

SUPPLEMENTARY MATERIAL

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

Jack Harrowfield^{A,C} and Pierre Thuéry^B

^AISIS, Université de Strasbourg, 8 allée Gaspard Monge, 67083 Strasbourg, France.

^BCEA, IRAMIS, CNRS UMR 3685 NIMBE, LCMCE, Bât. 125, 91191 Gif-sur-Yvette, France.

^CCorresponding author. Email: harrowfield@unistra.fr

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

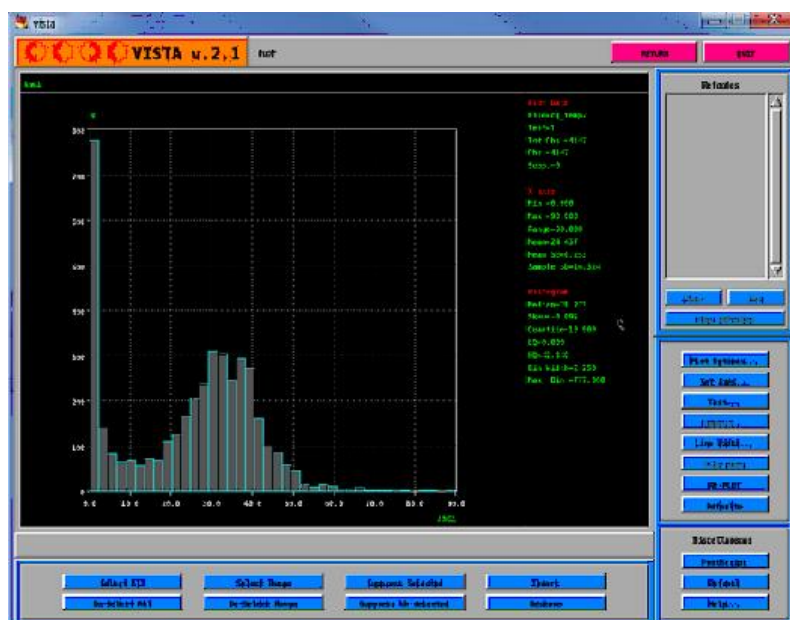
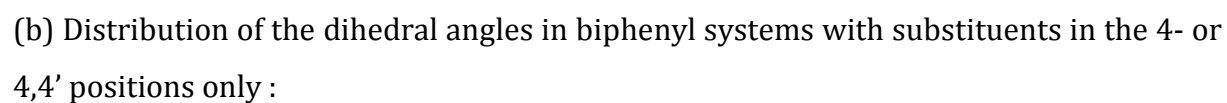
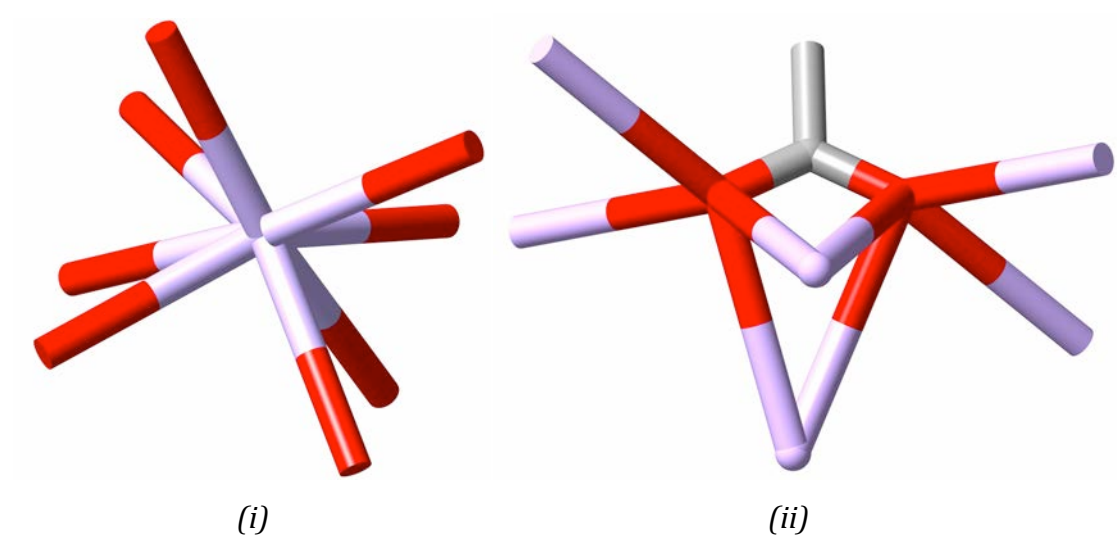


