

Supporting Information

Microhydration of Neutral and Charged Acetic Acid

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India

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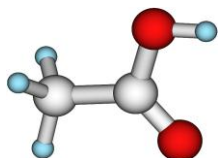
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Figure S1: Equilibrium structure and relative energy of conformers for different size of hydrated clusters of acetic acid **S2**

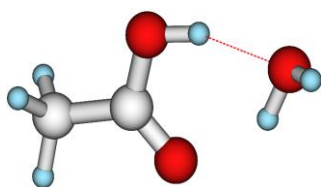
Figure S2: Simulated IR spectra of the most stable structure of acetic acid and its hydrated clusters calculated at ω B97X-D/aug-cc-pVDZ level of theory. **S14**

Figure S1. Equilibrium structure and relative energy (zero point energy corrected) of predicted minimum energy structures with respect to the most stable structure of acetic acid and its microhydrated clusters, $\text{CH}_3\text{COOH}\cdot n\text{H}_2\text{O}$ ($n=1-8$).

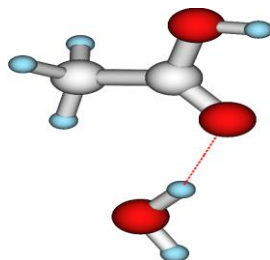
a) CH_3COOH



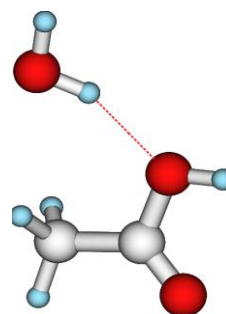
b) $\text{CH}_3\text{COOH}\cdot 1\text{H}_2\text{O}$



$\Delta E = 0$ kcal/mol

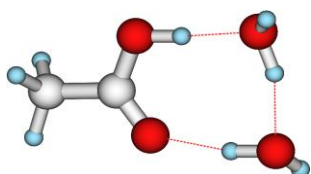


$\Delta E = +3.5$ kcal/mol

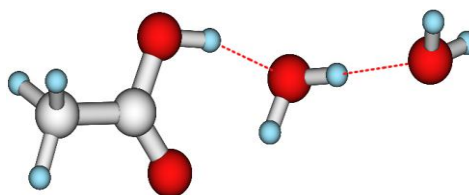


$\Delta E = +5.7$ kcal/mol

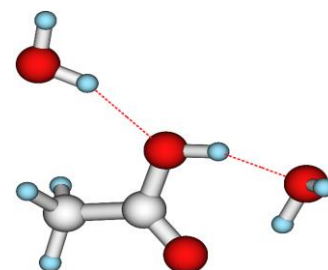
c) $\text{CH}_3\text{COOH}\cdot 2\text{H}_2\text{O}$



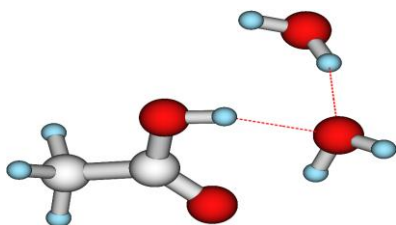
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$\Delta E = +5.2$ kcal/mol

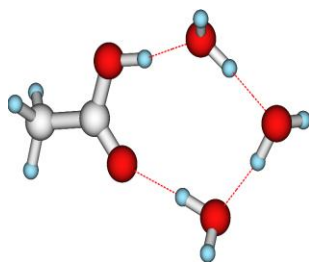


$\Delta E = +6.3$ kcal/mol

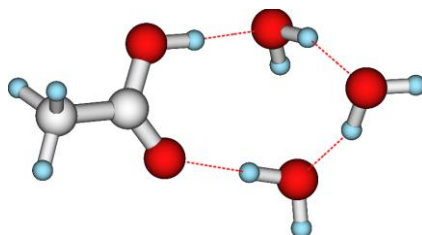


$\Delta E = +7.0$ kcal/mol

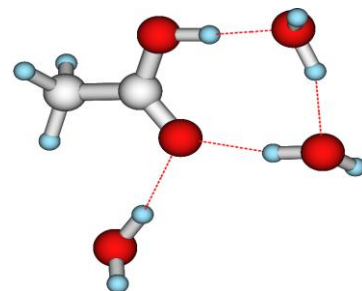
d) $\text{CH}_3\text{COOH} \cdot 3\text{H}_2\text{O}$



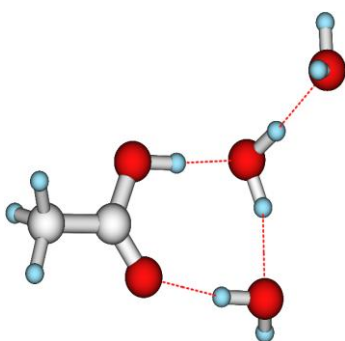
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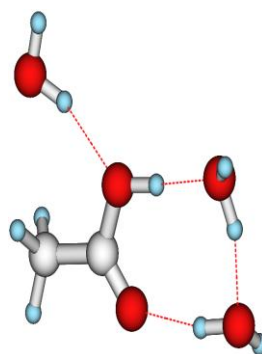
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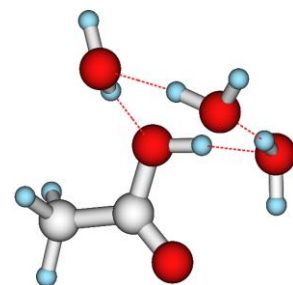
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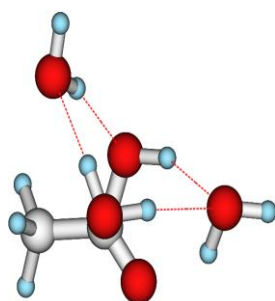
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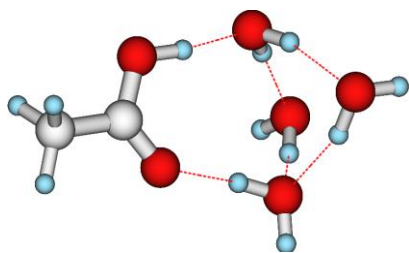


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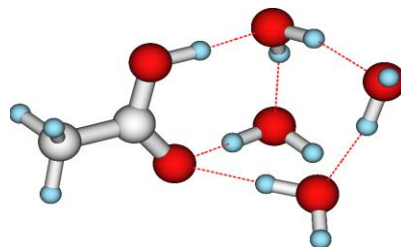


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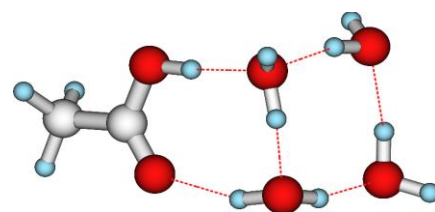
e) $\text{CH}_3\text{COOH} \cdot 4\text{H}_2\text{O}$



