Validation Studies of Hydrogen (H_2 and HD) in HITRAN

Line lists for H_2 electric quadrupole and HD electric dipole transitions were added to HITRAN2012 for the first time. In this update, a total number of 7195 electric quadrupole transitions of the HD molecule have been calculated and added to the HITRAN line list. The calculation has been carried out using the energy levels from the work by Pachucki and Komasa [1] and the quadrupole moment function by Wolniewicz *et al* [2].

For the purpose of validation, comparison between the HITRAN database, Kurucz database [3], and the most recent experimental results [4] has been performed for both electric dipole and electric quadrupole transitions of the HD molecule and the electric quadrupole transitions of H_2.

Figure 1 shows the comparison of the line positions for the first overtone electric dipole transitions of HD. It is clear that our results agree very well with the experimental results ($\leq$ 0.001 cm^{-1}). However the Kurucz database differs from both the experimental values and the HITRAN database by 0.03 cm^{-1} at the band origin, and the difference increases to almost 0.4 cm^{-1} for high-*J* P-branch lines. Indeed, based on the validation by experiment and the sophistication of the Pachucki and Komasa calculation, their energy levels are of unprecedented accuracy in comparison with previous calculations. Figure 2 shows the overall comparison for a large number of ro-vibrational transitions of the electric dipole transitions of HD. The differences are between -0.3 cm^{-1} and +0.6 cm^{-1} and generally increase with *J* within each band.

A recently developed accurate dipole moment function by Pachucki and Komasa [5] has been used in the calculation of the Einstein A coefficients of the electric dipole transitions of HD. In Figs. 3 and 4, we have compared the Einstein A coefficient between the HITRAN and Kurucz databases. Note that the Einstein A coefficients in the Kurucz database are from E. Roueff (private communication, 1991). Prior to this comparison, we have confirmed our intensity calculation with the experimental values of Kassi and Campargue [4]. However, large differences have been found for some of the transitions between the HITRAN and Kurucz databases.

We have also compared two databases for the HD electric quadrupole transitions in a similar fashion. Figure 5 shows the overall comparison for line positions. The range of the Y-axis of this figure is similar to that of Fig. 2, because the same energy levels have been used in calculating both electric dipole and quadrupole transitions. Figures 6 and 7 show the comparison of Einstein A coefficients of HD quadrupole transitions. It can be seen that the differences become larger towards higher wavenumber (Fig. 6) and weaker lines (smaller Einstein-A coefficients, see Fig. 7).

For the line list of the H_2 molecule, we also carried out similar comparison. Figure 8 shows the comparison of the line positions of the electric quadrupole transitions. We can see that the differences between the Kurucz and the HITRAN databases range from -0.02 to 0.6 cm^{-1}. For the Einstein A coefficient, because the same quadrupole moment function from Ref. [2] has been used, the difference between two databases arise only from different potential energy functions. In general, the differences of the Einstein A coefficients of H_2 between two databases are less than 2%.

