**Vibrational spectroscopic studies and DFT calculations on $NaCH_3CO_2$(aq) and $CH_3COOH$(aq).**

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## Supplementary Material

**Table S1.** Assignments of the normal modes of $CH_3CO_2^-$($D_2O$) measured in $NaCH_3CO_2$( $D_2O$).

| Raman | | | | | |
|---|---|---|---|---|---|
| $\nu_{max}$ / $cm^{-1}$ | fwhh / $cm^{-1}$ | $A_i$ | depol. ratio | symmetry | assignment |
| n.d. | - | - | - | a″ | $\tau CO_2$ |
| 474 | 23 | 0.442 | 0.70 | a′ | $\rho CO_2$ |
| 626.5 | 16 | 0.439 | 0.75 | a″ | $\rho CO_2$ |
| 661.5 | 20 | 4.138 | 0.340 | a′ | $\delta CO_2$ |
| 927.3 | 11.4 | 25.80 | 0.054 | a′ | $\nu$C-C/$\delta CO_2$ |
| 1022 | 26.5 | 0.691 | 0.70 | a′ | $\rho CH_3$ |
| 1053 | 27 | 0.054 | 0.75 | a″ | $\rho CH_3$ |
| 1349.5 | 11 | 4.259 | 0.367 | a′ | $\delta CH_3$ |
| 1417.8 | 22 | 33.50 | 0.26 | a′ | $\nu_s CO_2$ |
| 1429 | 28 | 1.926 | 0.75 | a″ | $\delta CH_2$ |
| 1444 | 17 | 2.003 | 0.50 | a′ | $\delta CH_2$ |
| 1563 | 42 | 4.248 | 0.60 | a′ | $\nu_{as} CO_2$ |
| 2936.0 | 23.5 | 100.0 | 0.008 | a′ | $\nu_s CH_3$ |
| 2983 | 24 | 4.391 | 0.75 | a″ | $\nu_{as} CH_3$ |
| 3016 | 35 | 4.006 | 0.70 | a′ | $\nu_{as} CH_3$ |

**Table S2 .** Geometrical parameters for the acetate of structure **II** of the $CH_3CO_2^-$ ion (dihedral angle = 29°): bond lengths $a_{ij}$ (in Å), angles $\alpha_{ijk}$ and dihedral angle $d_{4215}$ (see Fig. S2).

| parameter | gas phase molecule | molecule (with solvation sphere) |
|---|---|---|
| a12 | 1.561 | 1.534 |
| a23 | 1.253 | 1.260 |
| a24 | 1.253 | 1.260 |
| a15 | 1.091 | 1.089 |
| a16 | 1.091 | 1.089 |
| a17 | 1.094 | $1.092_5$ |
| α324 | 128.83° | 125.39° |
| α516 | 110.38° | 109.11° |
| α517 | 107.85° | 107.80° |
| α617 | 107.85° | 107.80° |
| d4215 | 29.04° | 29.13° |

**Table S3.** Geometrical parameters for the acetic acid derived from DFT method: bond lengths $a_{ij}$ (in Å), angles $\alpha_{ijk}$ and dihedral angles $d_{ijkl}$ of $CH_3COOH$ (see also Fig. 9).

| parameter | gas phase molecule | molecule (with solvation sphere) |
|---|---|---|
| a12 | 1.502 | 1.502 |
| a23 | 1.355 | 1.338 |
| a24 | 1.202 | 1.212 |
| a15 | 1.085 | 1.085 |
| a16 | 1.090 | 1.090 |
| a17 | 1.090 | 1.090 |
| a38 | 0.9678 | 0.9904 |
| α324 | 122.38° | 122.86° |
| α617 | 107.27° | 107.31° |
| α516 | 110.10° | 109.95° |
| α617 | 110.10° | 109.95° |
| α238 | 107.07° | 109.17° |
| d4215 | 0° | 0° |
| d4238 | 0° | 0° |