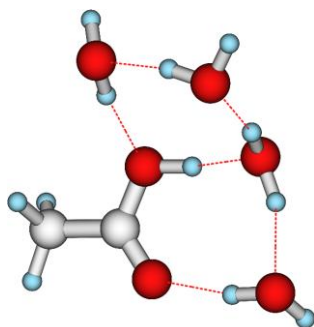
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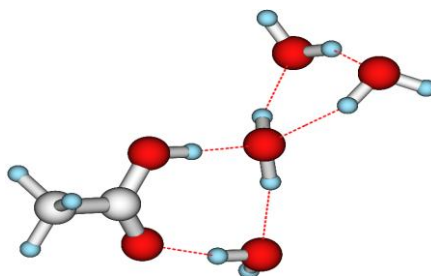
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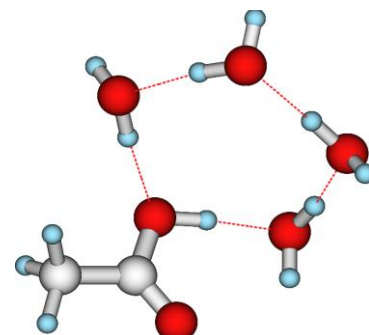
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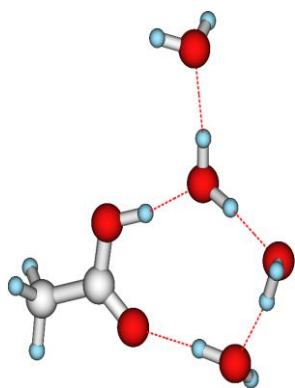
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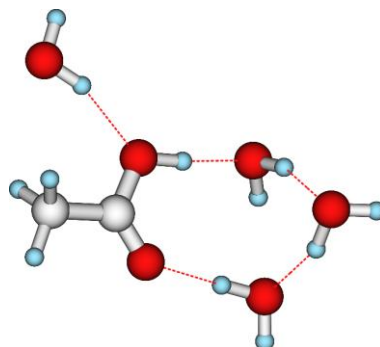
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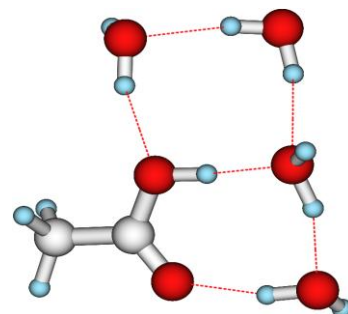
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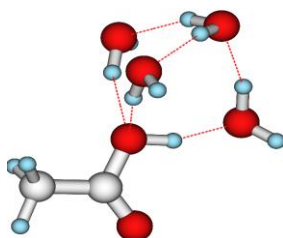
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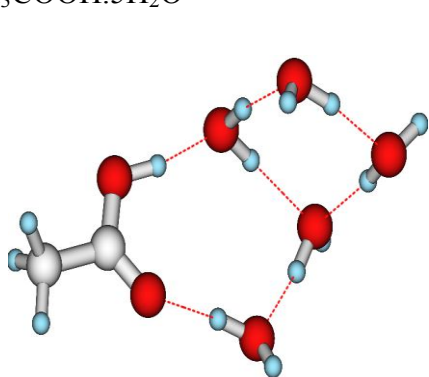


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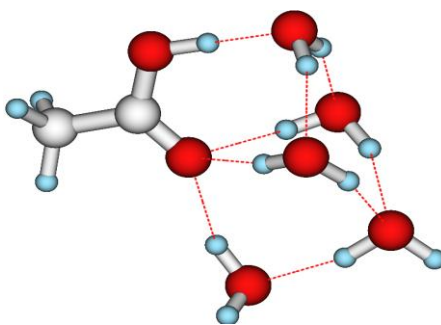


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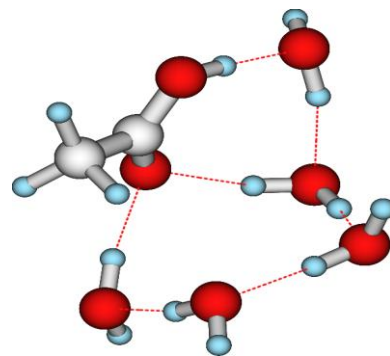
f) $\text{CH}_3\text{COOH} \cdot 5\text{H}_2\text{O}$



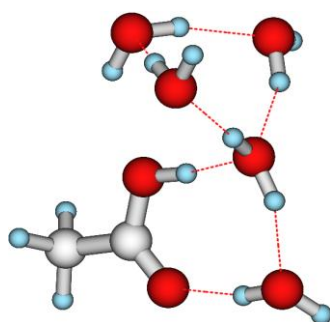
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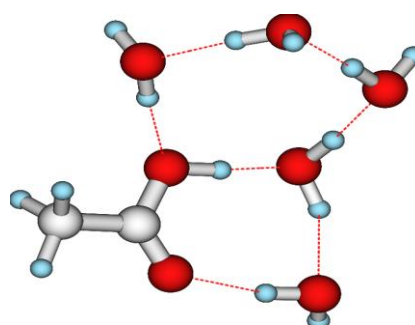
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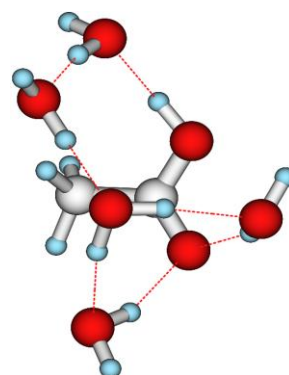
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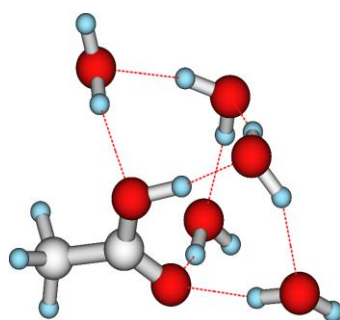
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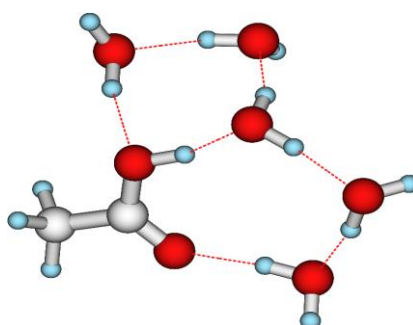
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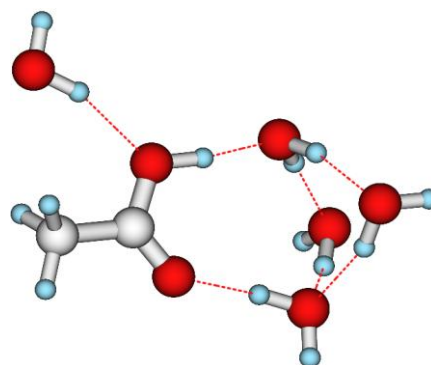
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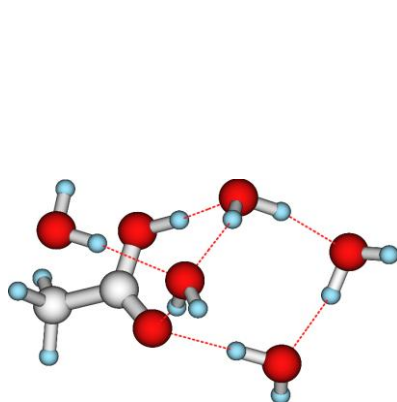
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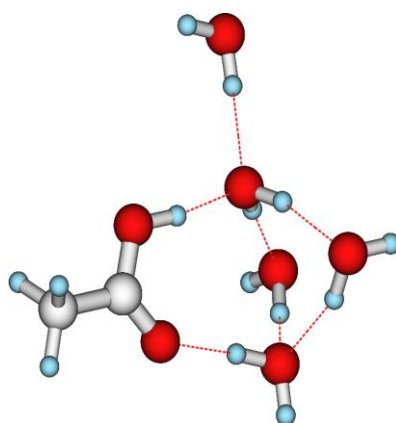
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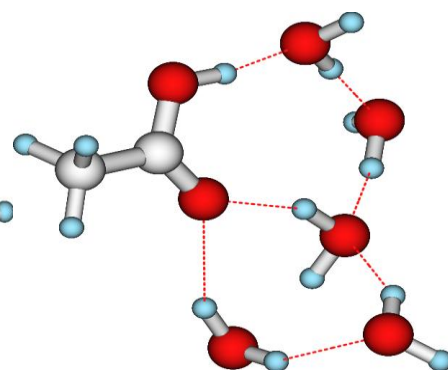
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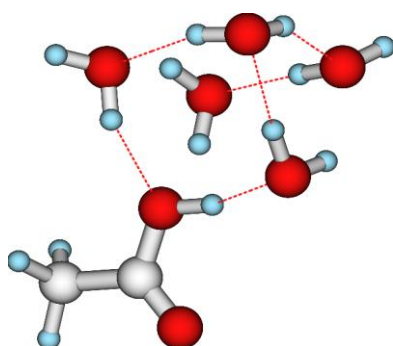
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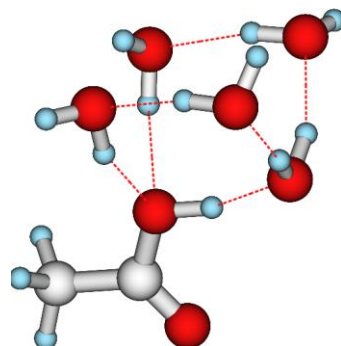
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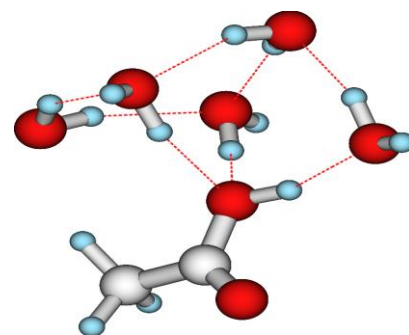
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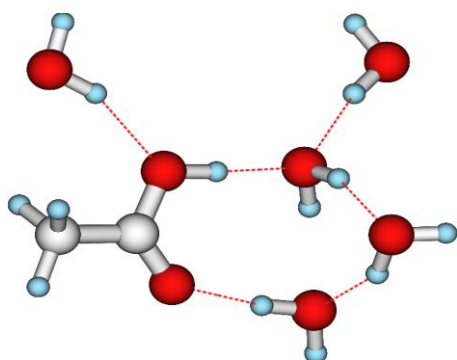
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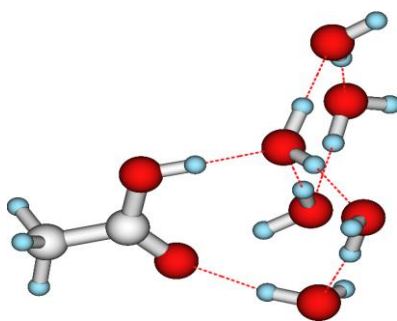


