

Supplemental Information for:

Spectroscopy of YO from first principles

**Alexander N. Smirnov^{a)}, Victor G. Solomonik,^{a)} Sergei N. Yurchenko,^{b)} and
Jonathan Tennyson^{b)}**

*^a Department of Physics, Ivanovo State University of Chemistry and Technology, Ivanovo
153000, Russia*

*^b Department of Physics & Astronomy, University College London, London WC1E 6BT, United
Kingdom*

This file includes 2 figures that show the CCSD/awCV5Z D_1 diagnostics of YO and the MRCI/aVTZ electronic angular momentum curves of YO.

Excel files containing CCSD(T)/CBS excitation energies (CC_en.xls), MRCI/aVTZ total energies (CI_en.xls), electric dipole moment (dm.xls), transition dipole moment (dmx.xls and dmz.xls), electronic angular momentum (lx.xls), and spin-orbit coupling (SOC.xlsx) matrix elements, are supplied separately.

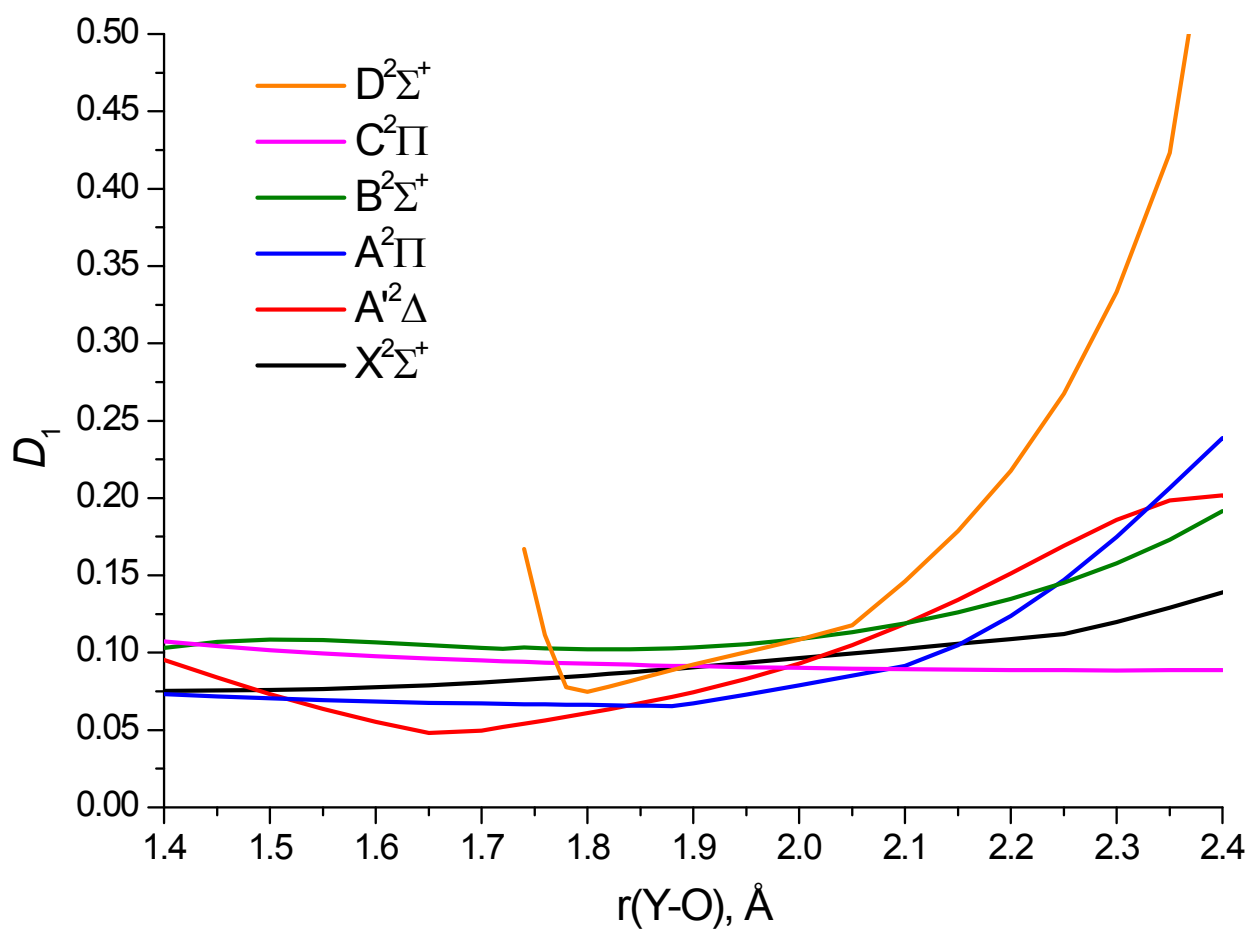


Figure S1. The CCSD/awCV5Z D_1 diagnostics of YO.

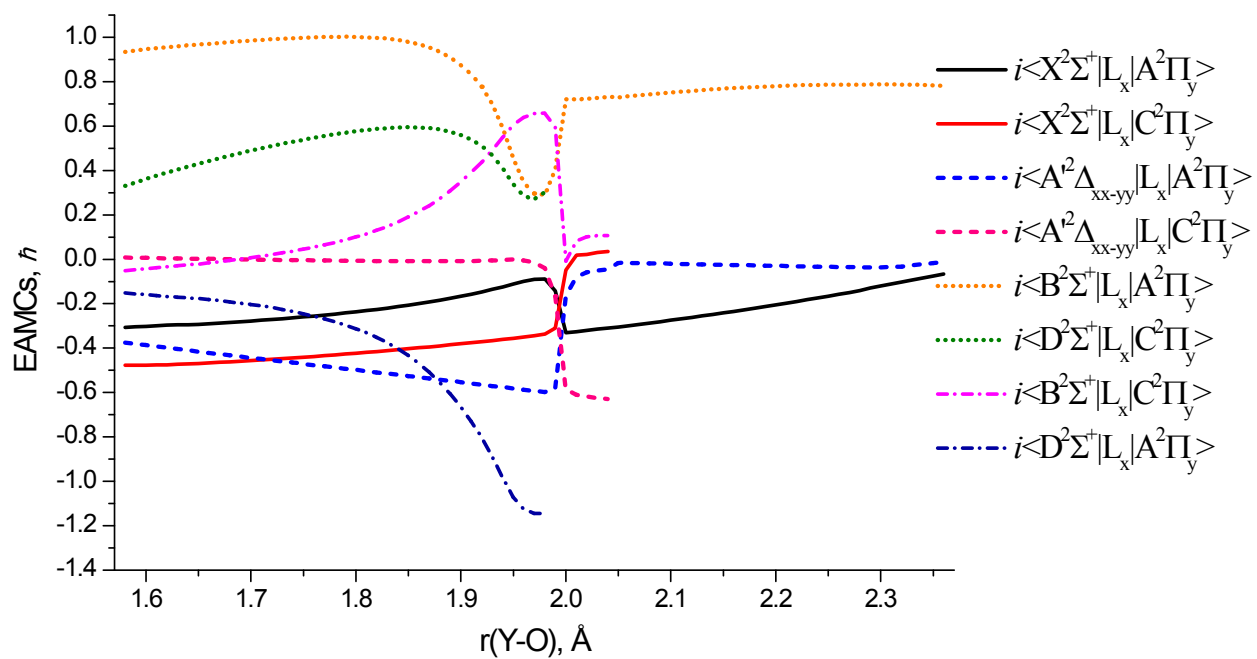


Figure S2. MRCI/aVTZ electronic angular momentum curves of YO.