

Counterion Quandary

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Charge balance is essential in crystal structures. But what do you do when co-crystallized ions create a tangle of uncertain identity, unreasonable bond angles, and special position problems? For example, a recent structure contained four co-crystallized species. One is a seemingly neutral Cu complex, one is clearly a chloride ion and requires a counter ion, but the identity of the other two species is not as obvious, and the most chemically reasonable model tends to produce abnormal bond lengths and angles. Could this be a case for SQUEEZE, or is it necessary to grapple with the counterion quandary?