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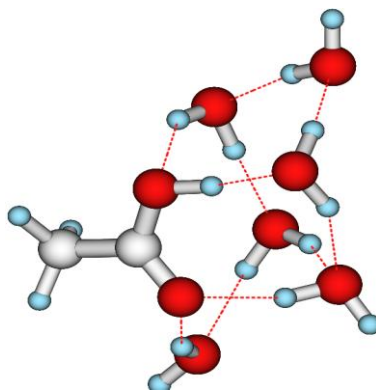


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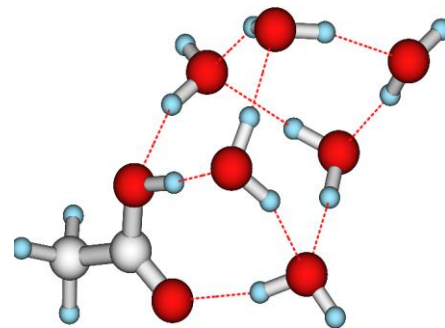
g) $\text{CH}_3\text{COOH} \cdot 6\text{H}_2\text{O}$



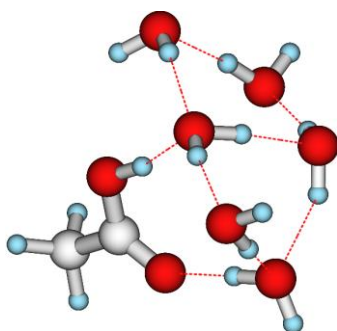
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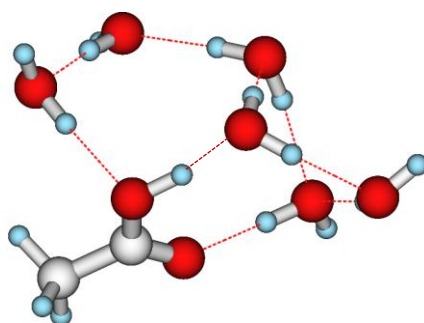
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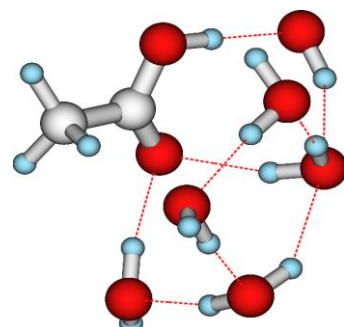
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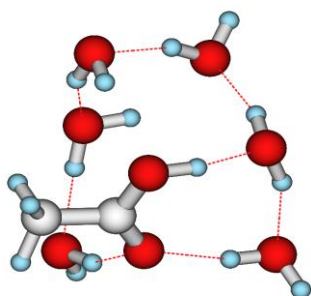
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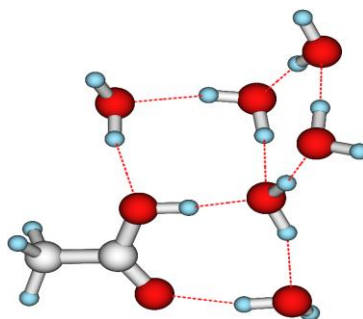
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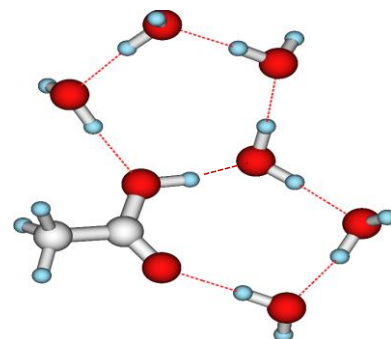
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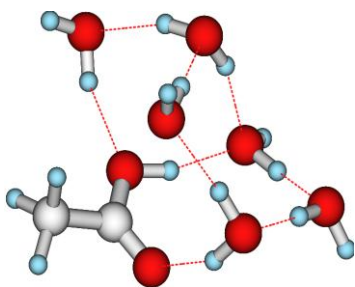
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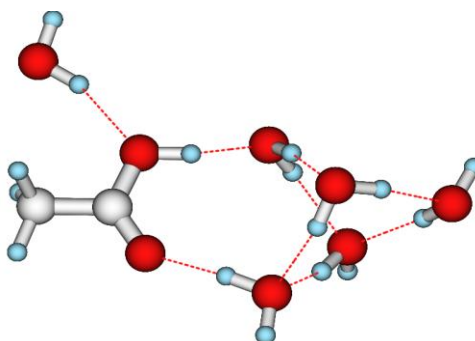
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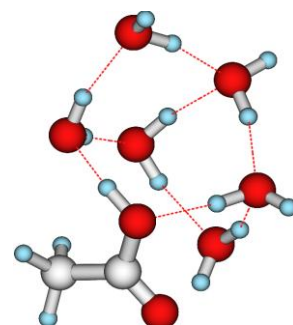
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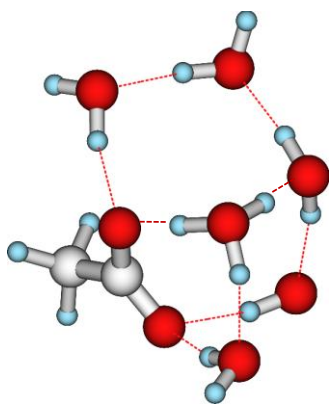
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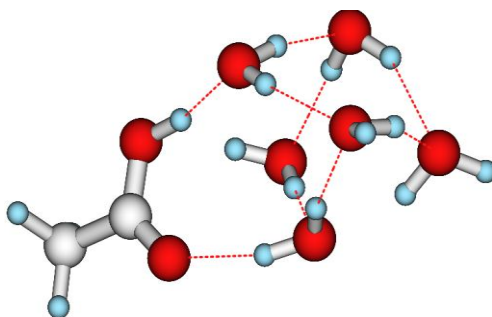
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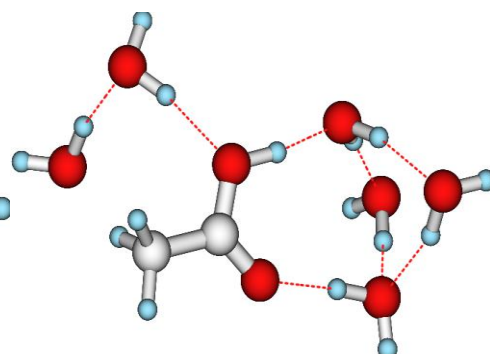
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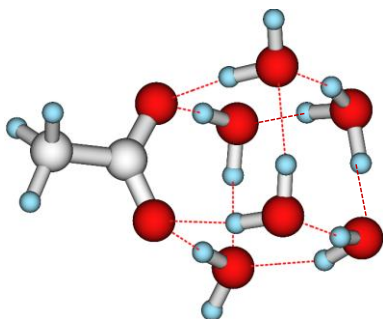
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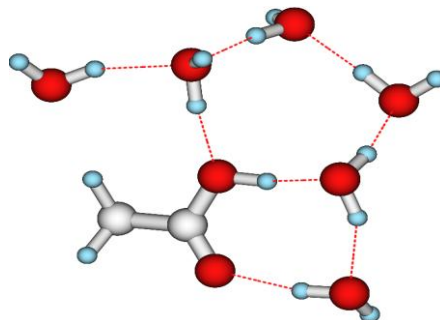
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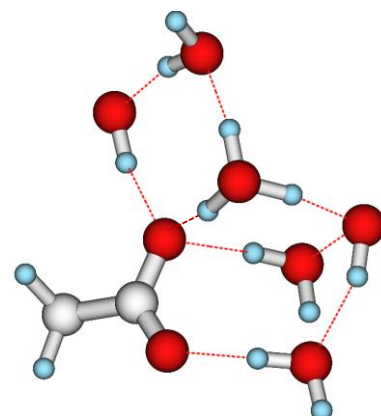
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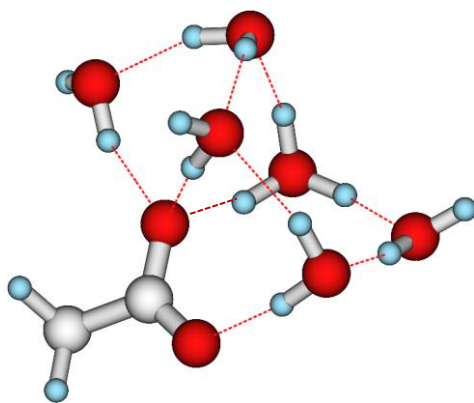
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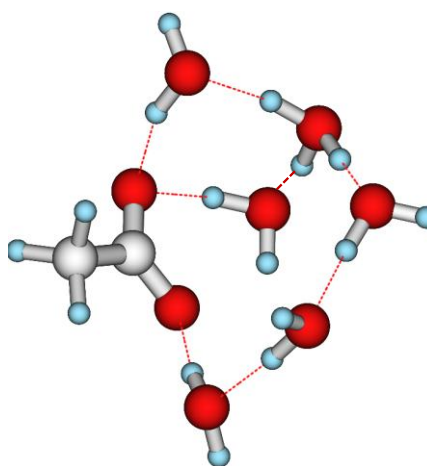
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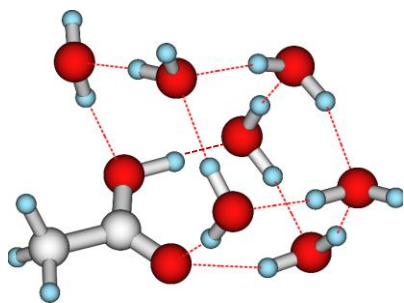


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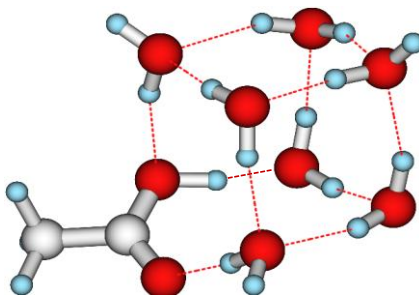