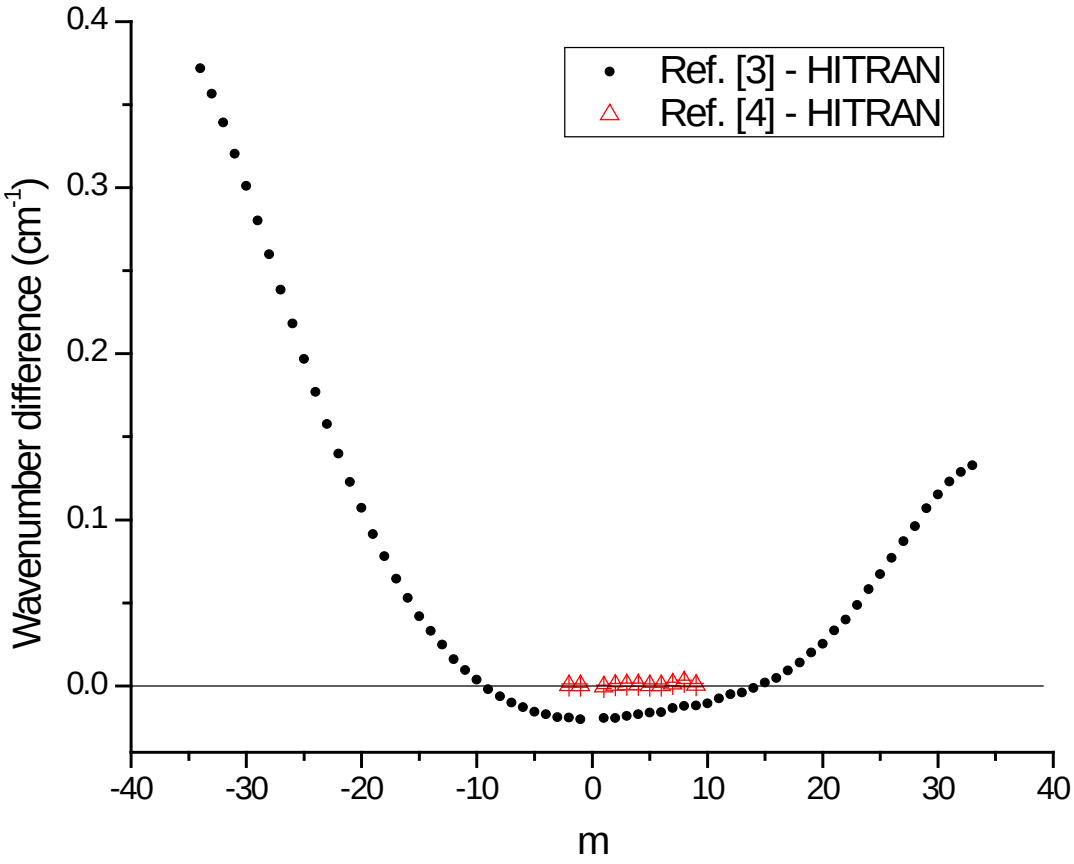

Figure 1. Comparison of the line positions for HD electric dipole transitions in the first overtone. $m = -J$ for P lines and $J+1$ for R lines.

