Comment on "Anomalous neutron Compton scattering from molecular hydrogen"

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Claims in the paper by Chatizidimitiou-Dreismann *et al.* [Phys. Rev. B **72**, 054123 (2005)] that our analysis of the keV neutron scattering data is incorrect are shown to be wrong. Their analysis neglects the effect of the neutron attenuation in the relatively thick samples, thus creating an artificial anomaly of ~21% in the scattering intensity ratio of H_2O relative to that of D_2O.

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We address a recent paper[1] containing a claim that our calculation of the neutron scattering cross section from H_2O and from D_2O in the ~40 keV range reported in Ref. 2 is incorrect. In the above work,[1] the authors studied molecular H_2 using the neutron Compton scattering (NCS) technique at epithermal neutron energies (10–200 eV). In their study some evidence was presented for the occurrence of an anomaly in which the *n*-*p* scattering cross section is reported to be lower than the normal value by ~30%. This report followed a series of papers using several H-containing samples and claiming the observation of a similar shortfall in the *n*-*p* scattering intensity in all the samples studied. In the same paper,[1] reference was given to our recent publication[2] in which the H_2O-D_2O system was studied at incident neutron energies of 24–140 keV, where no anomaly in the *n*-*p* scattering was observed. The authors of Ref. 1 claim that our data analysis as presented in Ref. 2 is wrong and that they have carried out a "complete analysis" of our results (of Ref. 2) reaching an entirely different conclusion. They state that their analysis based on standard NCS theory in the impulse approximation[3] revealed a strong *n*-*p* scattering anomaly of ~21% in our measured H_2O-D_2O ratio[2] carried out at higher neutron energies in the ~40 keV range. This alleged anomaly was reported to be in "surprisingly good agreement" with other anomalies which they observed at lower energies (10–200 eV) in several H-containing compounds.

In this connection, it should be remarked that in our work[2] a different scattering technique was employed together with a far simpler method of data analysis; the scattering intensity from the entire H_2O molecule within a certain angular range was compared to that from the entire D_2O molecule and also to a mixture of H_2O and D_2O. One of the main features of our work[2] was the use of a 20-cm-thick iron filter which fixed the final energy of the scattered neutrons at 24.3 keV, yielding an isolated *n*-*p* scattering peak (containing contributions from D and O) and having a high signal-to-noise ratio. Here we remind the readers that due to kinematics, the incident *n* energy in the laboratory system is higher than the final energy, being 24.3 keV. Thus, the incident neutron energies corresponding to scattering angles between 25° and 65° are, for H, 29.6–136 keV; for D, 26.7–45 keV, and for O, 24.6–26.1 keV. In addition, the *n*-*p* scattering intensity is highly peaked in the forward direction in the lab system compared to that of *n*-D and *n*-O.

Note that within the above energy ranges the neutron *total* *n*-*p* cross section decreases by about 36% while those of *n*-D and *n*-O are essentially constant, decreasing by ~1%.

In the present Comment we show that the allegation of Ref. 1, concerning the existence of an anomalous *n*-*p* scattering intensity at ~40 keV of Ref. 2, is incorrect and misleading. The claim of Ref. 1 is based on a calculation of the scattering intensities (from single scattering) in which the effect of neutron attenuation by the samples is ignored. This assumption is justifiable when using very thin samples as is usually the case in NCS studies.[3] In Ref. 2, however, the samples were relatively thick (0.18 cm). Hence the high total *n*-*p* cross section compared to that of *n*-D causes the *n* attenuation by the H_2O sample to be much higher than that by D_2O. This effect reduces the calculated *ratio* of scattering intensity from the two samples versus thickness as illustrated in Fig. 1. In this calculation, only first collision (single scattering) events are assumed and no multiple scattering is included. It may be seen that the scattering intensity ratio drops from 6.65 for very thin samples ($x \sim 0$) to a ratio of 5.5 for a sample 0.18 cm thick, used in Ref. 2. Note that when *n* attenuation in H_2O-D_2O samples is negligible, as in the case of very thin samples, an artificial ~21% increase in the ratio of the neutron scattering intensities from H_2O-D_2O is created. This explains the anomalous effect reported by the complete analysis of Ref. 1.

In Fig. 1, only single scattering events were taken into account as was done in Ref. 1. In the following we show that at a final energy of 24.3 keV, the same conclusion is ob-

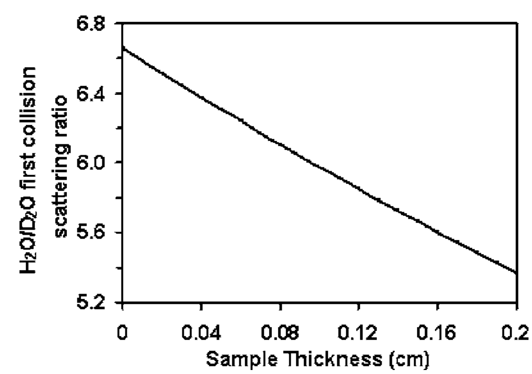

FIG. 1. Calculated ratios of scattering intensities from H_2O and D_2O samples versus thickness. The scattered neutrons have a final energy of 24.3 keV and the scattering angles are between 25° and 65°. The *n* flux varies with *E* as $E^{-0.65}$.