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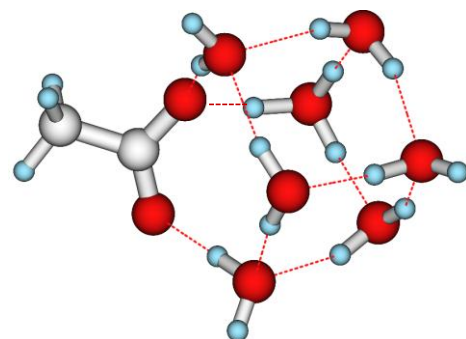
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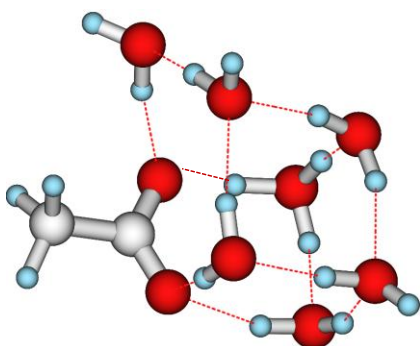
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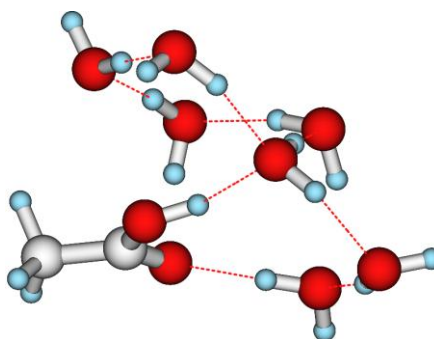
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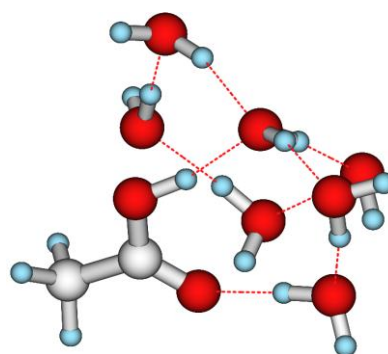
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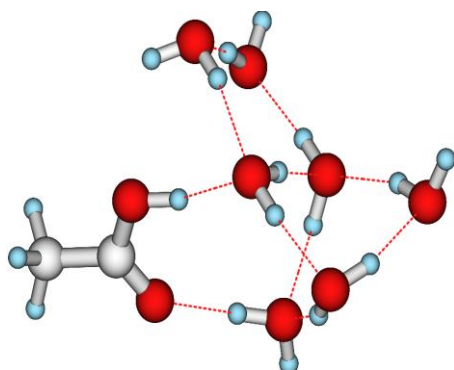
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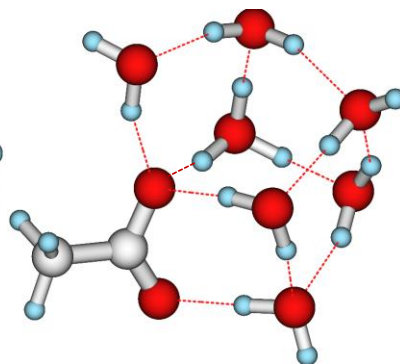
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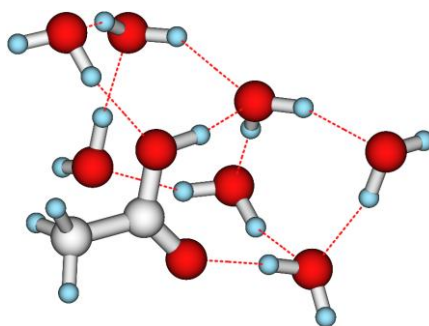
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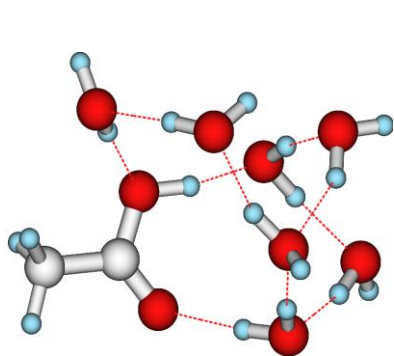
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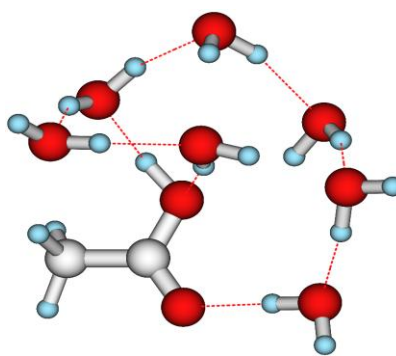
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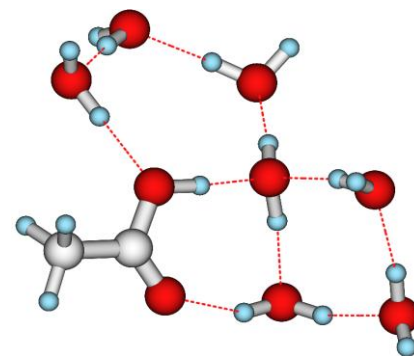
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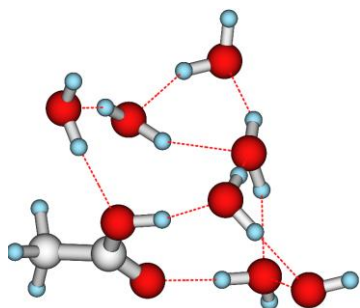
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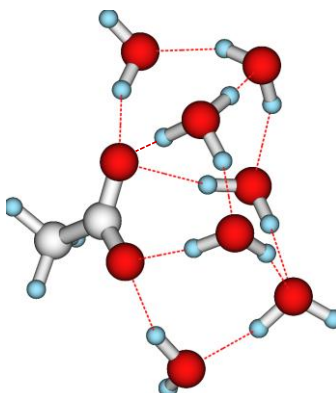
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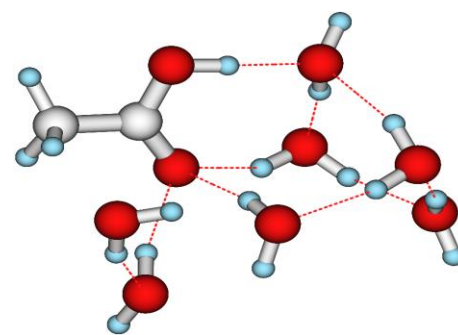
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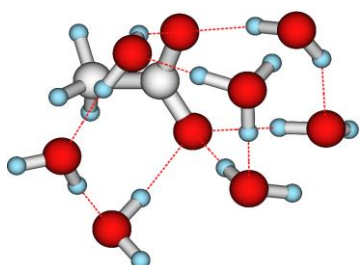
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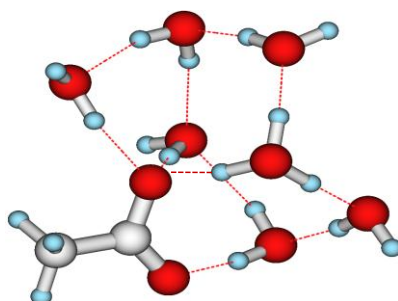
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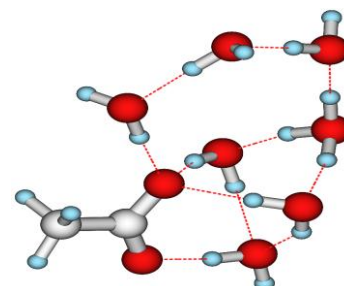
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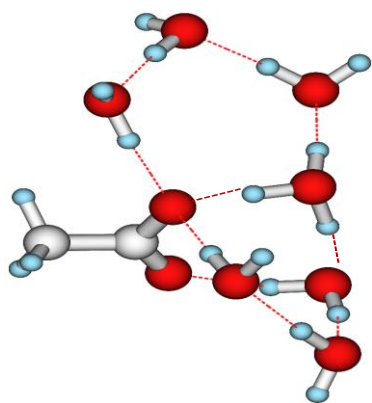
$\Delta E = 7.2$ kcal/mol