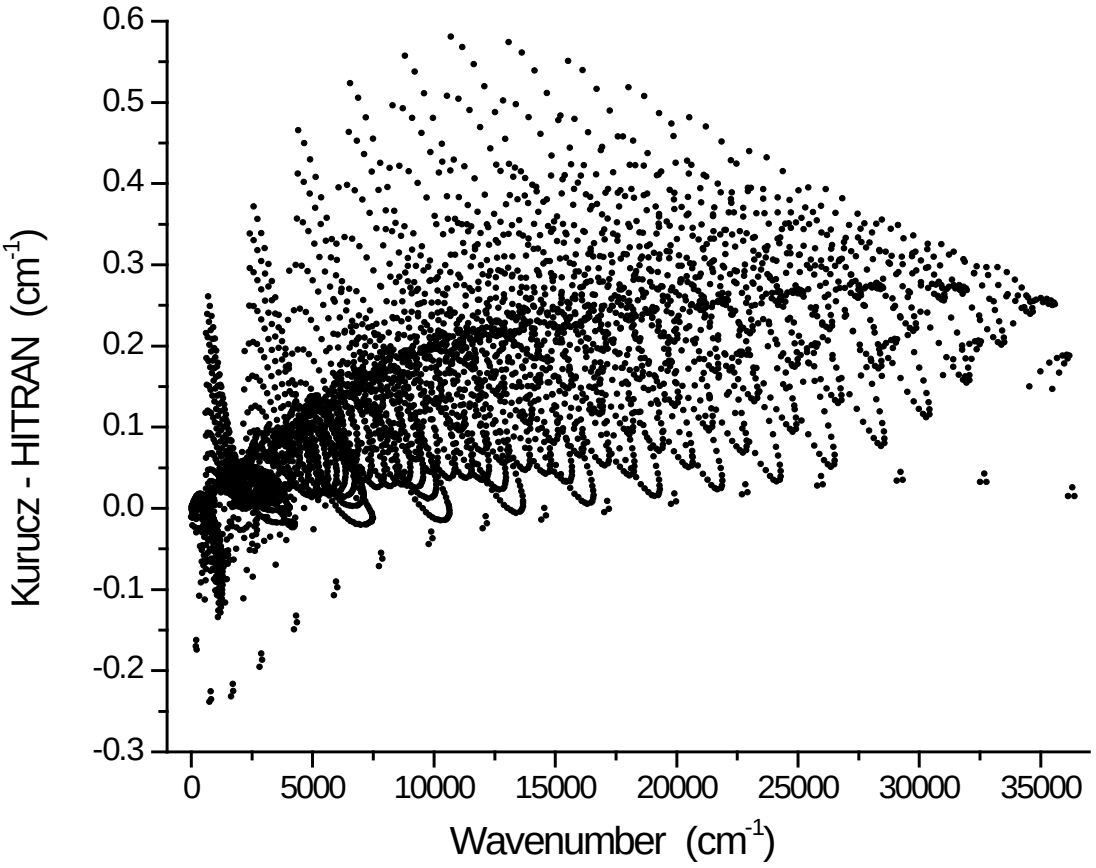

Figure 2. Comparison of the line positions for HD electric dipole transitions between the Kurucz database [3] and the HITRAN database.

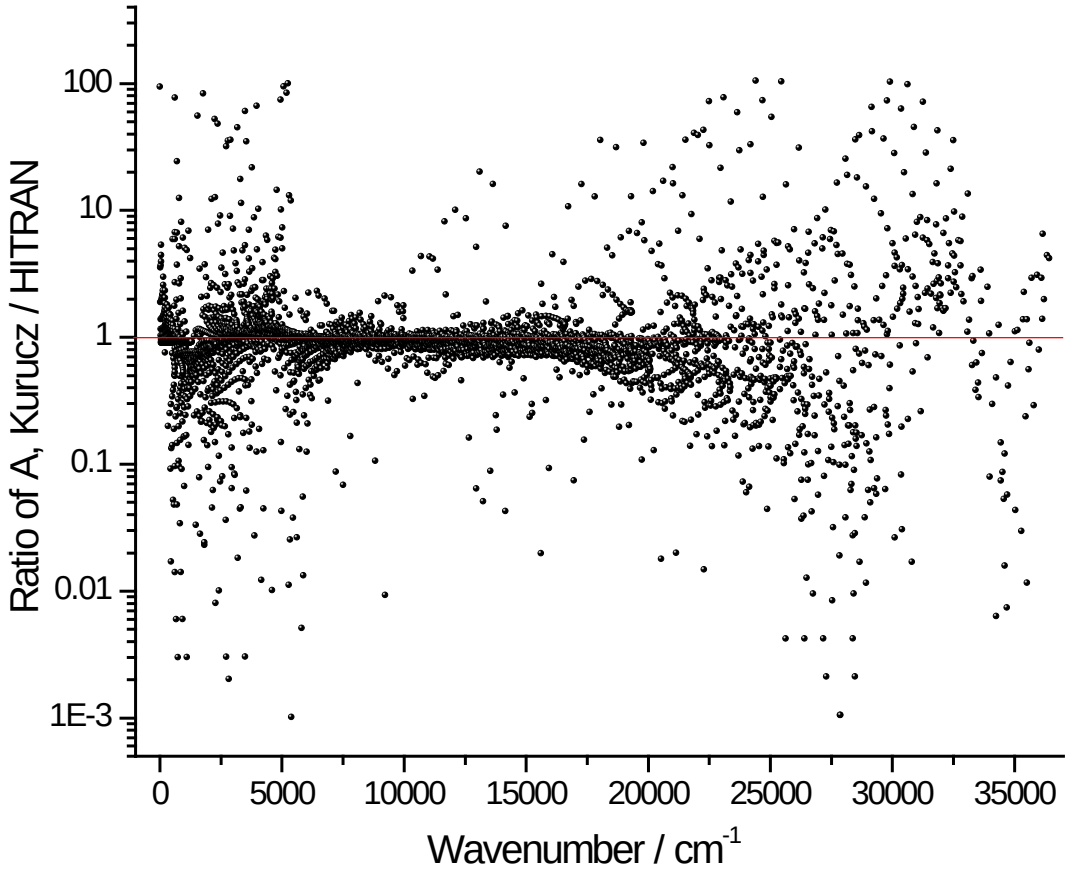

Figure 3. Comparison of the Einstein A coefficient for HD electric dipole transitions between the Kurucz database [3] and the HITRAN database.

