

MRCI Characterization of the Low Lying Quintet States of MoO Radical

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INTRODUCTION

In recent years several studies have been published on the properties of MoO. Early MCPF calculations by Langhoff and Bauschlicher¹ on the electronic structure of MoO examined a small set of states and characterized the ground state as $^5\Pi$ with configuration $(2\delta)^2(12\sigma)^1(6\pi)^1(13\sigma)^0$. Later, Hamrick and Morse² obtained a high resolution optical spectrum of jet-cooled MoO, and obtained several spectroscopic constants for several quintet states. Given the interest in these systems, we have studied them using multireference methods.

METHODS

The chosen basis was the aug-cc-pV5Z set for both atoms, with inclusion of ECP for Mo. The zeroth order wavefunction was obtained at the CASSCF level, and the resulting optimized MOs were used in MRCI calculations. The calculations were carried out using the MOLPRO program and the molecular constants have been calculated by solving the radial equation using the INTENSITY code.

RESULTS AND DISCUSSION

Table 1 shows our calculated spectroscopic constants, and Figure 1 shows our calculated potential curves for the quintet low lying states of MoO radical.

Table 1. Quintet electronic states of MoO.

state	$r_e(\text{Å})$	$T_e(\text{cm}^{-1})$	$\omega_e(\text{cm}^{-1})$	$\omega_e x_e(\text{cm}^{-1})$
$X^5\Pi$	1.713	0	924.0	2.90
$(1)^5\Sigma^-$	1.742	10877	862.1	4.26
$(1)^5\Sigma^+$	1.757	11896	859.6	0.51
$A^5\Delta$	1.752	16214	886.7	2.51
$B^5\Pi$	1.795	21747	788.0	9.30

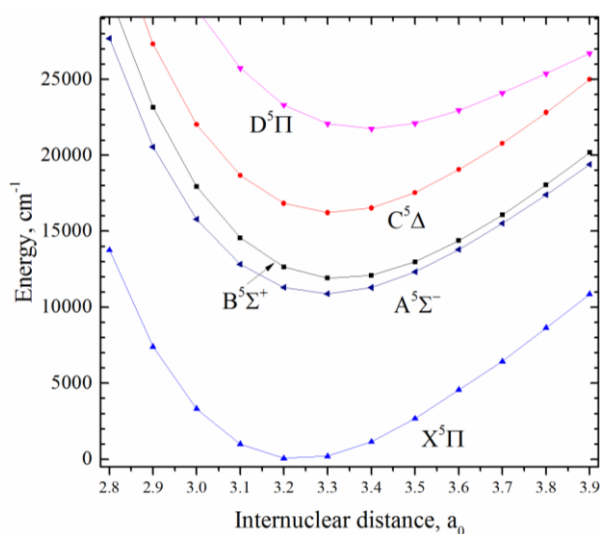


Figure 1. Calculated potential curves for MoO.

Our calculated harmonic frequency of 924 cm^{-1} matches the MCPF value of 850 cm^{-1} by Bauschlicher. We discuss the fact that this transition is apparently absent in the infrared spectrum obtained by Andrews and coworkers³.

CONCLUSIONS

We have studied MoO using multireference methods. We present a list of spectroscopic constants for this little known system.

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² Y.M. Hamrick, S. Taylor and M.D. Morse, J. Mol. Spectrosc. 146, 274 (1991).

³ W.D. Bare, P.F. Souter and L. Andrews, J. Phys. Chem. A 102, 8279-8286 (1998).