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SUPPLEMENTARY MATERIAL

Charge Localisation in Heavy Alkali Metal Ion Complexes of 4,4'- Biphenyldicarboxylate

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Figure S1

(a) Distribution of biphenyl-twist dihedral angles in the 22816 structures in the CSD containing the biphenyl unit with a wide variety of substituents :



(b) Distribution of the dihedral angles in biphenyl systems with substituents in the 4- or 4,4' positions only :

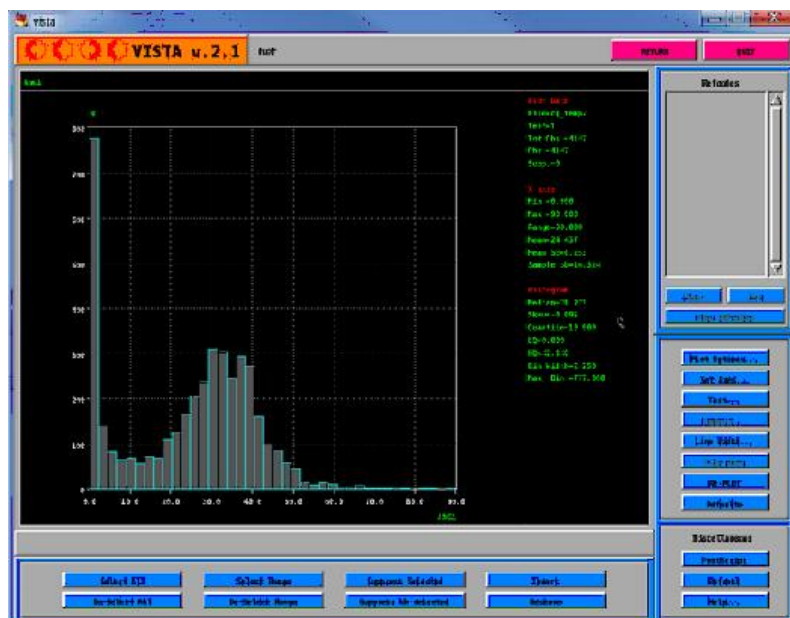
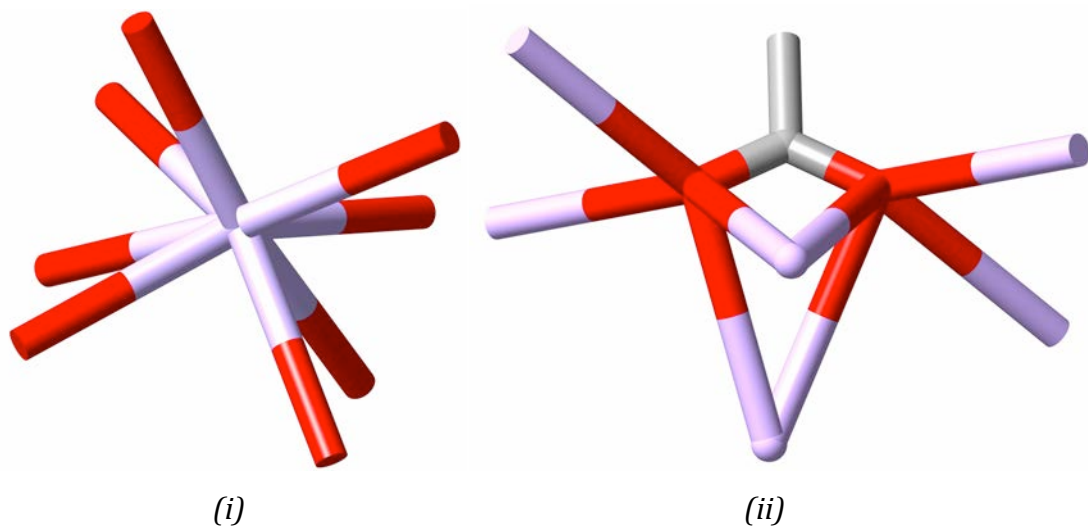


