

Carbonyl-Carbonyl Interactions in First-row Transition Metal Complexes

Hazel A. Sparkes^a, Mary F. Mahon^a, Paul R. Raithby^a, Frank H. Allen^b, Gregory P. Shields^b, ^a*University of Bath, Department of Chemistry, Claverton Down, Bath, BA2 7AY UK.* ^b*Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK.* E-mail: chphas@bath.ac.uk

Carbonyl-carbonyl interactions in organic species have been previously documented [1]. In theory, the strength of carbonyl-carbonyl interactions should be greater when the carbonyls are directly attached to a transition metal since the magnitude of the carbonyl dipole is greater than in purely organic compounds. The Cambridge Structural Database [2] was used to identify first row transition metal carbonyl species in which two carbonyl groups were separated by less than 3.6 Å and could potentially interact. Only two of the three main carbonyl-carbonyl interaction motifs previously identified for organic carbonyl species are possible in transition metal carbonyl compounds; these are illustrated Figure 1.

Data analysis suggests that transition metal carbonyl-carbonyl interactions in motifs A and B are more prevalent than organic carbonyl-carbonyl interactions, with around 33% of transition metal carbonyls suitably orientated to interact while only 8% of organic carbonyls can potentially interact. A comparison of the geometries of the interaction motifs is provided along with an analysis of accompanying theoretical calculations.

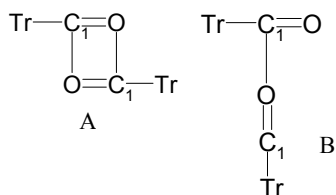


Figure 1 – interaction motifs in transition metal carbonyl species.

[1] Allen F.H., Baalham C.A., Lommerse J.P.M., Raithby P.R., *Acta Cryst.*, 1998, **B54**, 320. [2] Allen F.H., *Acta Crystallogr.*, 2002, **B58**, 380.

Keywords: database manipulation, transition metal complexes, interatomic interactions