

## MS23 Charge and spin density of materials at extreme conditions

Figure 1.

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### MS23-O1 Anagostic Interactions under Pressure: Attractive or Repulsive?

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The expression “anagostic interactions” was introduced to distinguish *sterically enforced*  $M\cdots H-C$  contacts ( $M = Pd, Pt$ ) in square-planar transition metal  $d^8$  complexes from *attractive*, agostic interactions. This classification raised the fundamental question whether axial  $M\cdots H-C$  interaction in planar  $d^8-ML_4$  complexes represent (i) repulsive anagostic  $3c-4e$   $M\cdots H-C$  interactions or (ii) attractive  $3c-4e$   $M\cdots H-C$  hydrogen bonds.

We reveal, however, that square-planar  $d^8-ML_4$  complexes might display subtle but noticeable *local* Lewis acidic sites in axial direction in the valence shell of the metal atom. These sites of local charge depletion provide the electronic prerequisites to establish **weakly attractive**  $3c-2e$   $M\cdots H-C$  agostic interactions in contrast to earlier assumptions in the literature (see above). We therefore suggest as a new characterization method to probe the response of these  $M\cdots H-C$  interactions under pressure via combined high pressure IR and diffraction studies [1].

[1] W. Scherer, A. C. Dunbar, J. E. Barquera-Lozada, D. Schmitz, G. Eickerling, D. Kratzert, D. Stalke, A. Lanza, P. Macchi, N. P. M. Casati, J. Ebad-Allah, Ch. Kuntscher, *Angew. Chem. Int. Ed.* **2015**, *54*, 2505-2509.