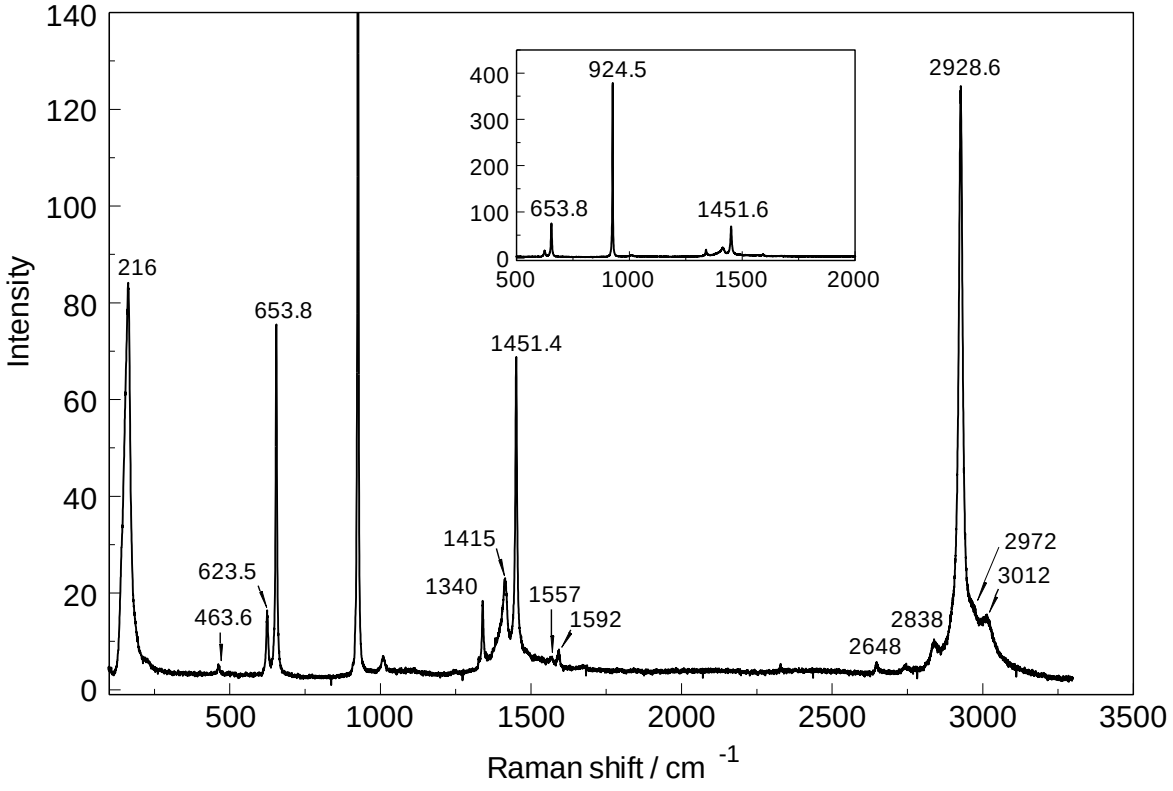


**Figure S1.** Overview Raman spectrum of crystal powder of anhydrous $Na(CH_3CO_2)$ at 23 °C.

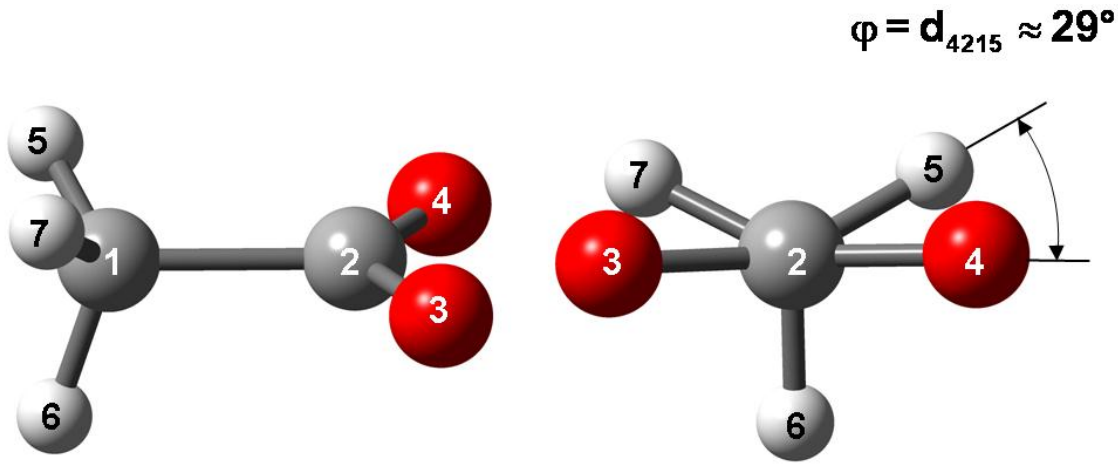


**Figure S2.** Gas phase geometry of $CH_3CO_2^-$ for φ = 29°.

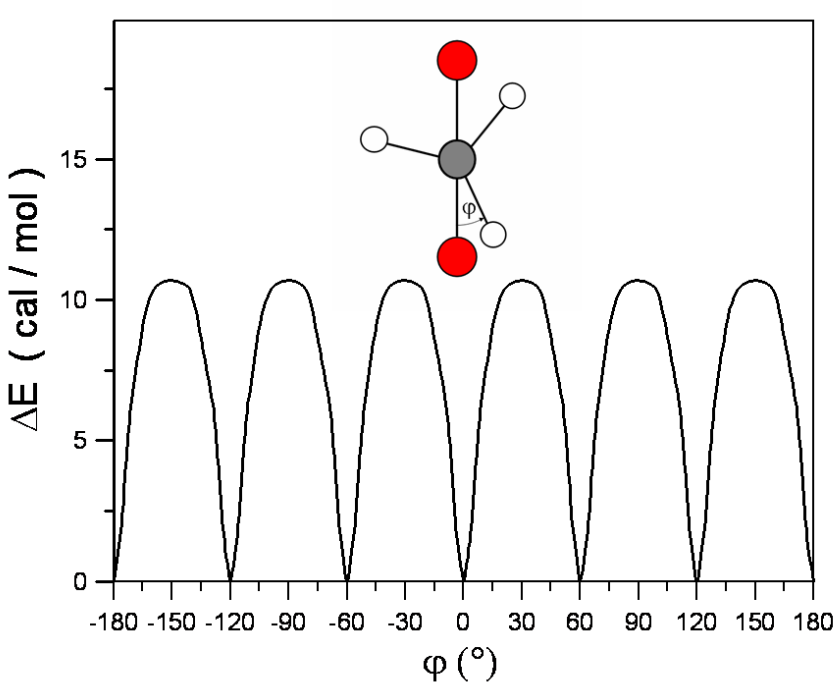