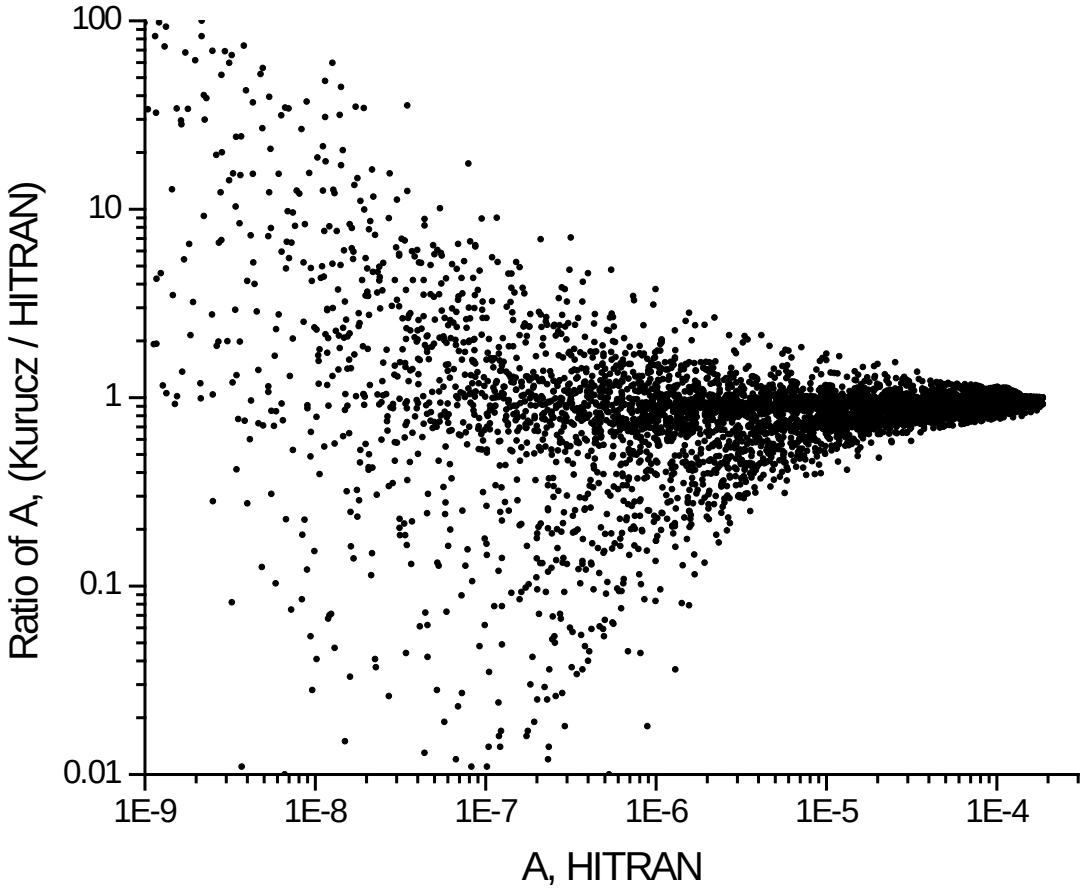

Figure 4. Comparison of the Einstein A coefficient for HD electric dipole transitions between the Kurucz database [3] and the HITRAN database.

