



Hydration of NaHCO_3 , KHCO_3 , $(\text{HCO}_3^-)_2$, HCO_3^- and CO_3^{2-} from molecular dynamics simulation and speed of sound measurements.

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Streszczenie

Car–Parrinello molecular dynamics and acoustic method have been applied to determine the hydration of and ions in aqueous solution. From CPMD simulations the hydration numbers are 5.3 and 8.5 for the and ions, respectively. From speed of sound and density measurements the hydration numbers for and are 5.5 and 10.2, respectively. Our attempt to answer the old question concerning the status of in solution quite well support the earlier spectroscopic results that no $(\text{O})_2$ is present in the solution but the existence of the minor amount of dimers cannot be definitely excluded.

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