Title:	From the propargyl alcohol–water complex to the propargyl alcohol dimer: where does the propargyl alcohol–methanol complex fit in?†
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Abstract:	This work describes the matrix isolation infrared and ab initio studies on the complexes of propargyl alcohol (PA) with methanol (MeOH). Our experiments revealed two isomeric 1 : 1 PA–MeOH complexes, which were evidenced by red shifts in the O–H stretch and blue shifts in the C–O stretch of the PA submolecule and red shifts in the C–O stretch of the MeOH submolecule, in the complexes. The experimentally observed shifts in the vibrational wavenumbers for both these complexes were in agreement with the computed shifts. Computations were performed using the M06-2X, ωB97X-D and MP2 methods employing the aug-cc-pVDZ basis set. Calculations showed that the two complexes observed in our experiments were nearly isoenergetic and most strongly bound. These complexes manifested dual contacts; one was an O–H···O interaction involving the O–H of PA interacting with the oxygen of MeOH, while the second was an O–H···π contact involving the O–H of MeOH and the acetylenic π cloud of PA, as confirmed by both AIM and NBO analysis. We also investigated the cooperativity effects between these dual interactions in PA–MeOH and compared them with our earlier studied PA–H2O system. At the MP2/aug-cc-pVDZ level, nine other local minima were also located for the PA–MeOH complexes, which showed the presence of O–H···O, C–H···O, [triple bond, length as m-dash]C–H···O, O–H···π and C–H···π contacts. As a result of this study, an interesting correlation was recognized between the structures of PA–H2O, PA–MeOH and PA dimer complexes; a correlation that could help in predicting the structures of larger systems in a systematic way.
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