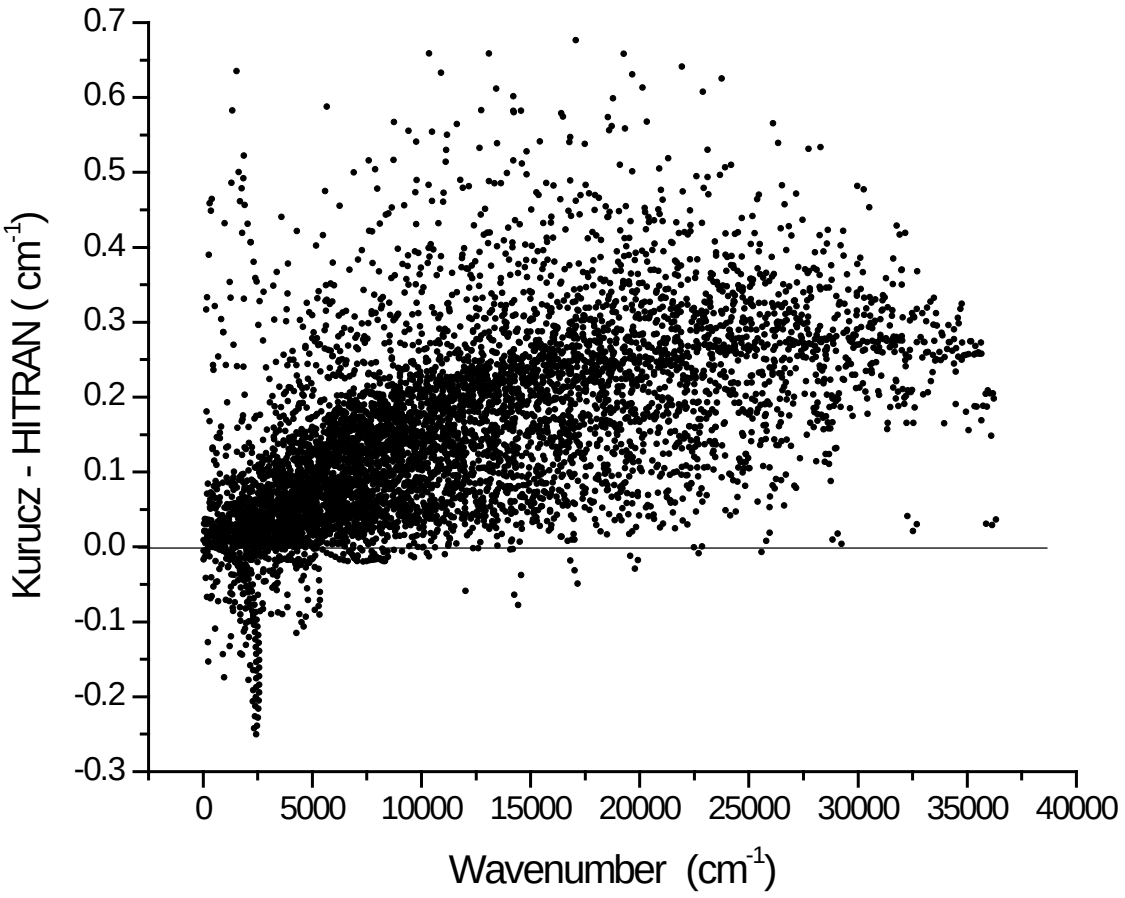

Figure 5. Comparison of the line positions for HD electric quadrupole transitions between the Kurucz database [3] and the HITRAN database.