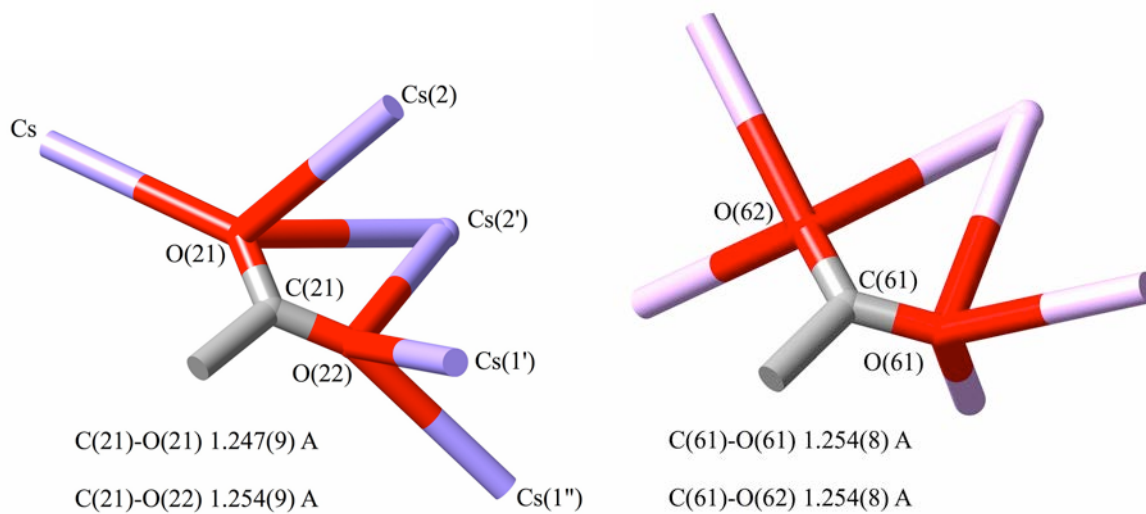
Figure S2 (i) Eight-coordinate Cs(I) and (ii) five-coordinate O in anhydrous CsO_2CCH_3 .²⁵



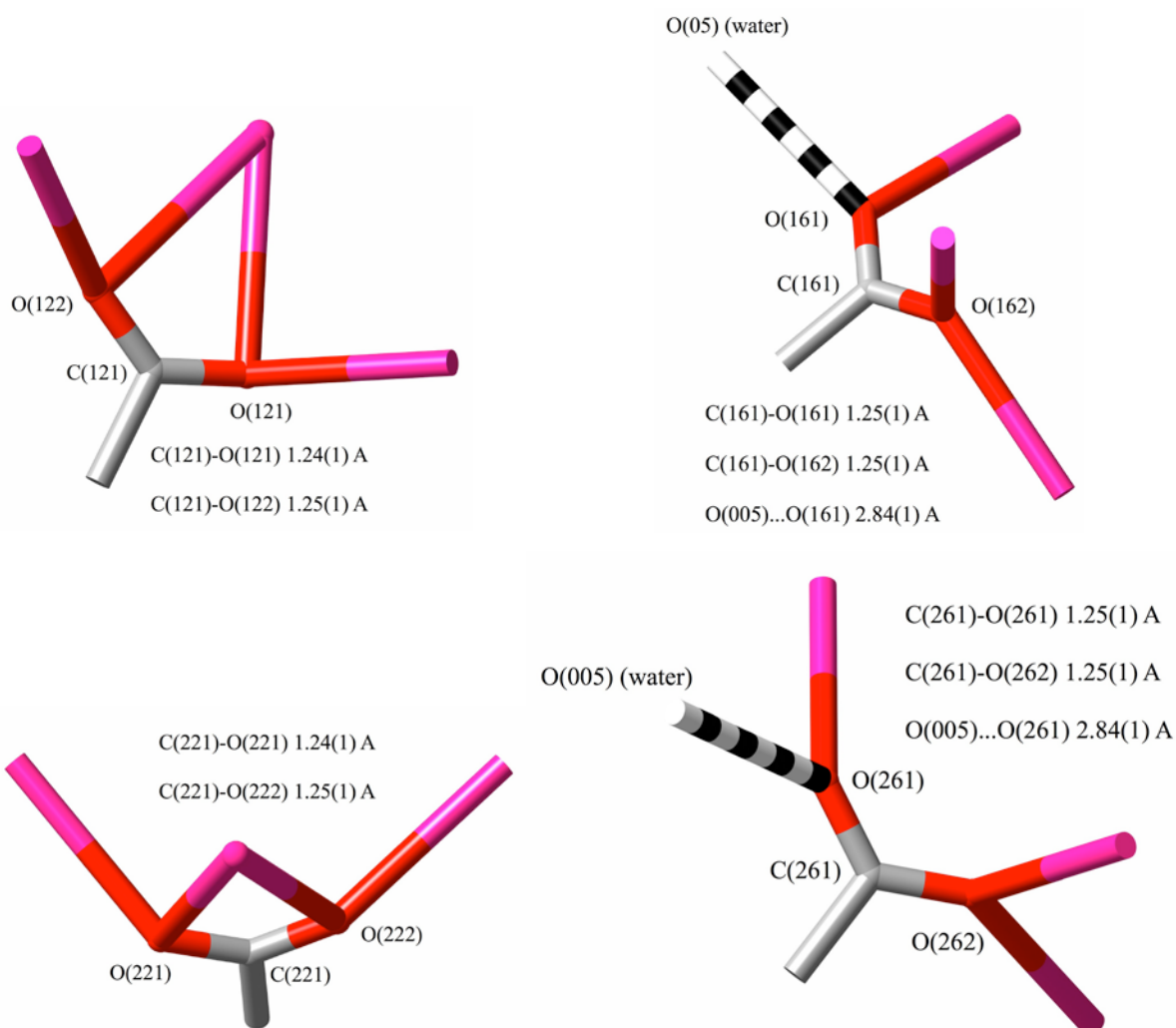
Carboxylate C-O 1.240(10), 1.270(6) Å.

