

Poster Presentation

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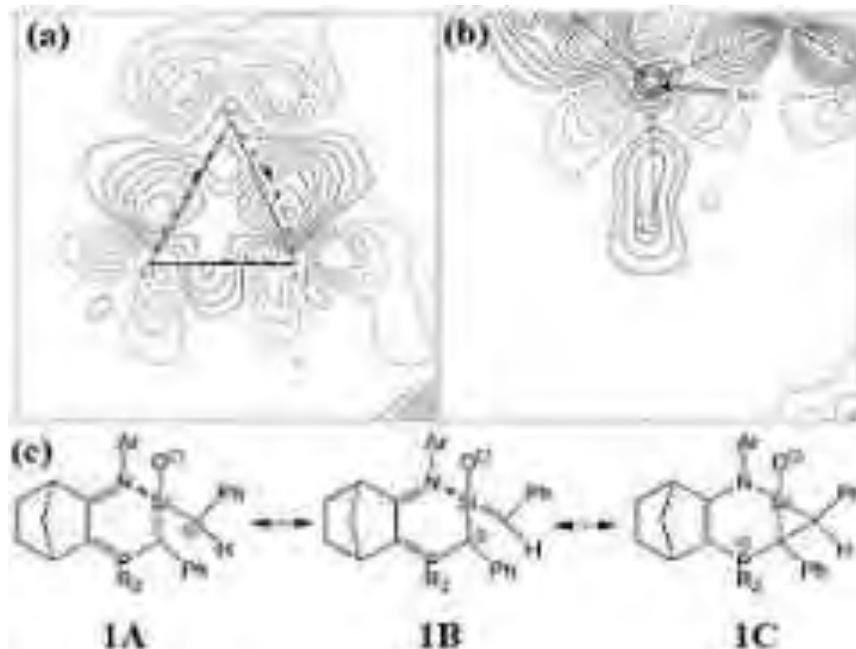
Bonding modes of some labile Si compounds studied by charge density analysis

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Some organic molecules containing Si atom(s) are very labile, even if the corresponding carbon analogs are very stable. To gain information on bonding modes of such compounds, we analyzed valence density distribution, which play critical roles in chemistry of molecule, by applying multipole expansion method. Very recently, an imine coordinated silacyclopropan-1-one, **1**, has synthesized by Baceiredo, Kato and co-workers.[1] To clarify the bonding mode of **1**, the electron density distributions of **1** and its precursor have analyzed by a multiple expansion method using single crystal X-ray diffraction data. As shown in static model density maps, bonding electrons of Si-C bonds distribute on the outside of the silacyclopropane ring (Si1-C1-C2 ring) (Fig. 1a) with largely extent, in compared with that of the precursor, indicating an in-plane pi-interaction on the Si1-C1 and Si1-C2 bonds. On the other hand, the C1-C2 bonding electrons distribute on the bond, and the bond critical point (BCP) is located on the inside of the three membered ring. In addition, the C1-C2 bonding electrons elongates inside the ring toward the Si1 atom, indicating electron donation from sigma(C1-C2)-bond to the Si1 (Fig. 1b). Consequently, these maps propose greater contribution of canonical structures in Fig. 1c.

[1] R. Rodriguez, T. Troadec, D. Gau, et al, *Angew. Chem. Int. Ed.*, 2013, 52, 4426-4430



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