OCSO 在固態 Ar 間質中的紅外吸收光譜

羅文瑞

慈濟技術學院通識教育中心

摘要

用輸出波長 308 奈米 (308 nm) 的氯化氙(XeCl)準分子雷射照射含有臭氧(O3) 和羰基硫(OCS) 的固態氬(Ar)間質後，位於 2058.1, and 1032.9 cm-1 處產生新的紅外吸收譜線。根據同位素 13C- and 18O-的實驗與理論計算結果，這些譜線被指派為 OCSO 的 C=O 伸縮振動(C=O stretching)及 S-O 伸縮振動(S-O stretching) 模式。以密度泛函理論[density functional theory (B3LYP/6-311+G(3df))]預測 OCSO 兩種最穩定的同分異構物(isomer)：O(OCS)與 OCSO。根據理論計算的結果，OCSO 是最穩定的同分異構物。OSCO 為具有鍵長 1.15 Å (C-O)、1.67 Å (C-S)、1.50Å (S-O) 與鍵角 ÐCSO @ 110.40˚的平面結構。OSCO 比 O(OCS) 大約穩定 50.8 kJ mol-1。理論計算所得到的 OCSO 振動波數(vibrational wave numbers)、紅外吸收強度、13C- and 18O-同位素位移與實驗的結果也相當吻合。

關鍵字：羰基硫,密度泛函理論,OCS,OCSO

Isomer of OCSO: IR absorption spectra of OCSO in solid Ar

Wen-jui Lo

General Education Center Tzu Chi College of Technology

Abstract

Irradiation of an Ar matrix sample containing O3 and OCS with a XeCl excimer laser at 308 nm yielded new lines at 2058.1 and 1032.9 cm-1. These lines are assigned to C=O stretching and S-O stretching modes of OCSO, based on results of 13C- and 18O-isotopic experiments and quantum-chemical calculations. These calculations using density functional theory (B3LYP/6-311+G(3df)) predict two stable isomers of OCSO: According to calculations, OCSO is the most stable isomer. OSCO is planar, with bond lengths of 1.15 Å (C-O),1.67 Å (C-S), and 1.50Å (S-O) bond angle ÐCSO @ 110.40°; it is more stable than O(OCS) by ~50.8 kJ mol-1. Calculated vibrational wave numbers, IR intensities, 13C- and 18O-isotopic shifts for OCSO fit satisfactorily with experimental results.

Keywords：carbonyl sulfide, density functional theory, OCS, OCSO