# Accurate and consistent prediction of molecular IR line lists based on ab initio theory and high-resolution experimental data

Xinchuan Huang,<sup>1</sup>,<sup>2</sup> David W. Schwenke,<sup>3</sup> and Timothy J. Lee<sup>4</sup> <sup>1</sup>SETI Institute, Mountain View, CA, USA; xhuang@seti.org

<sup>2</sup>Mail Stop 245-6, NASA Ames Research Center, Moffett Field, CA, USA; Xinchuan.Huang-1@nasa.gov

<sup>3</sup>Mail Stop 258-2, NASA Ames Research Center, Moffett Field, CA, USA; David.W.Schwenke@nasa.gov

<sup>4</sup>Mail Stop 245-3, NASA Ames Research Center, Moffett Field, CA, USA; Timothy.J.Lee@nasa.gov

In the last 10 years, the prediction oriented "Best Theory + High-resolution Abstract. Experimental Data" strategy has been extended from water to  $NH_3$ ,  $CO_2$ , and  $SO_2$ . To compute the molecular infrared (IR) opacity, the accuracy of experimental line positions is combined with the consistency of high quality ab initio theory. The Ames IR line lists computed on the empirically refined ab initio potential energy surface (PES) go beyond the reproduction of existing data to make predictions as accurate as 0.01-0.02 cm<sup>-1</sup> for line positions and  $\sigma$ <5-10% for line intensity. They provide valuable reference data and assignments for missing IR bands or minor isotopologues, identify the defects and unreliable extrapolations of existing effective Hamiltonian (EH) models, and improve molecular IR opacity databases. Recent experiments have verified the accuracy, consistency and completeness of the Ames IR list predictions. Examples are given to demonstrate the EH database deficiencies, experimental difficulties, and the prediction accuracy & consistency of our work. Our latest study has pushed the strategy to a higher level: the microwave (MW) spectra of the SO<sub>2</sub> minor isotopologues can be predicted with 1-5 MHz accuracy in the range of J<20 and  $K_a < 10-15$ , and 0.01-0.02 MHz for rotational constants  $A_0/B_0/C_0$ . The Ames IR intensity predictions have very high consistency across all isotopologues. These data provide quality control over experimental data or effective dipole moment (EDM) models, and allow future "refinement" on intensities when much more accurate experimental intensity data become available. See http://huang.seti.org for the latest updates of the Ames molecular IR line lists.

## 1. The Strategy to Tackle Database Deficiencies

Highly accurate Infrared line lists including line positions, intensity, and line shapes parameters are necessities for the characterization and studies of molecular isotopologues in astronomical environments (Freedman et al 2008; Marley & Robinson 2015; Fortney et al 2016; Tennyson & Yurchenko 2017). The experimental IR analysis fits measured line positions and intensities to reduced EH and EDM models. The models use the fitted parameters to derive the line positions and intensities for thousands of transitions, which are collected in popular databases such as HITRAN2008-2016

(Rothman et al 2008, 2012; Gordon et al 2016), CDSD (Tashkun et al 2015; Tashkun & Perevalov 2011), and CDMS (Müller et al 2001, 2005; Endres et al 2016). These fast-growing infrared databases are still not complete nor accurate enough to subtract the IR contributions of astrophysical molecules so that scientists may identify the "hidden flowers", or to carry out complete and accurate IR simulations for hot exoplanets or dwarf stars. Due to various difficulties associated with laboratory IR measurements and analyses, it has been concluded that the only viable solution for astrophysical molecular opacity is to combine the accuracy of experimental data with the consistency and global picture of theoretical computations. The prediction oriented "Best Theory + High-resolution Experimental Data" strategy was first applied in the Ames group for H<sub>2</sub>O IR line lists (Partridge & Schwenke 1997). Over the last 10 years this approach has been improved and extended to NH<sub>3</sub> (Huang, Schwenke & Lee 2008, 2011a,b; Sung et al 2012), CO<sub>2</sub> (Huang, Schwenke & Lee 2012; Huang et al 2013, 2014, 2017), and SO<sub>2</sub> (Huang, Schwenke & Lee 2014, 2015, 2016).



Figure 1. "Best Theory + High-res Expt Data" on  ${}^{14}NH_3$ : Two orders of magnitude improvement on the accuracy, from the pure ab initio potential energy surface (PES) HSL-0 to the empirically refined HSL-2 using less than 500 HITRAN levels. Reprinted from Huang et al (2011a), with the permission of AIP Publishing.