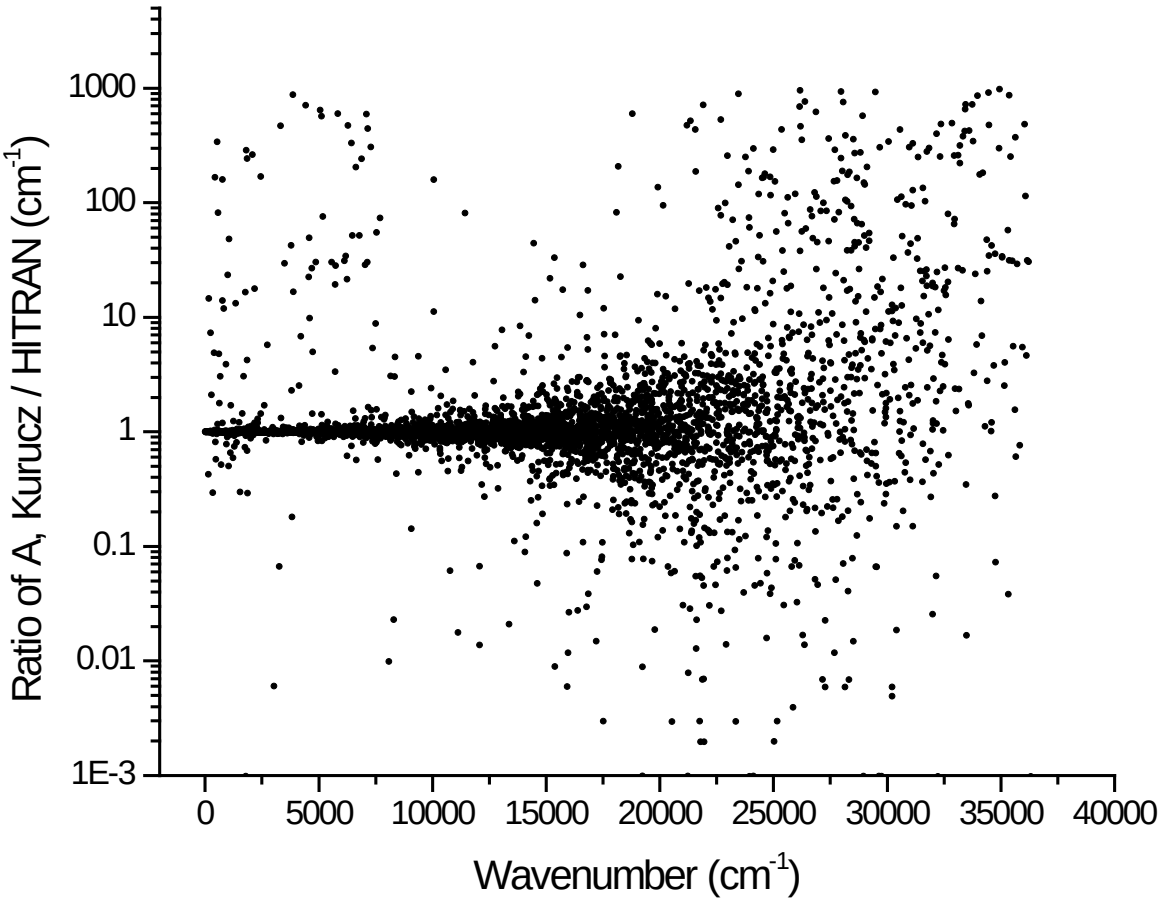

Figure 6. Comparison of Einstein A coefficient for the electric quadrupole transitions of HD between the Kurucz database [3] and the HITRAN database.