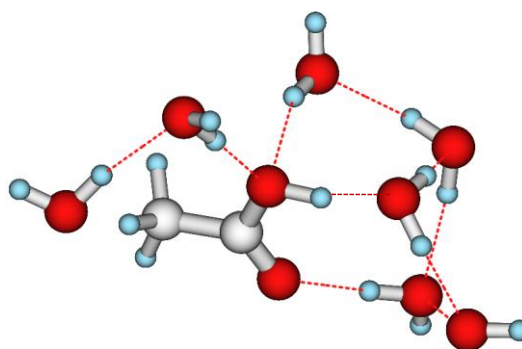
$\Delta E = +7.4$ kcal/mol



$\Delta E = +7.9$ kcal/mol

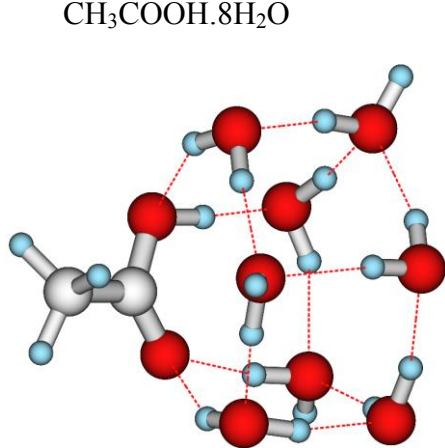


$\Delta E = 8.1$ kcal/mol

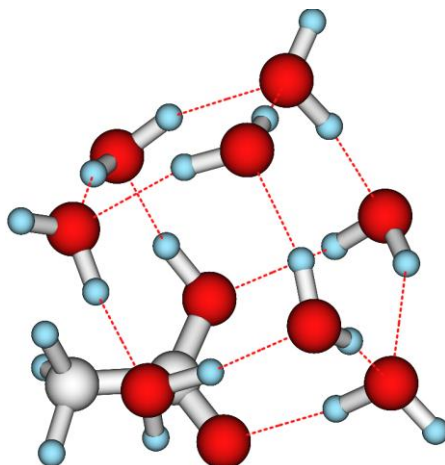


$\Delta E = +8.9$ kcal/mol

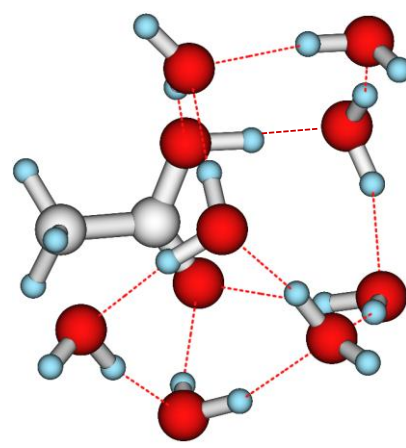
i) $\text{CH}_3\text{COOH} \cdot 8\text{H}_2\text{O}$



