Optimization at the UM06-2X/AUG-cc-pVTZ level yielded geometries for trans-diacetyl, cis-diacetyl, water, DTW, DBW, gem-diol I, gem-diol-II complexes. IR spectra obtained for the complexes showed a good indicator for the trans-diacetyl was a red-shift at the C—C and C—O stretches,

This study was meant to lay a foundation for further understanding of diacetyl water complexes and the breadth of its findings may be useful in future experimentation including matrix isolation IR in solid inert gases, isotopic substitution studies and the characterization of diacetyl hydrate reaction vibrations.