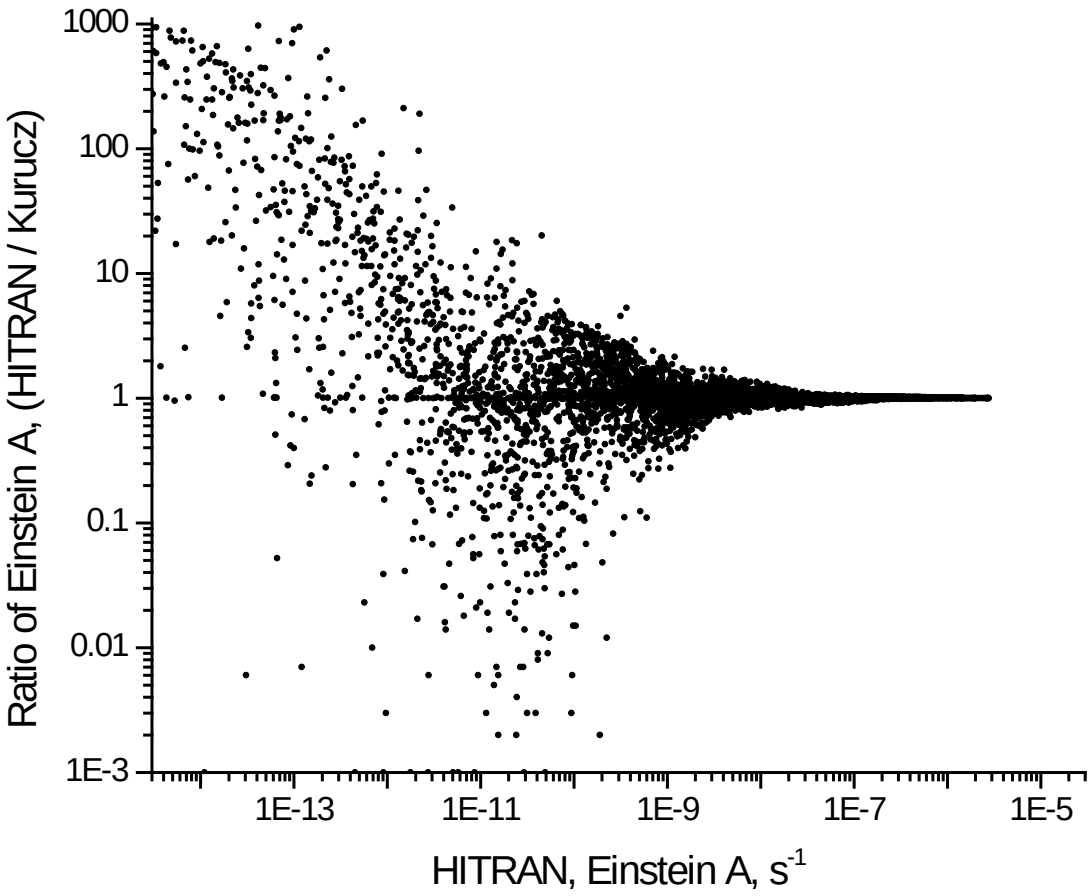

Figure 7. Comparison of Einstein A coefficient for the electric quadrupole transitions of HD between the Kurucz database [3] and the HITRAN database.

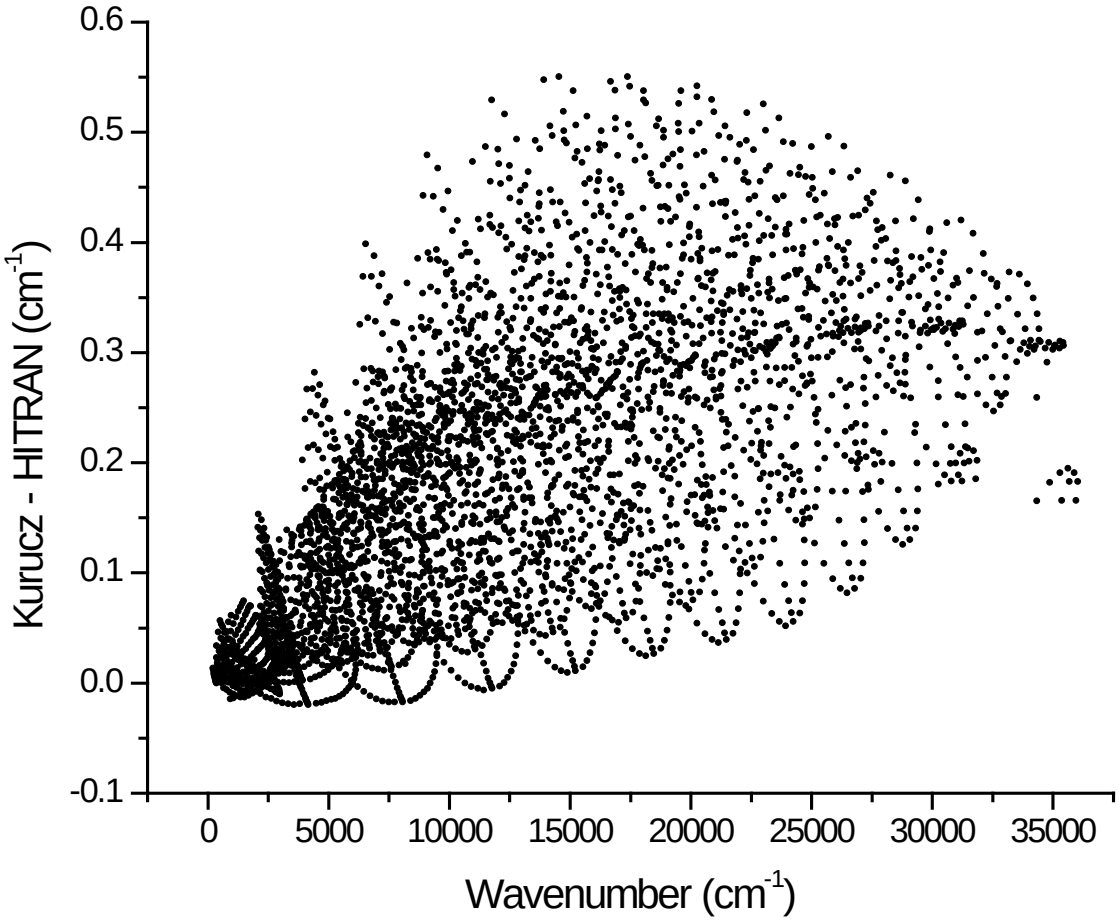

Figure 8. Comparison of the line positions for the electric quadrupole transitions of the H_2 molecule between the Kurucz database [6] and the HITRAN database.

References

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