Fig.1 illustrates the two orders of magnitude improvement we have achieved for  $NH_3$  (Huang et al 2011a). The basic idea is that the *ab initio* PES is systematic, consistent, complete but lacks very high accuracy. However, it can be refined with a few hundreds of rovibrational energy levels taken from the most reliable high-resolution IR data. With an exact molecular rovibrational Hamiltonian implemented within the Born-Oppenheimer approximation, we can reproduce thousands of measured transitions first. But most importantly, we can make reliable predictions with the same or similar accuracy for the missing bands of higher rovibrational quanta, lower intensity, or isotopologues. The prediction accuracy, reliability and consistency achieved, have allowed us to identify defects, unreliable assignments, over extrapolations, and suspicious data and analyses from EH models and existing databases. Here are a few examples.

The primary deficiency of most experimental data based IR line lists is the very limited coverage. For example, only 7 discrete segments can be found in HITRAN2016 (Gordon et al 2016) for  ${}^{32}S^{16}O_2$ , see Fig.2 (Huang et al 2014). Very little or no data at all exists for other minor isotopologues (Müller et al 2005). Data for CO<sub>2</sub> minor isotopologues also requires significant improvement (Huang et al 2014, 2017).

For existing EH models, the main issue related to line positions is the over extrapolation beyond the original experimental data included in the EH fit. For example, the old EH model of  ${}^{32}S^{16}O_2$  was fit with data K<sub>a</sub> up to 23 so its accuracy degrades significantly near K<sub>a</sub> =30, but the model was over extrapolated to generate transitions



Figure 2. Ames 296K IR line list for  ${}^{32}S^{16}O_2$  (red) v.s. the 7 segments in HITRAN (green). Remake of Fig.4 in Huang et al (2014).

with  $K_a$  as high as 35-40. Ulenikov et al (2013) published a new EH (or  $H_{EFF}$ ) model including data with  $K_a$  up to 34. It significantly increased the reliable range of the EH model from less than 30 to near 40, and confirmed the consistency and reliability of our theoretical line lists computed on the empirically refined PES. See Fig.3a. In some extreme cases, the EH model was not appropriately constructed, e.g. the <sup>14</sup>NH<sub>3</sub> 2 $\nu_4$ levels computed from the existing EH model are inconsistent with other bands. See Fig.3b. Other examples include certain parameters wrongly fixed, etc.



Figure 3. (a) Ames line lists vs. two EH models of  ${}^{32}S^{16}O_2$ , the EH model quickly loses accuracy at higher K<sub>a</sub>. Reprinted from Huang et al (2014) with the permission of AIP publishing; (b) defected EH model for  ${}^{14}NH_3 2v_4$  band. Reprinted from Huang et al (2011b), with the permission of AIP publishing;

The EDM model for intensity should have all critical effective dipole terms reliably determined. If certain terms were missing or unreliable, the predicted intensity may be off by orders of magnitude. For example, the CO<sub>2</sub> band at  $1.1\mu$ m was underestimated by 2 orders of magnitude in HITRAN2008, which was fixed in HITRAN2012 as new experiment confirmed our intensity predictions (Huang et al 2013). See Fig.4.

Second issue about IR intensity is that some EDM models do not have adequate higher order terms, which means less accurate intensity at higher quanta and higher temperature simulations. An example is the  ${}^{32}S^{16}O_2$  microwave spectra, i.e. the line position and intensity differences between our IR list and database. Excellent intensity

agreement is found for the 518 measured transitions (left panel), with  $|\delta| \pm \sigma_{RMS} = 1.42 \pm 1.77\%$ , but the relative intensity deviation can be as large as 20-60% when compared to the full EH model in the CDMS (Müller et al 2005) and HITRAN (Gordon et al 2016) databases. See Huang et al (2014) for more details.



Figure 4.  ${}^{12}12C^{16}O_2$  IR simulation at 296K, Ames IR lists (red) vs. HITRAN2008 (black) and 2012 (blue), note the fixes near 9000 cm<sup>-1</sup>.

From one isotopologue to another, the EDM models usually do not have very good consistency. Their consistency is also dependent on specific vibrational bands. We can test the isotopologue consistency of EDM models by computing their relative deviations with respect to Ames intensities, because the Ames intensities are highly consistent across isotopologues. Fig.5a shows the CO<sub>2</sub>  $v_2$  band. In the 13 isotopologues, the 627 and 628 are obvious outliers. Their linear dipole term may need a small fix. Note some CO<sub>2</sub> EDM models could be off by orders of magnitude on certain isotopologues, e.g. the vibration-induced rotational band of asymmetric isotopologues (Huang et al 2017). Fig. 5b plots the 110 ( $v_1 + v_2$ ) band intensities for 4 SO<sub>2</sub> isotopologues: 626, 646, 628 and 828. Reasonable agreement is found for the 626 and 646 transitions, while fairly large systematic deviations (>100%) for 628 and 828 clearly indicate inconsistency of reported data (Ulenikov et al 2017).



