Chatzidimitriou-Dreismann *et al.* Reply: The point of the Comment by Torii [1] is that our results [2] of the Raman cross sections σ_{H} and σ_{D} of the OH and OD stretching vibrations in liquid H_2O-D_2O mixtures may have a simple conventional interpretation, provided by standard quantum chemical calculations in the frame of the conventional Born-Oppenheimer scheme. More concretely, Torii applied the package GAUSSIAN 94 at the Hartree-Fock (HF) level to the *isolated* (gas-phase) molecules H_2O, D_2O, and HDO, and he found (i) that the Raman activity of the OH stretching mode of HDO is smaller by $\Delta A_H = -3.9\%$ than the average of the OH stretching modes of H_2O and (ii) that the Raman activity of the OD stretching mode of HDO is larger by $\Delta A_D = +7.4\%$ than the average of the OD stretching modes of D_2O [1]. Torii then concludes [1] that these numerical values may "explain" qualitatively the experimental results $\Delta\sigma_{\mathrm{H}} \approx -7.5\%$ and $\Delta\sigma_{\mathrm{D}} \approx +10\%$, for an equimolar H_2O-D_2O mixture [2].

In our opinion, such HF calculations are inappropriate for the physical context under consideration; e.g., the calculated values of bond lengths, bond angles, and vibrational frequencies depend much on the basis set chosen. Moreover, from the viewpoint of present-day theory, these values differ inacceptably from the corresponding experimental "gas-phase" values (see below).

Nevertheless, we tested the calculations described in [1], applying the same package GAUSSIAN 94 at the HF level, and using the basis set 6-311G** (which includes polarization functions), and which is essentially similar to that of [1]. GAUSSIAN 94 has a built-in option to calculate Raman activities at the HF level.

Recall that the "standard procedure" of quantum chemistry determines the bond lengths and angles that minimize the total electronic energy of the molecule, by considering the nuclei as classical mass points. However, HF calculations provide always an "incorrect" molecular geometry of the water molecule, e.g., in our case (basis set 6-311G**): bond length = 0.941 Å; bond angle = 105.46°. As mentioned above, these values (and also those of [1]) are significantly—and, to present-day valid computational standards, unacceptably—different from the experimental values as follows.

(1) Experimental gas phase geometry [3]: bond length = 0.957 Å, bond angle = 104.5°. Therefore, to improve somewhat the calculated geometry, we performed with GAUSSIAN 94 associated calculations using the DFT (with SVWN) method, and we obtained (2) the calculated (DFT) gas phase geometry: bond length = 0.969 Å, bond angle = 103.71°. These values (2) are closer to the experimental values (1) than the HF values given above. Note, however, that the DFT algorithm of GAUSSIAN 94 has no option for the calculation of Raman activities.

Now, applying the considered numerical procedure (GAUSSIAN 94, HF/6-311G**), and using the offered option "1SCF" on the calculated geometry (1), we obtain $\Delta A_H = -4.8\%$ and $\Delta A_D = +9.0\%$, which are similar to the results of [1]. Surprisingly, application of exactly the *same* numerical procedure to the experimentally known geometry (2) yields $\Delta A_H = -2.1\%$ and $\Delta A_D = +3.95\%$. In simple words, assuming the experimental gas-phase geometry, the calculated "anomalies" of the Raman activities of HDO become reduced by more than 50%.

Moreover, due to the reaction $H_2O + D_2O \rightleftharpoons 2HDO$, in an equimolar H_2O-D_2O liquid mixture only 50% of the molecules are HDO's. Thus, in order to compare quantum chemical calculations of HDO with our experimental findings [2], the calculated anomalies of Raman activities of HDO must be divided by 2. For the equimolar H_2O-D_2O mixture, therefore, the above quantum chemical calculations may explain only an "anomalous" decrease of $\Delta A_H \approx -1.1\%$ and an anomalous increase of $\Delta A_D \approx +2\%$, which are significantly smaller than the experimentally determined values [2]. In view of the aforementioned weakness of the numerical procedure, these small values may as well represent numerical "artifacts."

Summarizing, in contrast to [1] we conclude that the calculations presented above, or those of the Comment [1] (as well as similar quantum chemical calculations), fail to provide a conventional interpretation of the striking Raman findings [2]. Further experimental evidence for protonic quantum entanglement in liquid H_2O-D_2O has been recently provided using the novel neutron Compton scattering technique [4].

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