chem-bla-ics

Preferential positions of phophate counter ions

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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 has asked me to look at data in the CSD, and in particular the prefered position of phosphate counter ions. It was a fun research, and almost made it into a paper, if we were not just beating by a few months by a group of Russians who just published the same.

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 :)