Figure 5. Relative intensity deviations (%) of the EDM models, with respect to Ames line list intensities (a)  $CO_2 v_2$  band, 13 isotopologues; Reprinted from Huang et al (2017), Copyright (2017), with permission from Elsevier; (b)  $SO_2 v_1 + v_2$  band, 4 isotopologues, strong deviations in the lower K<sub>a</sub> region of 628 and 828 Expt. data.

## 2. Prediction Accuracy and Consistency of Ames IR Line Lists

The quality of the Ames IR line list predictions have been verified in many experiments. For example, the <sup>14</sup>NH<sub>3</sub> accuracy in Fig.6 is still the best available predictions for 1.5 $\mu$ m region, and the comparisons in Fig.7 include 13 isotopologues of CO<sub>2</sub>. It has been our "normal" expectation to achieve  $\sigma_{RMS}$ =0.01-0.02 cm<sup>-1</sup> for band origins,  $\sigma_{RMS}$ =0.01-0.03 cm<sup>-1</sup> for line list positions, and  $\delta$ S within ±5-10% for intensities.



Figure 6. Best accuracy achieved for <sup>14</sup>NH<sub>3</sub> levels at 1.5  $\mu$ m: (a) J=0-8 levels of 6 bands computed on the Ames-Pre3 PES, Reprinted from Sung et al (2012), Copyright (2012), with permission from Elsevier; (b) inversion splits of the  $2v_3^2$  band predicted using the HSL-2 PES nicely match with JPL experiments (Sung et al 2012)

Fig.6 is a perfect demonstration for the power of "Best Theory + High-res Expt Data" strategy. The HSL-2 PES was refined using HITRAN2008 based energy levels  $< 5300 \text{ cm}^{-1}$  (Huang et al 2011a,b), . It achieved 0.01-0.02 cm<sup>-1</sup> accuracy for most <sup>14</sup>NH<sub>3</sub> levels below 5500 <sup>-1</sup> or even 6000 cm<sup>-1</sup>, but band origins in 1.5-1.6µm region would degrade to about 1-2 cm<sup>-1</sup> (Huang, Schwenke & Lee 2011a). However, the inversion split predictions are still as accurate as  $\Delta_{Ames-Expt} = -0.001 \pm 0.024 \text{ cm}^{-1}$ . This is one order of magnitude smaller than the 0.140±0.124cm<sup>-1</sup> in UCL BYTe list (Yurchenko et al 2011), indicating higher accuracy and better consistency.

More importantly, by including a few higher energy levels experimentally determined at  $1.5-1.6\mu$ m region, the new HSL-Pre3 PES refinement successfully extended the 0.01-0.02 cm<sup>-1</sup> prediction accuracy to 7000 cm<sup>-1</sup> (Sung et al 2012). This means we can make more accurate predictions and spectra for even higher energy regions, i.e. providing more valuable reference data for experimental and astrophysical studies. Those data acquired at higher energies or from weaker bands will feed back to our strategy for the next cycle of improvement. Such kind of mutually beneficial interactions between theoreticians and experimentalists are critical for our approach, as we go far beyond simple reproduction of existing data. For our approach, prediction matters!

In Fig.7, the left panel shows the CO<sub>2</sub> isotopologue band origins are well reproduced without nonadiabatic corrections. This is different from the NH<sub>3</sub> case. But higher J (>30) rotational levels will need mass-dependent correction terms to get uniform  $\sigma_{RMS}$  from 626 to 828, as confirmed in our refinement tests (Huang et al 2017). In general, the <sup>17/18</sup>O substitution needs larger nonadiabatic corrections than <sup>13/14</sup>C.

The Ames-2016 CO2 line lists at 296K are compared with CDSD database (Tashkun et al 2015), with results shown in Fig.7 (b). It should be noted the intensity data in

CDSD are all based on EDM models fitted from experimental transmission measurements. The uncertainties are usually 1-20%. Some band intensities were pure predictions with no real measurement. Isotopologue inconsistency is not rare in EDM models, either. So the relative  $\Delta$ S% distribution is already satisfactory enough.



