題名:台灣地區城鄉差距影響牙醫師對愛滋病,B型肝炎及感染控制認知與態度之研究

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摘要:DFT calculations were carried out to study (183)W NMR chemical shifts in the family of the Keggin anions with formula alpha-[XW(12)O(40)](q-) (X=B, Al, Si, P, Ga, Ge, As, Zn), in the beta- and gamma-[SiW(12)O(40)](4-) geometric isomers, in the derivative Dawson anion [P(2)W(18)O(62)](6-), and in the most symmetrical Lindqvist [W(6)O(19)](2-) anion and its derivative [W(10)O(32)](4-). In this article, we show that the geometry employed in the calculation of NMR chemical shifts in polyoxotungstates is extremely important if we want to be quantitative. Using very large basis sets of QZ4P quality and taking into account the conductor-like screening model (COSMO) to account for solvent effects (aqueous and organic solutions), good geometries were found for the polyoxoanions. From these optimal geometries the (183)W NMR chemical shifts were computed with the more standard basis sets of TZP quality and including spin-orbit corrections inside the zero-order regular approximation (ZORA) to describe the relativistic effects of the internal electrons. With this strategy the mean absolute error between experimental and theoretical values was found to be less than 10 ppm, which is similar to the experimental error. We also discuss how the geometry of the polyoxoanion influences on the shielding.