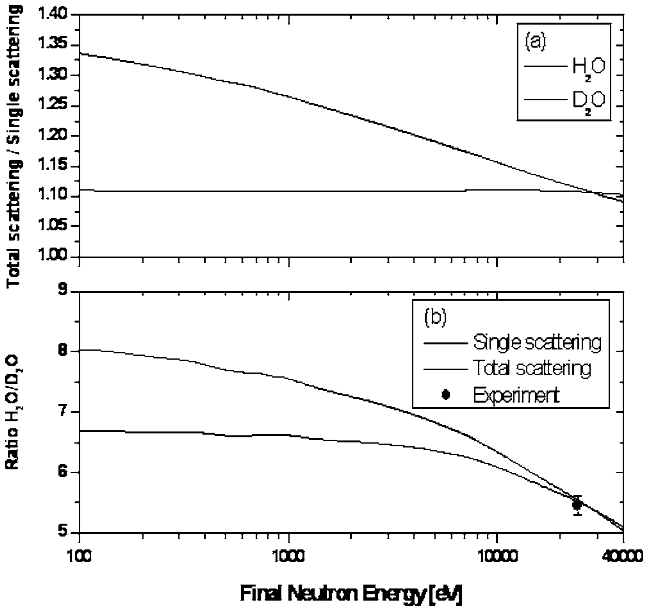

FIG. 2. (a) Effect of neutron MS on the scattered intensity from H_2O and D_2O versus the neutron final energy. The samples were 0.18 cm thick and the scattering angle 45°. (b) Calculated ratio of total scattering intensities (including the MS effect). The calculations were made using the MCNP computer code (Ref. 4).

tained when multiple scattering (MS) of neutrons in the samples is accounted for. We do so using the Monte Carlo MCNP general purpose computer code[4] of Los Alamos mentioned in Ref. 2. We focus our attention on a scattering angle of 45°, being the medium between the two extreme angles 25° and 65° used in Ref. 2. The results of the MS calculation are illustrated in Fig. 2(a) and show the relative contribution of MS versus the final n energy for the H_2O-D_2O samples, each 0.18 cm thick. At 24.3 keV, the MS effect causes the scattering intensity from H_2O to increase by ~10%. This increase happens to be practically the same as that for D_2O. Thus the calculated ratio of the total scattering intensities is 5.5 [see Fig. 2(b)]; it is essentially equal to the calculated ratio of the single scattering intensities. Both the single and total scattering intensity ratios coincide with the measured values. Thus at 24.3 keV and 45°, the calculated effect of MS on the ratio of scattered intensities is negligible even though the MS effect in each sample is quite large. Note that at lower energies, e.g. 100 eV, a strong MS effect of 20% is obtained for the ratio of scattered intensities because the MS in H_2O is 35% while that in D_2O is ~12%.

The fact that the calculated MS result shows no effect at 24.3 keV can readily be understood. It may be qualitatively explained by noting that the two factors governing the ratio of multiple to single n scattering in samples of H_2O and D_2O (of equal numbers of molecules and the same geometry) are the scattering cross section and the number of neutrons being multiply scattered. Now, the n energies involved in n-p multiple scattering are much higher than those in n-D multiple scattering. At high energies both the n-p scattering cross section and the n flux decrease steeply with increasing E, compared to that of n-D scattering. The n flux varies with energy as $E^{-0.65}$. The two factors work in such a way that at 24.3 keV the MS effect of n-p scattering in H_2O happens to be practically equal to that of n-D in D_2O. In view of the above remarks, it may be seen that at a final energy of 24.3 keV no anomaly in the n-p scattering intensities occurs and all the contents and conclusions given in Ref. 2 remain intact.

Finally, it is important to mention that in a recent publication,[5] we reported a strong confirmation of our previous result[2] as to the absence of any anomaly in the n-p scattering measurements by working at lower final energies (64 eV–2.6 keV) and using CH_2-C samples of about the same n attenuation and hence nearly the same MS effect.

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[1] C. A. Chatzidimitriou-Dreismann, T. Abdul-Redah, and M. Krzystyniak, Phys. Rev. B **72**, 054123 (2005).
[2] R. Moreh, R. C. Block, Y. Danon, and M. Neuman, Phys. Rev. Lett. **94**, 185301 (2005).
[3] J. Mayers and T. Abdul-Redah, J. Phys.: Condens. Matter **16**, 4811 (2004).
[4] J. Sweezy *et al.*, Los Alamos Report No. LA-UR-03-1987, 2003 (unpublished).
[5] R. Moreh, R. C. Block, Y. Danon, and M. Neuman, Phys. Rev. Lett. **96**, 055302 (2006).