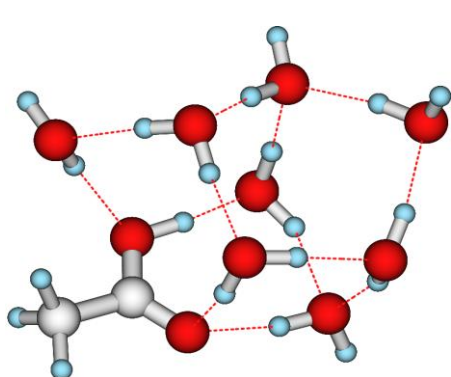
$\Delta E = 0$ kcal/mol



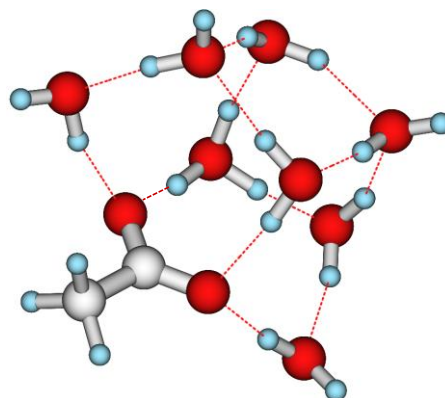
$\Delta E = +2.6$ kcal/mol



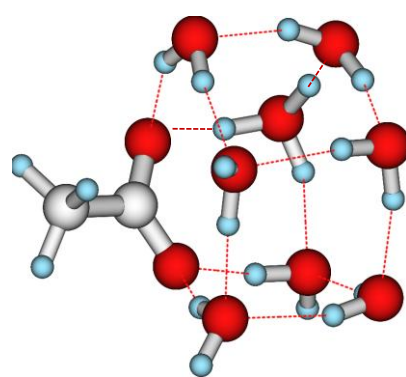
$\Delta E = +2.8$ kcal/mol



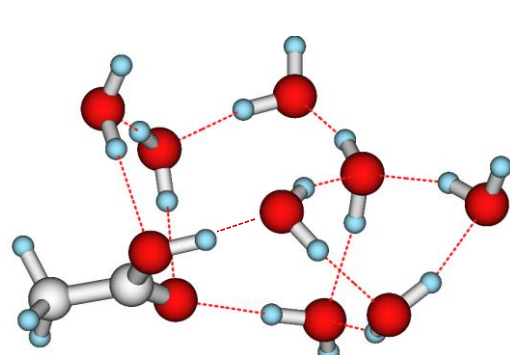
$\Delta E = +2.9$ kcal/mol



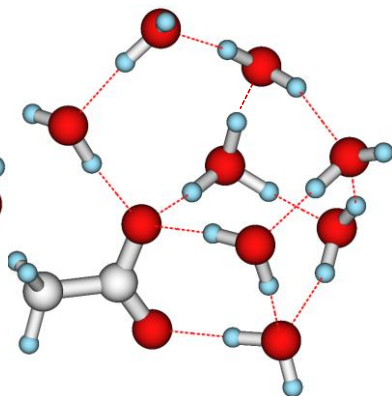
$\Delta E = +3.3$ kcal/mol



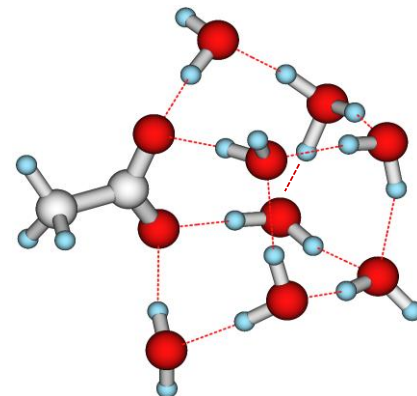
$\Delta E = +3.9$ kcal/mol



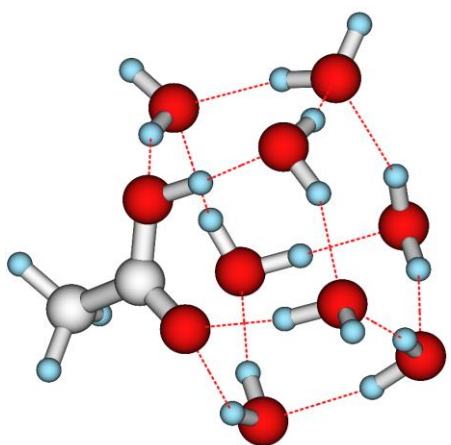
$\Delta E = +4.3$ kcal/mol



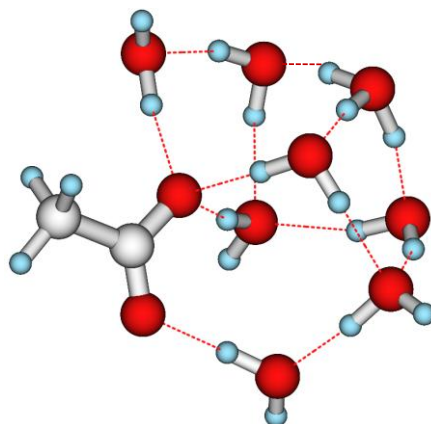
$\Delta E = +4.3$ kcal/mol



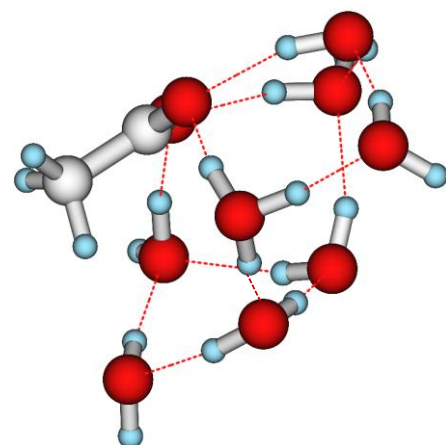
$\Delta E = +5.0$ kcal/mol



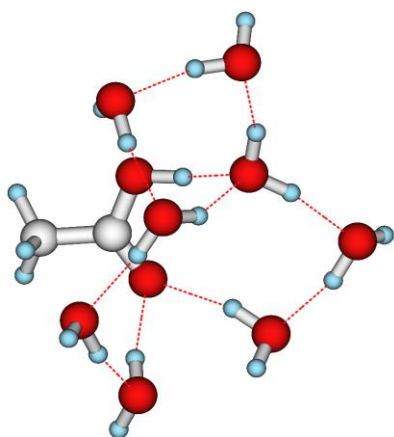
$\Delta E = +5.4$ kcal/mol



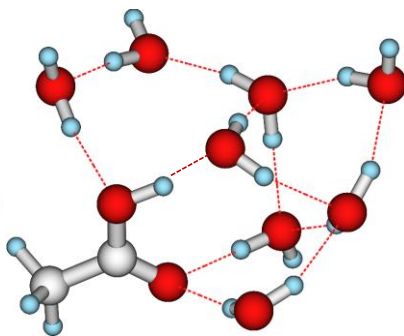
