

# Surprising robustness of a unit cell: Isomorphism in caesium 18-crown[6] complexes with aromatic polycarboxylate anions of varying shape and size

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## ELECTRONIC SUPPORTING INFORMATION (5 pages)

Comparison between experimental diffraction patterns recorded on products obtained by grinding (blue lines) and from crystallization (red lines) and diffraction patterns computed on the basis of the single crystal structures for complexes **2**, **3**, **4**, **5**, **6** and **8**.

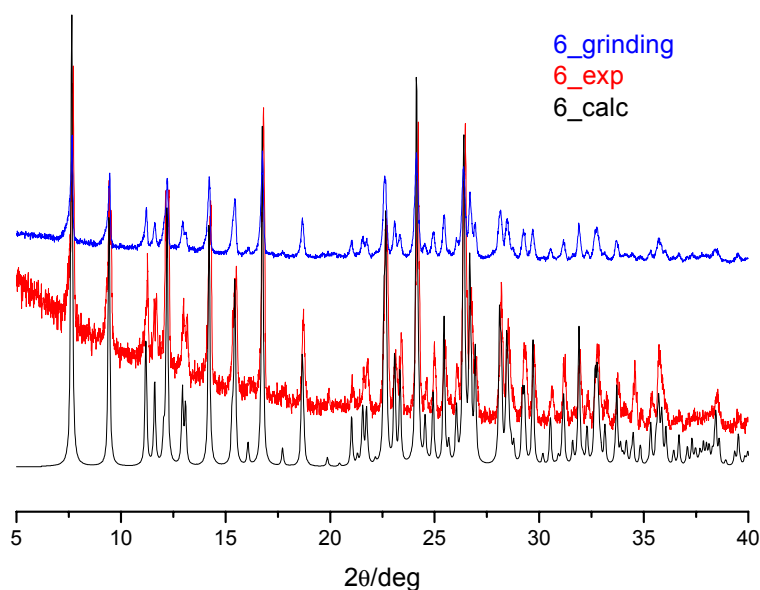


Figure ESI-1. 18-crown[6] · Cs[OH-isoH] (**2**).

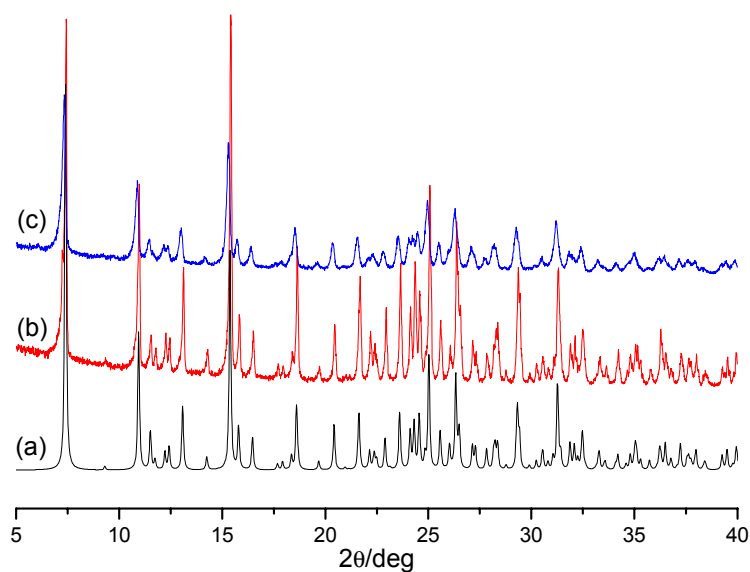


Figure ESI-2. 18-crown[6] · Cs[CH<sub>3</sub>-isoH] (**3**).

(a) Calculated, (b) exp. from solution, (c) exp. from grinding.

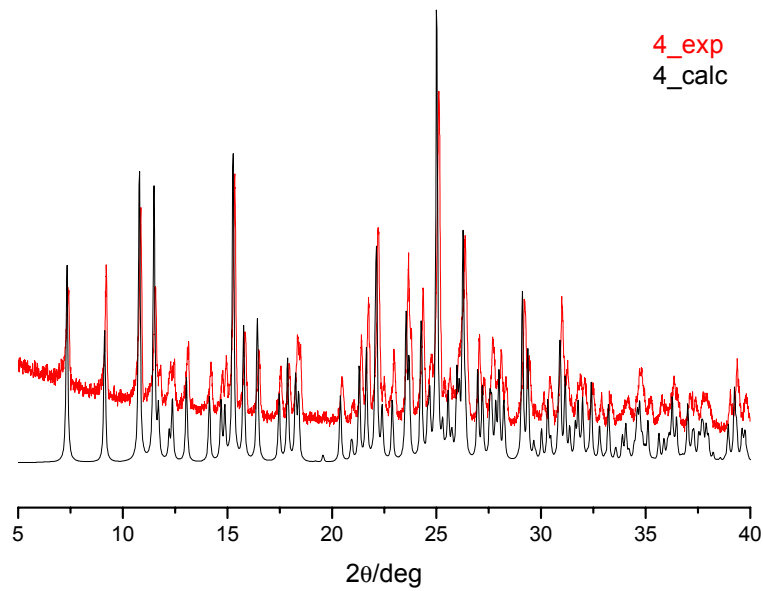


Figure ESI-3. 18-crown[6]·Cs[Br-isoH] (4).