Figure S3 Carboxylate coordination arrays in :

(a) Caesium chelidamate, $\text{Cs}_2\text{C}_7\text{H}_3\text{NO}_5$



(b) Rubidium chelidamate, $\text{Rb}_3(\text{C}_7\text{H}_3\text{NO}_5)(\text{C}_7\text{H}_4\text{NO}_5) \cdot 6\text{H}_2\text{O}$



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

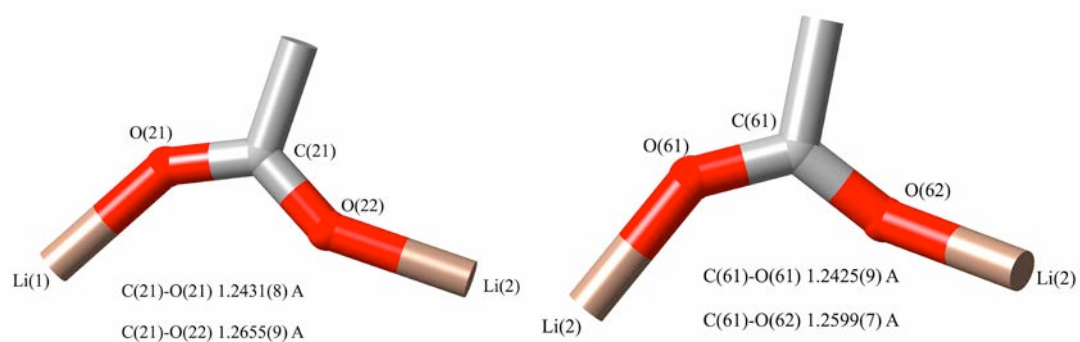
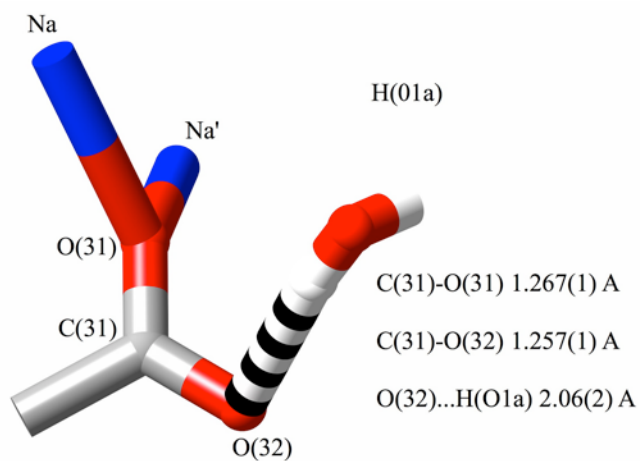


Figure S4 Carboxylate coordination arrays in :

(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)

