

Supplementary Information

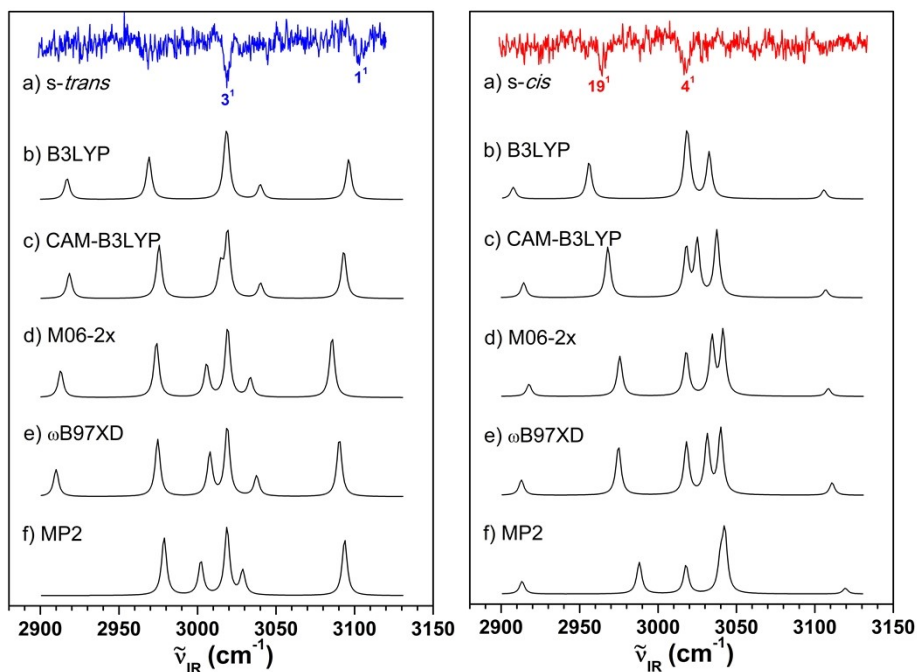
## **Identification of Individual Conformers in C<sub>4</sub>H<sub>6</sub>O Isomers Using Conformer-Specific Vibrational Spectroscopy**

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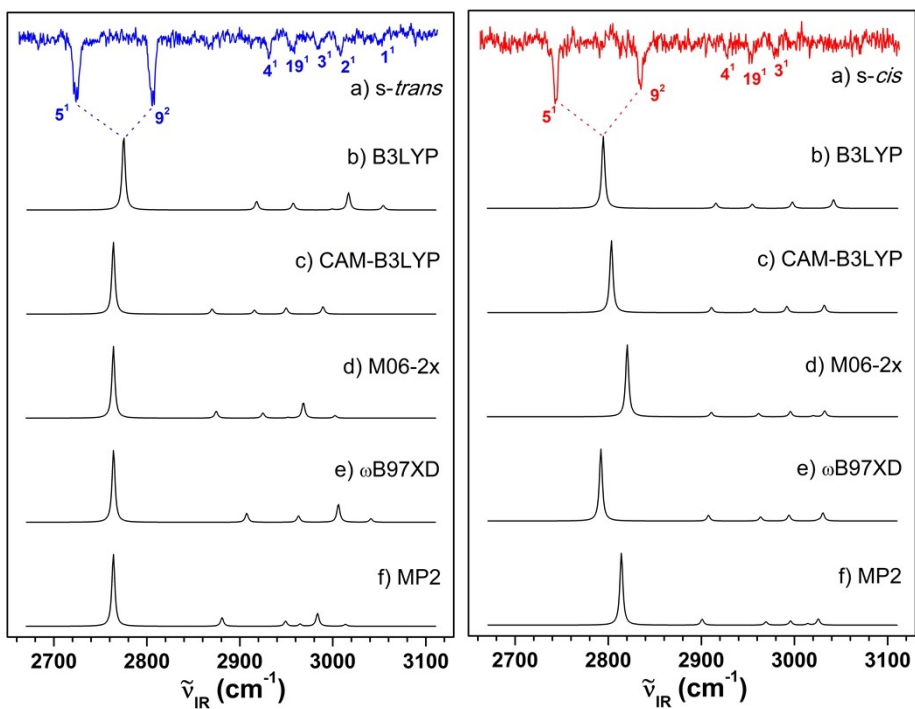
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**Figure S1.** IR dip VUV-MATI spectra measured by monitoring the origin bands ( $77,861$  and  $78,216\text{ cm}^{-1}$ ) of the *s-trans* (left) and the *s-cis* (right) conformers in MVK. IR spectra of the neutral *s-trans* (left) and neutral *s-cis* (right) conformers calculated at the (b) B3LYP, (c) CAM-B3LYP, (d) M06-2X, (e)  $\omega$ B97XD, and (f) MP2 levels using the aug-cc-pVTZ basis set with *s-trans* (*s-cis*) scaling factors of 0.9606 (0.9612), 0.9525 (0.9546), 0.9478 (0.9525), 0.9513 (0.9554), and 0.9430 (0.9495), respectively.



**Figure S2.** IR dip VUV-MATI spectra measured by monitoring the origin bands ( $78,638$  and  $78,734$   $\text{cm}^{-1}$ ) of the *s-trans* (left) and the *s-cis* (right) conformers in CA. IR spectra of the neutral *s-trans* (left) and neutral *s-cis* (right) conformers calculated at the (b) B3LYP, (c) CAM-B3LYP, (d) M06-2X, (e)  $\omega$ B97XD, and (f) MP2 levels using the aug-cc-pVTZ basis set, with *s-trans* (*s-cis*) scaling factors of 0.9667 (0.9667), 0.9421 (0.9555), 0.9395 (0.9519), 0.9544 (0.9549), and 0.9392 (0.9468), respectively.