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Non-Covalent Interactions in Carbon Dioxide Clusters: Comparison Between the Thiophenol-CO_2 and Benzylmercaptan-CO_2 Dimers Using Microwave Spectroscopy

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\title{Non−Covalent Interactions in Carbon Dioxide Clusters: Comparison Between the Thiophenol−CO_2 and Benzylmercaptan−CO_2 Dimers Using Microwave Spectroscopy}
Carbon dioxide (CO_2), as a greenhouse gas causing global warming, has received great attention concerning its pollution effects and reactivity.\footnote{S. C. Peter, {\it ACS Energy Lett.\/}, {\bf 3}, 1557−1561 (2018).\label{HQ}} Hence, various strategies have been implemented to reduce the atmospheric concentration of CO_2 for instance, separation, storage, and utilization.\footnote{Z. X. Sun, Y. H. Hu, {\it Acc. Mater. Res. \/}, {\bf 2}, 48−58 (2021).\label{HQ}} The investigation of the noncovalent interactions involving CO_2 could help understanding CO_2 aggregation and reactivity in the atmosphere. Presently, only a few clusters of CO_2 and sulfur molecules have been studied using rotational resolution.\footnote{ J. K. Rice, L. H. Coudert, K. Matsumura, et al. {\it J chem. Phys. \/}, {\bf 92}(11), 6408−6419 (1990).\label{HQ}}, \footnote{L. Sun, I. I. Ioannou, R. L. Kuczkowski, {\it Molec. Phys. \/}, {\bf 88}, 255 (1996).\label{HQ}} In this work, we have measured the microwave spectra of the clusters of thiophenol−CO_2 and benzylmercaptan−CO_2 using broadband chirped-pulsed microwave spectroscopy. Only one isomer was observed for both clusters, with dominant C···π and C···S non-bonding interactions. The experiments are supplemented density functional theory and Natural Bond Orbital (NBO) calculation. Details of the experimental and computational results on this problem will be offered during the conference.

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