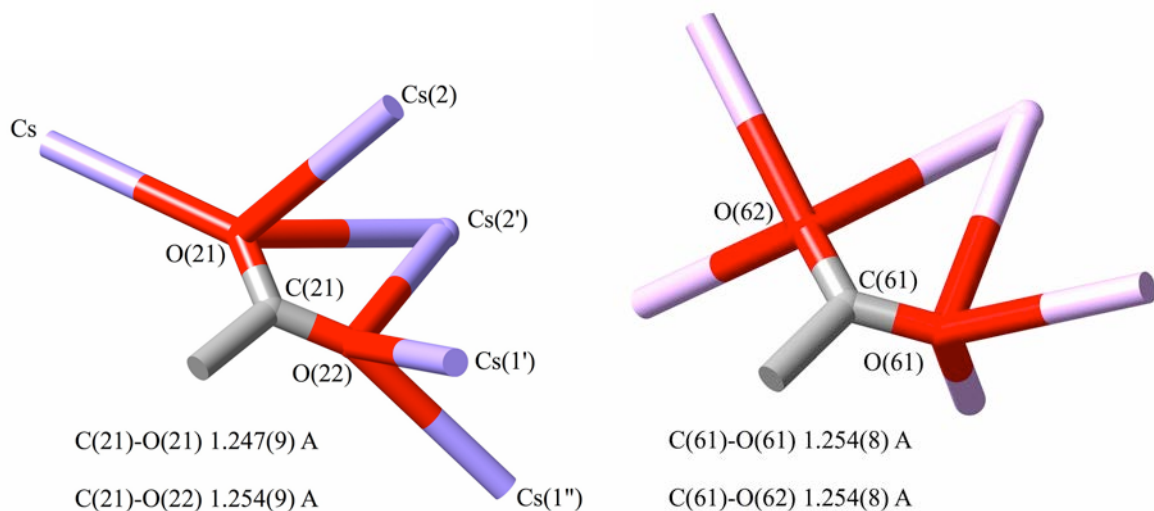
Figure S2 (i) Eight-coordinate Cs(I) and (ii) five-coordinate O in anhydrous CsO_2CCH_3 .²⁵



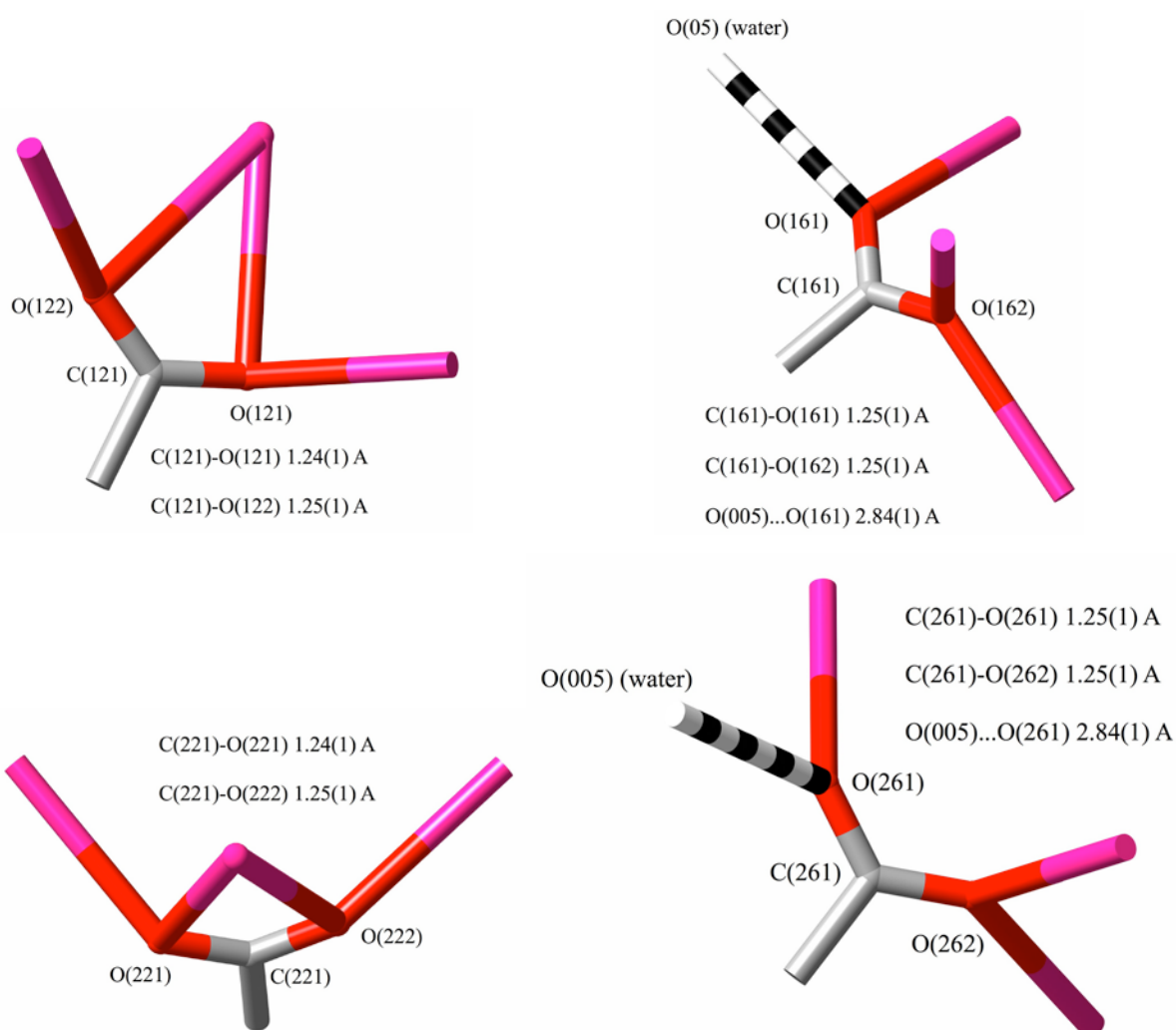
Carboxylate C-O 1.240(10), 1.270(6) Å.