Figure 7. Accuracy of Ames  $CO_2$  IR lists (a) J=0 band origins of 13 isotopologues; (b) Statistics of line position deviations (left) and relative intensity deviations (right) for transitions (top) or bands (bottom), vs. CDSD (Tashkun et al 2015). Both are reprinted from Huang et al (2017), Copyright (2017), with permission from Elsevier.

The reliability and consistency of Ames IR list predictions comes from several aspects: use of an exact quantum rovibrational Hamiltonian within the Born-Oppenheimer approximation (plus nonadiabatic corrections when necessary), high quality ab initio PES and dipole moment surface (DMS), nonlinear least-squares refining algorithm applied to the most important short-range potential terms (usually up to quartic level). Both the PES and DMS formula are invariant to permutations of any two alike atoms. The polynomial expansion of all Ames DMS are about the pseudo point charges on nuclei, instead of fitting three dipole vectors which leads to 3 separate sets of dipole coefficients. This is closer to physical reality. Note the Ames  $CO_2$  lists match several state-of-the-art highly accurate IR intensity measurements within  $\pm 1\%$ , or better.



Figure 8.  ${}^{12}C^{16}O_2$  IR simulation at 4000K, Ames lists vs. CDSD-4000 (Tashkun & Perevalov 2011). Reprinted from Huang et al (2017), Copyright (2017), with permission from Elsevier.

One important check for prediction quality is IR simulations at high temperature comparing with experiments or other databases. Huang et al (2013) showed at 1773K,

Ames CO<sub>2</sub> lists are at least comparable or even better than EDM model based databases. In Fig.8, a recent 4000K comparison (Huang et al 2017) confirms that Ames IR lists are much more complete than the CDSD-4000 (Tashkun & Perevalov 2011) above 5800 cm<sup>-1</sup>. Additional rovibrational calculations at higher energy, 24000 - 44000 cm<sup>-1</sup>, will help improve Ames intensities so it can better compare with future high temperature spectra.



Figure 9. (a)  $CO_2$  728  $2v_3$  band, Ames (red) vs. JPL Expt. IR analysis residuals (blue). The band is missing in CDSD and HITRAN. Top: overall comparison; middle: intensity pattern matches; bottom: line position matches. The S(Ames) intensities are given in cm/molecule, and with 100% abundance.; (b) Differences on extrapolated (predicted)  $CO_2$  band origins, Ames vs. EH models (CDSD). Reprinted from Huang et al (2017), Copyright (2017), with permission from Elsevier.

Our complete set of Isotopologue line lists is very helpful in mixed isotopologue IR analysis, e.g. a  $CO_2$  728 band was found in JPL IR analysis residuals. See Fig.9a. But to ensure consistent accuracy in the high energy region, it is important for both experimentalists and theoreticians to collaborate through mutually beneficial interactions to determine highly accurate band origins, see Fig.9b, and reliable intensity measurements for those high lying weak bands.

Ames-296K Line lists for SO<sub>2</sub> isotopologues have also proven to be useful in mixed isotopologue IR analysis. The Ames IR line lists do provide more complete and consistent IR simulations, especially for those weak transitions or lower abundance isotopologue signals. Combining the Ames IR line lists for three SO<sub>2</sub> isotopologues, 626, 628 and 828, our mixed isotopologue IR simulation was able to provide more robust analysis for about 25 high-resolution IR features in a narrow window of 0.25 cm<sup>-1</sup>, plus a more reliable abundance ratio. On next page, Fig.10 illustrates how the observed iso-mixed IR features can be explicitly decomposed and re-assigned, e.g. the strong peak at 1340.00 cm<sup>-1</sup> was experimentally assigned to 628, but it is mainly a 828 transition. Detailed analysis can be found in Huang et al (2016).

# 3. Higher Level "Best Theory + High-res Expt. Data" Application: Best Spectroscopic Constants and Intensity for Isotopologues

Using the refined PES and ab initio DMS, we have computed IR lists for 30 isotopologues of SO<sub>2</sub>, i.e. 5 S isotopes from  ${}^{32}$ S to  ${}^{36}$ S x 6 combinations of two  ${}^{16/17/18}$ O atoms. This complete set can push the "Best Theory + High-res Expt Data" strategy



Figure 10. Ames-296K list based IR simulations (Top) vs. experimental spectrum analysis (Bottom). Discrepancies between the Ames analysis and the reported experimental assignments are as obvious as the very good agreement.  $\sigma = 0.001 \text{ cm}^{-1}$  in the Ames Gaussian convolution. Reprinted from Huang et al (2016). Copyright (2016), with permission from Elsevier.

to higher level, providing far more accurate predictions for the spectroscopic constants and intensity. Here we choose the  $SO_2$  pure rotational bands as an example.



