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Charge density as a powerful tool to predict reactivity

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The structure of a compound, composed from the various atom types and the divers bonding, determines its reactivity and properties. This renders the electron density one of the most informative observables of natural sciences. Since X-rays are mainly scattered by electrons X-ray diffraction techniques provide one of the most powerful tools to investigate and understand the relation between structure and chemical behaviour. However, despite all developments and improvements the phase problem is still operational and a model is still required to refine the electron density distribution (EDD) against measured data. In most cases the independent atom model (IAM) is used to describe the EDD. The more detailed multipole model describes the aspherical valence density by spherical harmonics. Of course such a model holds special requirements for the data quality and experimental errors needs to be minimized (Krause et al., 2015). Once this can be granted the model can be analysed beyond bond lengths and angles considerations. Especially the non-bonding regions and the localisation of lone-pairs are rewarding to predict reactivity. Some low-valent examples like the silylones Si(cAAC)2 (cAAC=cyclic amino alkyl carbene), containing a central silicon atom in oxidation state zero with two lone pairs (Niepötter et al., 2014) and the sec. phosphane P(bth)(Hbth) (bth=benzothiazol-2-yl), containing a central divalent phosphorus atom with two lone pairs (Hey et al., 2013), will be discussed.

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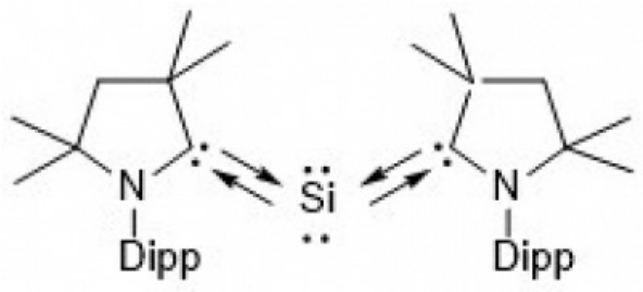

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