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Assessment of the O-O bond in terminal dioxygen first row transition metal complexes: A CSD/DFT study

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Dioxygen, a readily available raw material for most oxidation processes, has been the focus of research in inorganic chemistry, material science and catalysis in recent times. The molecule undergoes multielectron reduction reactions and is used in proton exchange membrane (PEM) fuel cell to generate electrical energy. Triplet oxygen is also used in combination with photosensitizers and visible light to generate singlet oxygen which is employed in photodynamic therapy (PDT). Other areas of research include the study of biochemical systems such as oxygen transport and electron transport using dioxygen complexes of transition metals such as iron and copper in combination with porphyrins. Recently, vanadium(IV)/(V)-dioxygen complexes are being explored as insulin mimetics to lower blood sugar levels. In most of thes studies, FTIR data on increased bond lengths of the coordinated O 2 is largely explained by the donation of π-electrons from metal d-orbitals into empty π* ligand orbitals.
A search in the CSD version 5.39 (November) + 1 update using the ConQuest version 1.20 software revealed 250 first row tranistion metal complexes with terminal dioxygen ligands. These crystal structures were then analysed using mercury 3.10 software of the CCDC. Statistical analysis show strong correlation between O-O bond lengths and O-M-O bond angles. DFT analyses of a vanadium (V)-dioxygen complex (refcode: VEMRUA) and its optimised analogues reveal possible σ-donor, π-donor weakening of the O-O bond and not the usual σ-donor, π-acceptor model used in explaining this phenomenon.

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