**Figure S3.** The potential energy of $CH_3CO_2^-$(g) as a function of the dihedral angle φ. The energy of the conformation with φ = 0° was set at zero.

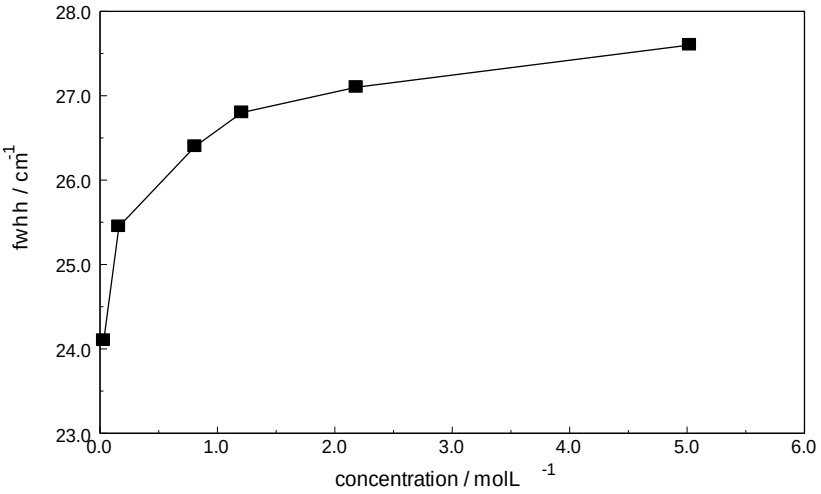


**Figure S4.** The fwhh (in $cm^{-1}$) of the $\nu_s$ $CO_2$ stretching mode of $CH_3CO_2^-$(aq) as a function of the concentration of the solute, sodium acetate.