

## Infrared spectra of the diatomic Hg-O molecule in noble gas matrices

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Mercuric oxide forms stable solids, but the diatomic molecule Hg-O is not stable enough to survive detection in the gas phase. However, laser-ablation of Hg atoms from a dental amalgam target<sup>1</sup> into argon or neon containing about 0.3 % of <sup>16</sup>O<sub>2</sub> or of <sup>18</sup>O<sub>2</sub> during their condensation into a matrix at 4 K allows the formation of O atoms which react on annealing to make ozone and new IR absorptions in solid argon at 521.2 cm<sup>-1</sup> for Hg-<sup>16</sup>O or at 496.4 cm<sup>-1</sup> for Hg-<sup>18</sup>O with the oxygen isotopic frequency ratio 521.2/496.4 = 1.0500. Solid neon gives a 529.0 cm<sup>-1</sup> absorption with a small 7.8 blue shift. These observed frequencies have the isotopic shift predicted for Hg-O and are within the range of recent high-level frequency calculations for the Hg-O molecule.<sup>2</sup> Infrared spectra will also be presented here for the related molecular mercury superoxide and ozonide species.

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<sup>1</sup> Andrews L.; Wang X.; Gong Y; Schlöder T.; Riedel S.; Franger M. J. Spectroscopic observation of a group 12 oxyfluoride: a matrix-isolation and quantum-chemical investigation of mercury oxyfluorides. *Angew. Chem. Int. Ed.* **2012**, *51*, 8235.

<sup>2</sup> Peterson K. A.; Shepler B. C.; Singleton J. M. The group 12 metal chalcogenides: an accurate multireference configuration interaction and coupled cluster study. *Mol. Phys.* **2007**, *105*, 1139.