle_torsion.xlsx, containing the citrate bond distances, angles, and torsion angles in the experimental and DFT-optimized structures. hw5048sup3.xlsx

Table S2 A MS Excel spreadsheet Group1_H-bonds.xlsx, containing the hydrogen bond geometries, overlap populations, and graph sets. hw5048sup4.xlsx

Table S3 A MS Excel spreadsheet M-O_DFT.xls, containing the metal-oxygen bond geometrical parameters and other related quantities. hw5048sup5.xls

Table S4 A SigmaPlot notebook citrate_conformations.jnb, containing the torsion angles and energies of low-energy conformations of citrate acid and various citrate anions. Individual sheets are also included as MS Excel spreadsheets citrate-1_cen.xls, citrate-1_end.xls, citrate-2.xls, and citrate-3.xls. hw5048sup6.jnb, hw5048sup7.xls, hw5048sup8.xls, hw5048sup9.xls hw5048sup10.xls

Table S5 A SigmaPlot notebook Energy.jnb, containing the various energy-related quantities. The individual sheets are also included as MS Excel spreadsheets energy_1.xls and energy_2.xls. hw5048sup11.jnb, hw5048sup12.xls, hw5048sup13.xls.