$\Delta E = +5.9$ kcal/mol



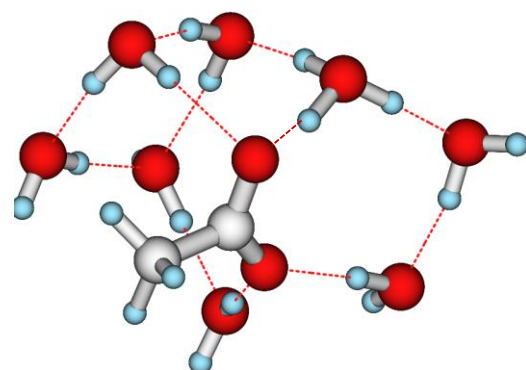
$\Delta E = +6.0$ kcal/mol



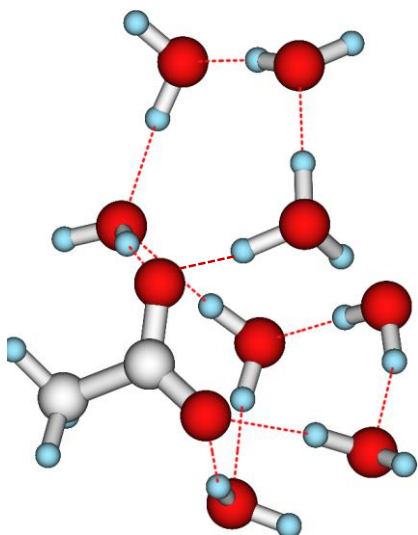
$\Delta E = +6.1$ kcal/mol



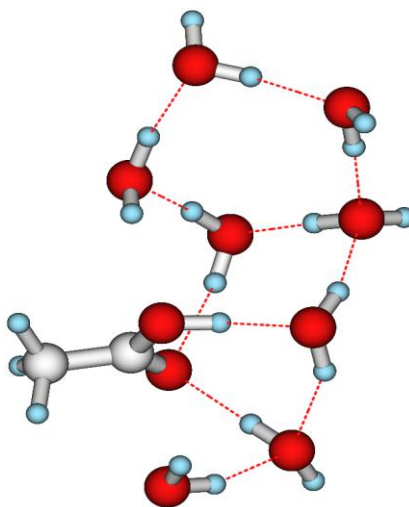
$\Delta E = +7.0$ kcal/mol



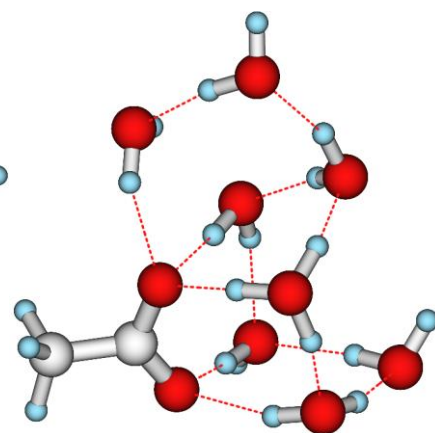
$\Delta E = +7.3$ kcal/mol



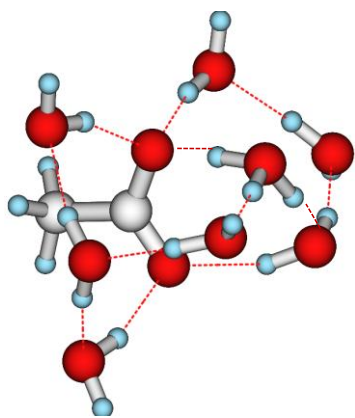
$\Delta E = +7.5$ kcal/mol



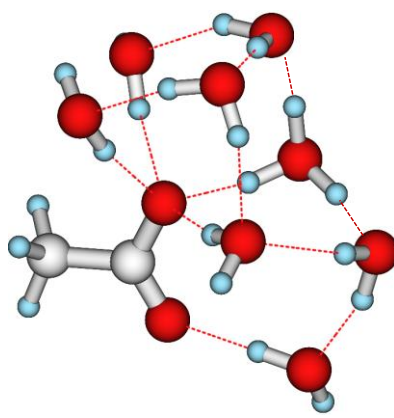
$\Delta E = +7.6$ kcal/mol



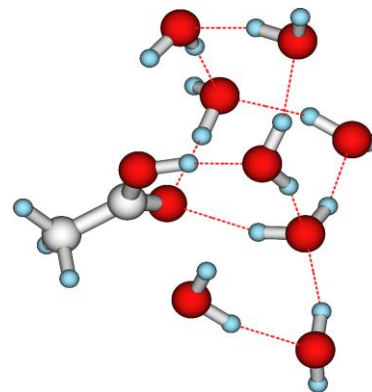
$\Delta E = +7.9$ kcal/mol



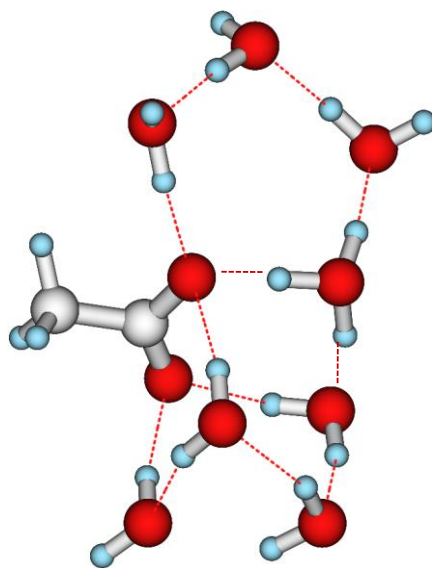
$\Delta E = +8.3$ kcal/mol



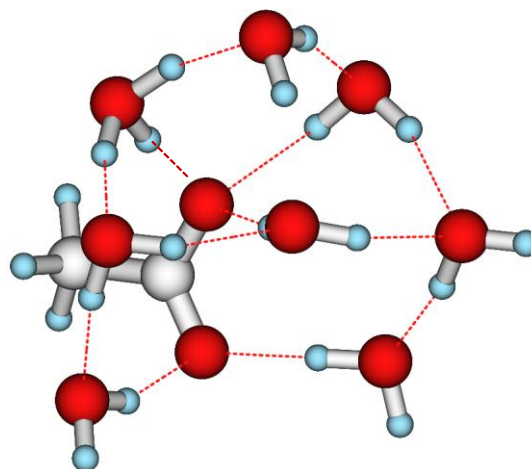
$\Delta E = +9.3$ kcal/mol



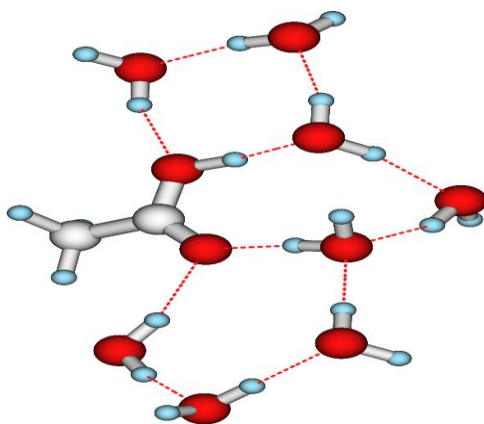
$\Delta E = +9.3$ kcal/mol



$\Delta E = +9.4$ kcal/mol