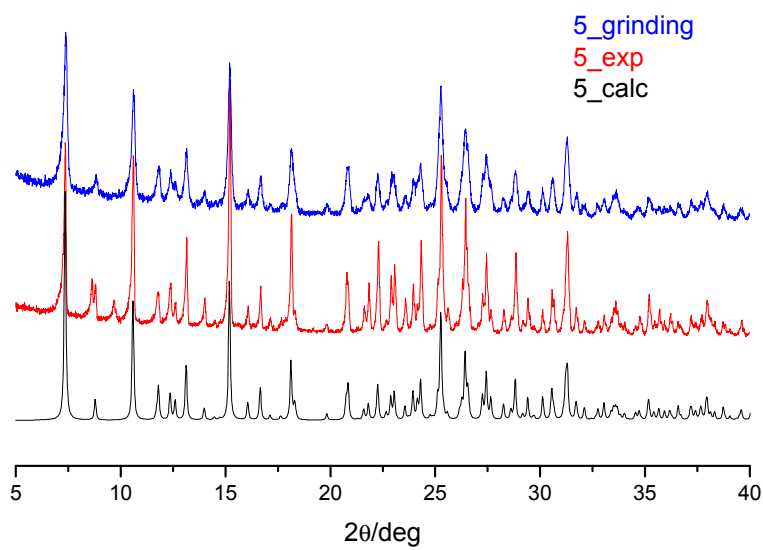


Figure ESI-4. 18-crown[6]·Cs[OCH<sub>3</sub>-isoH] (5).

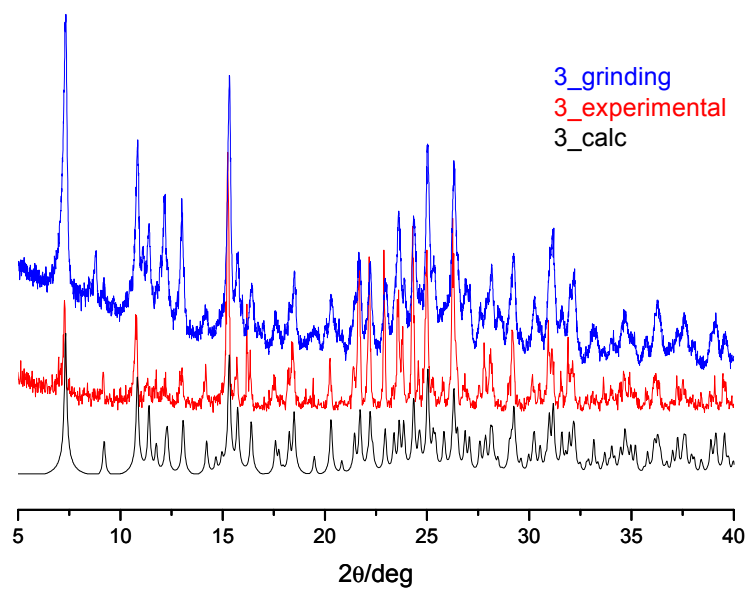
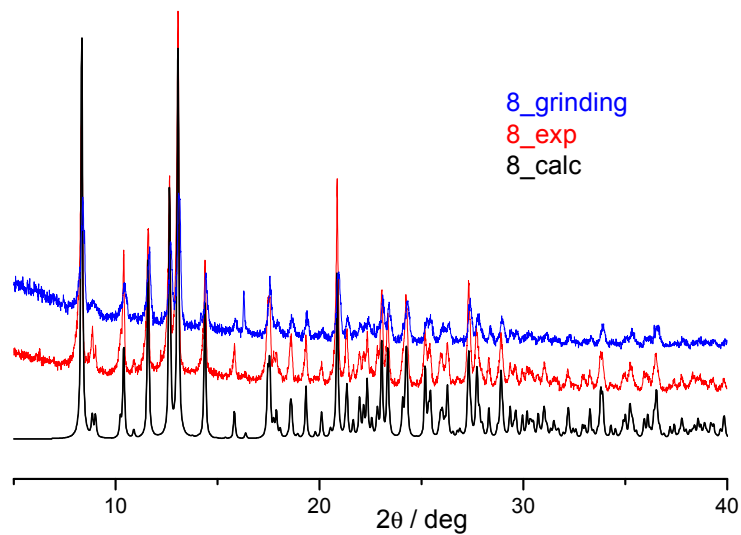
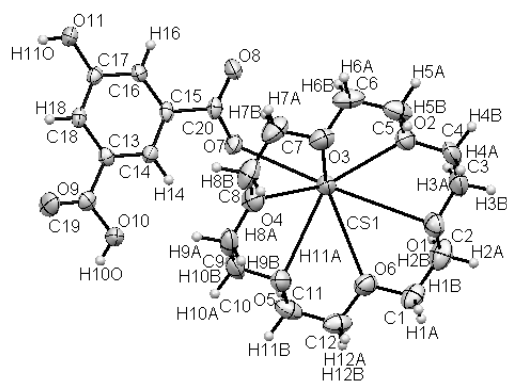


Figure ESI-5. 18-crown[6]·Cs[NO<sub>2</sub>-isoH] (6).

