Infrared spectroscopic and theoretical studies of iridium oxyfluoride molecules

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Transition metal oxyfluorides are attracting considerable attention due to their applications in energy production and storage, microelectronics, and catalysis. While the extensive studies of their crystal structures of most transition metal oxyfluorides have provided insights into the relevant chemical and physical properties of solid state oxyfluorides, only limited information is available for these compounds at the molecular level.

The iridium oxyfluorides have not yet been confirmed experimentally not only in molecular level but also in the solid state, although some methods and approaches have been proposed over the years. Therefore, it is essential to develop facile procedures to produce iridium oxyfluorides.

Recent studies in our research group[1,2] revealed that the oxyfluorides of group 10 and group 11 metal atoms can be prepared by the reaction of metal atoms with gaseous OF_2 and isolated in solid noble-gas matrices. The successful preparation and identification of such compounds suggest the possibility of synthesizing iridium oxyfluorides in a similar fashion.

In this work,[3] we describe for the first time the synthesis of molecular iridium oxyfluorides by two methods: laser-ablated iridium atoms with OF_2 and iridium dioxide (IrO_2) with F_2 in excess neon and argon under cryogenic conditions. Furthermore, the newly formed compounds were identified spectroscopically using isotope labeling ($^{18}OF_2$) experiments and supported by high-level *ab initio* calculations.

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[2] Li, L.; Beckers, H.; Stüker, T.; Lindič, T.; Schlöder, T.; Andrae, D.; Riedel, S. Molecular oxofluorides OMFn of nickel, palladium and platinum: oxyl radicals with moderate ligand field inversion. *Inorg. Chem. Front*. **2021**, *8*, 1215.

[3] Lu, Y.; Tsegaw, Y. A.; Riedel, S. Unpublished work.