

Preferential positions of phosphate counter ions

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Abstract

A long time ago ('96 or so?), as a student with the no longer existing CAOS/CAMM (Google shows some traces, like this chapter describing the centre), I did a short internship with Hilbert Bruijn-Slot (I hope I remember his name correctly), where he has asked me to look at data in the CSD, and in particular the preferred position of phosphate counter ions.

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chem-bla-ics

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Today, [Neil asked me](#) to look at another Nature Chemistry paper (DOI:[10.1038/nchem.100](#)), and in particular [its Chemical Compounds table](#). I could not directly spot the thing not in the table I discussed, but did notice the phosphate salts in the table. Not uncommonly, the counter ions are not near the phosphate in this diagram and I wondered how they did this in 3D.

Well, bringing back good memories to that internship I mentioned, [the 3D model](#) shown by Jmol actually does show the salt, and with the two sodiums near the phosphate; even better, they sit at very recognisable positions :)