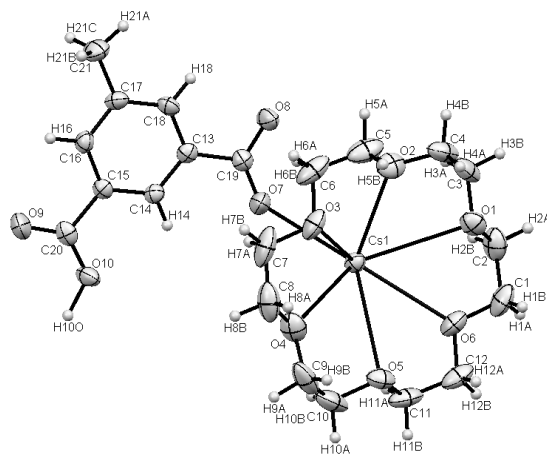


**Figure ESI-6.** 18-crown[6]·Cs[t-Butyl-isoH] (**8**).

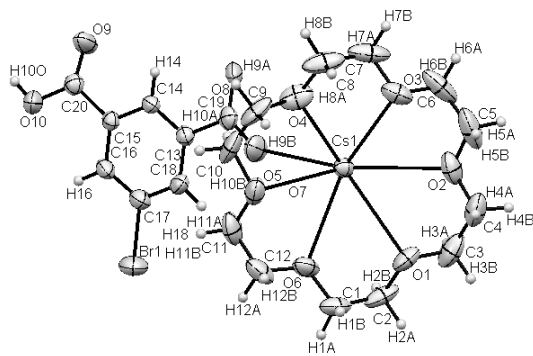
### ORTEP drawings



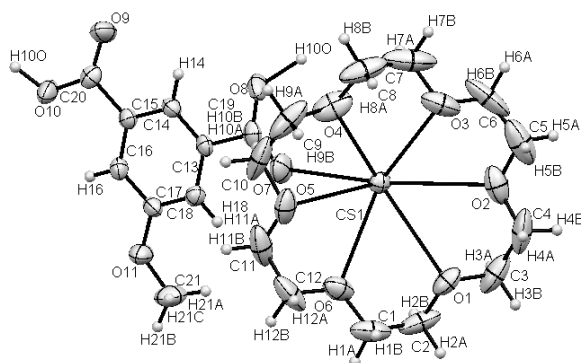
ORTEP representation of complex **2**



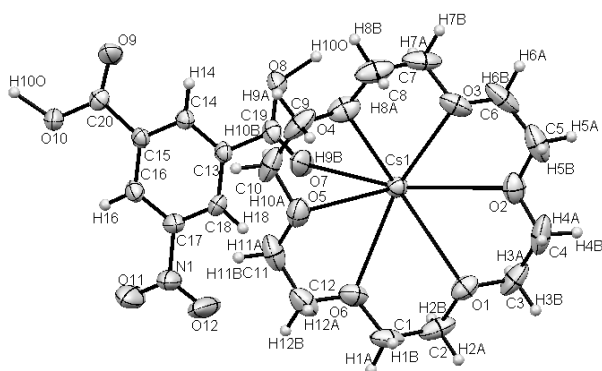
ORTEP representation of complex **3**



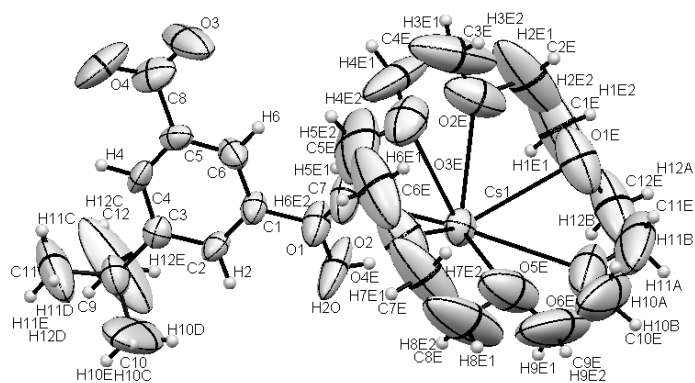
ORTEP representation of complex 4



ORTEP representation of complex 5



ORTEP representation of complex 6



ORTEP representation of complex 8