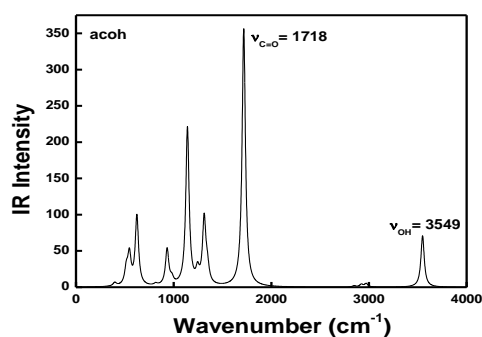


$\Delta E = +9.5$ kcal/mol

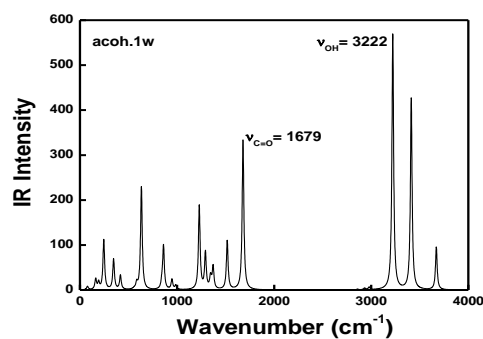


$\Delta E = +12.8$ kcal/mol

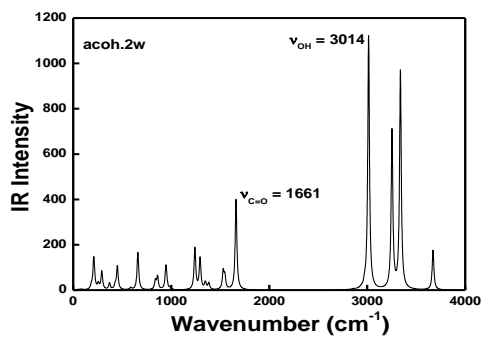
Figure S2. Simulated, scaled (scaling factor 0.93) IR spectra of the most stable structure of a) acoh; b) acoh.1H₂O; c) acoh.2H₂O; d) acoh.3H₂O; e) acoh.4H₂O; f) acoh.5H₂O; g) acoh.6H₂O; h) acoh.7H₂O and i) acoh.8H₂O calculated at ω B97X-D/aug-cc-pVDZ level of theory.



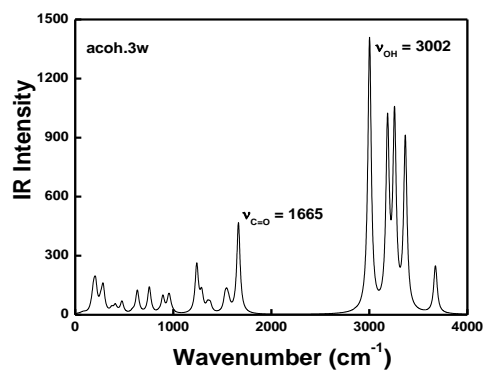
a



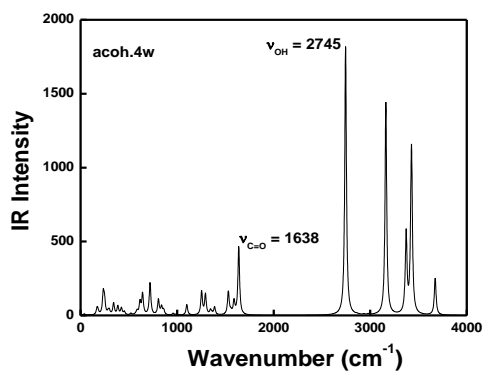
b



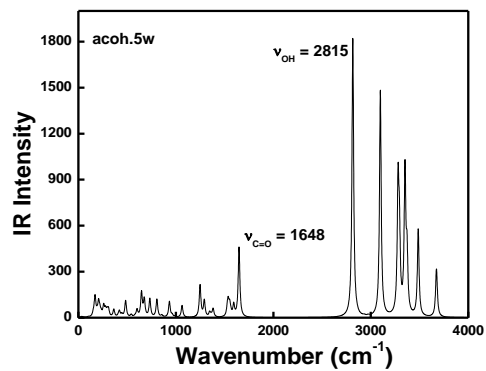
c



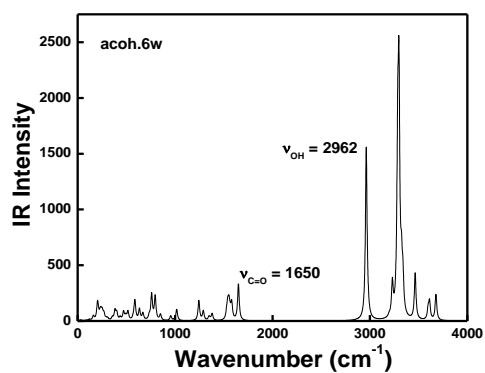
d



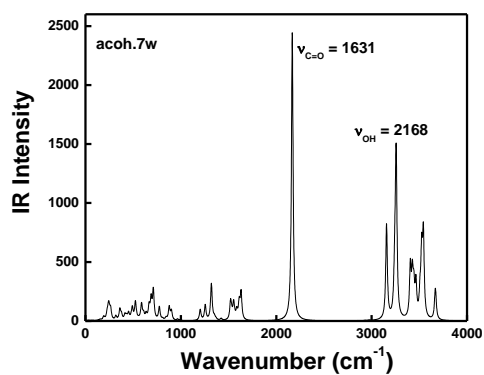
e



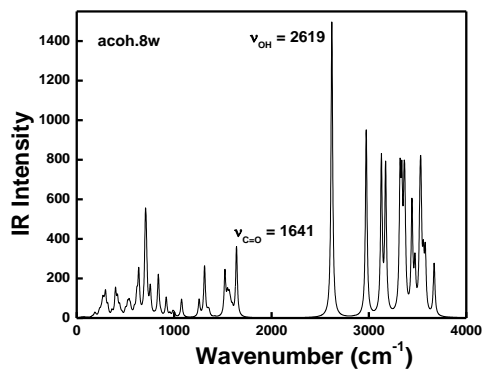
f



g



h



i