Figure 11. Isotopologue intensity consistency of Ames SO<sub>2</sub> transition at 296K: (a) intensity ; (b) Einstein-A coefficient, and linear & quadratic fitting residuals .

#### Prediction Accuracy and Consistency of Ames IR Line Lists

At 296K, the <sup>*R*</sup>*R* J"<sub>*Ka,Kc*</sub>=12<sub>12,0</sub> are the strongest transitions of the GS<-GS and  $v_2 <-v_2$  bands. In Fig.11a, the nuclei spin statistical weights are excluded and the  $v_2 <-v_2$  intensities (x 1E21) are given on the lower right side. Intensity variations in both groups are explicitly correlated with isotope substitutions. Actually, the Einstein-A coefficients for the 30 isotopologues show a simpler linear correlation in Fig.11b. A linear fit  $\sigma_{rms}$  is 0.3%, and a simple quadratic fit can reduce it to 0.05% or less. What does it mean? It simply means the Ames (or similar) isotopologue IR lists have an intensity consistency obviously better than the experimental data based EDM models, and much smaller noise than experimental uncertainties. It is straightforward to identify bad intensity data or suspicious EDM models. In future, one can deliberately calibrate all Ames intensity predictions using a few highly accurate experimental intensity data.



Figure 12. Top panels: the S and O isotope effects are nearly linear on  $\Delta A/B/C$  constants. Lower panels are  ${}^{34}S^{16}O_2$  prediction using  ${}^{32}S^{16}O_2$  and  ${}^{33}S^{16}O_2$  data : left - best prediction accuracy for A/B/C and  $D_J$ ,  $D_{JK}$ ; middle and right - line position deviations are as small as 1-5 MHz with the "Predicted" lower order EH<sub>Ames</sub> terms.

We use SPFIT (Pickett 1991) to fit the Ames GS<-GS band of each isotopologue to the same EH model that CDMS adopted for 646 and 628, and computed the  $\Delta$  between Ames fitted and Expt-based EH parameters. The S and O isotope effects on  $\Delta A/B/C$  are nearly linear, see Fig.12 top panels. The A/B/C constants of all other isotopologues can be reliably predicted by combining the S and O isotope effects. This  $\pm 0.01$ -0.02 MHz accuracy represents a two orders of magnitude improvement.

Such "empirically corrected" Ames EH parameters will bring much more accurate line positions. Fig.12 bottom panels report a simple test: using  ${}^{32}S^{16}O_2$  and  ${}^{33}S^{16}O_2$ data to predict  ${}^{34}S^{16}O_2$  EH constants and line positions. The A/B/C and quartic terms are called "lower order" terms, while the rest are "higher order" terms. The left figure shows the isotope- $\Delta$  method did well on quartic terms, especially  $D_J$  and  $D_{JK}$ , but not impressive on the higher order part. For lower order terms, we have original EH<sub>Ames</sub> constants (denoted "Ames"), or the EH<sub>Ames</sub> constants corrected using the isotope- $\Delta$ relation (denoted "Predicted"). For higher order terms, we have either original EH<sub>Ames</sub> or EH<sub>Expt</sub>, denoted "Ames" or "Expt/CDMS", respectively. Combinations of lower and higher order terms gives different EH parameter sets, and SPCAT (Pickett 1991) uses it to predict  ${}^{34}S^{16}O_2$  line positions. Taking the original EH<sub>Expt</sub> model (i.e. "Expt/CDMS" + "Expt/CDMS") based positions as reference, the  $\Delta$  deviations of 3 EH sets are plotted in the right panels. The errors are as small as 1-5 MHz for most J $\leq$ 30, K<sub>a</sub><10-15 transitions. Note the high K<sub>a</sub> tail in the middle panel is a result of the EH<sub>Expt</sub> over extrapolation. A paper is in preparation for the ongoing, more thorough investigation.

### 4. Summary

Prediction oriented "Best Theory + High-res Expt. Data" Strategy has been improved and extended to  $NH_3$ ,  $CO_2$  and  $SO_2$  and their isotopologues. The accuracy, consistency and completeness of Ames IR line lists now provide more powerful tools in astrophysical spectroscopic analysis and simulations. It is critical to have mutually beneficial interactions among theoreticians, experimentalists, and observers. The 0.01-0.02 cm<sup>-1</sup> (IR) and 5 MHz (Microwave) accuracy will become the new "normal" for empirical IR lists contributing to the opacity community. The latest updates on weaker or higher energy bands, more accurate line positions or intensities, and new molecules are available at http://huang.seti.org.

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