Figure S3 Carboxylate coordination arrays in :

(a) Caesium chelidamate, $Cs_2C_7H_3NO_5$



(b) Rubidium chelidamate, $Rb_3(C_7H_3NO_5)(C_7H_4NO_5) \cdot 6H_2O$



(c) Lithium chelidamate, $\text{Li}_2\text{C}_7\text{H}_3\text{NO}_5 \cdot 3\text{H}_2\text{O}$

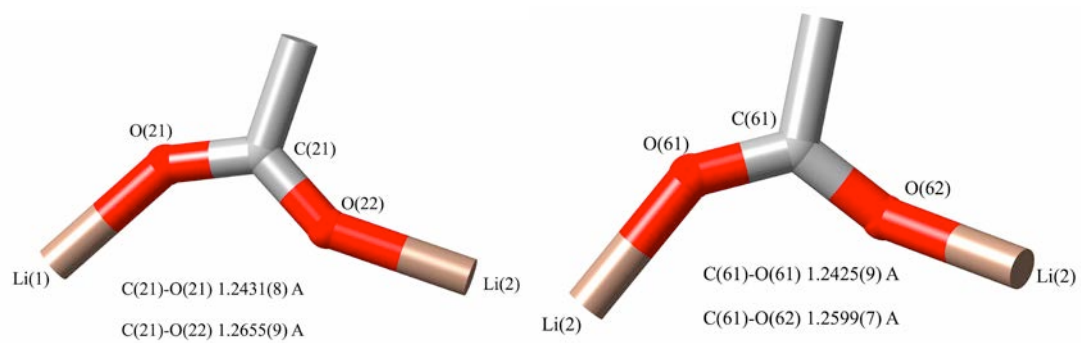
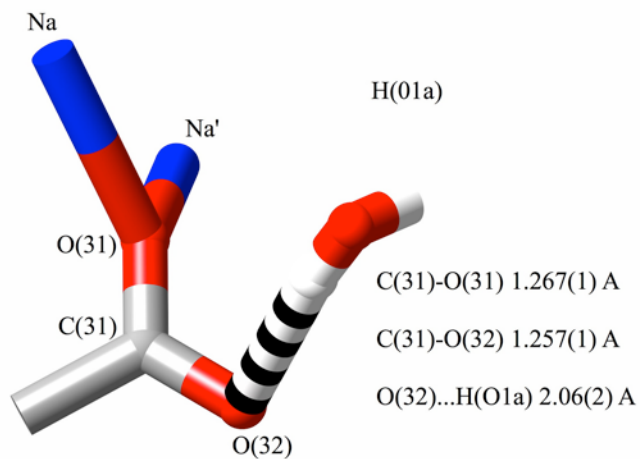


Figure S4 Carboxylate coordination arrays in :

(a) Sodium 2,2'-bipyridine-3,3'-bicarboxylate tetrahydrate (isomorphous with the potassium analogue)



(b) Rubidium 2,2'-bipyridine-3,3'-bicarboxylate monohydrate (isomorphous with the caesium analogue)

