

# HITRAN2020 supplementary material:

## Supporting information regarding the broadening of water vapor lines

### 1. Comparison of the MCRB calculations with experimental data

Figures 1a and 1b show the agreement of the MCRB calculations and the values from the prediction routine compared with the measurement database. Shown are the measured  $\nu_2$  transitions (blue open circle symbols with error bars), the MCRB calculated values (black solid circle symbols), and the prediction algorithm values (red open diamond symbols). The values are plotted against a “line count” which is a sequential line number if one ordered them on the descending magnitude of the MCRB half-widths. Figure 1a shows the air-broadened half-width in  $\text{cm}^{-1}\text{atm}^{-1}$  versus a line count and Fig. 1b is a similar figure for the line shifts. As can be seen, there is excellent agreement for both the MCRB calculated values and the predicted values.

### 2. Summary of water vapor line shape data

A summary of the water vapor line-shape data (assuming Voigt profile) considered for the HITRAN2020 data set is presented in Table S1. These data sets were taken and Python dictionaries were made using the ro-vibrational quantum numbers as the key. A Python algorithm was written that loads into memory, for all isotopologues of  $\text{H}_2\text{O}$ , the database dictionaries described above and then reads the HITRAN2020 water-vapor line file and selectively adds the line-shape data to each transition in the prioritized scheme discussed in the manuscript.

### References for supplementary material

- [1] N. Stolarczyk, F. Thibault, H. Cybulski, H. Józwiak, G. Kowzan, B. Vispoel, I.E. Gordon, L.S. Rothman, R.R. Gamache, P. Wcisło, . Evaluation of different parameterizations of temperature dependences of the line-shape parameters based on *ab initio* calculations: Case study for the HITRAN database. *Journal of Quantitative Spectroscopy and Radiative Transfer* 2020;240:106676. URL: <http://www.sciencedirect.com/science/article/pii/S0022407319304480>. doi:10.1016/j.jqsrt.2019.106676.

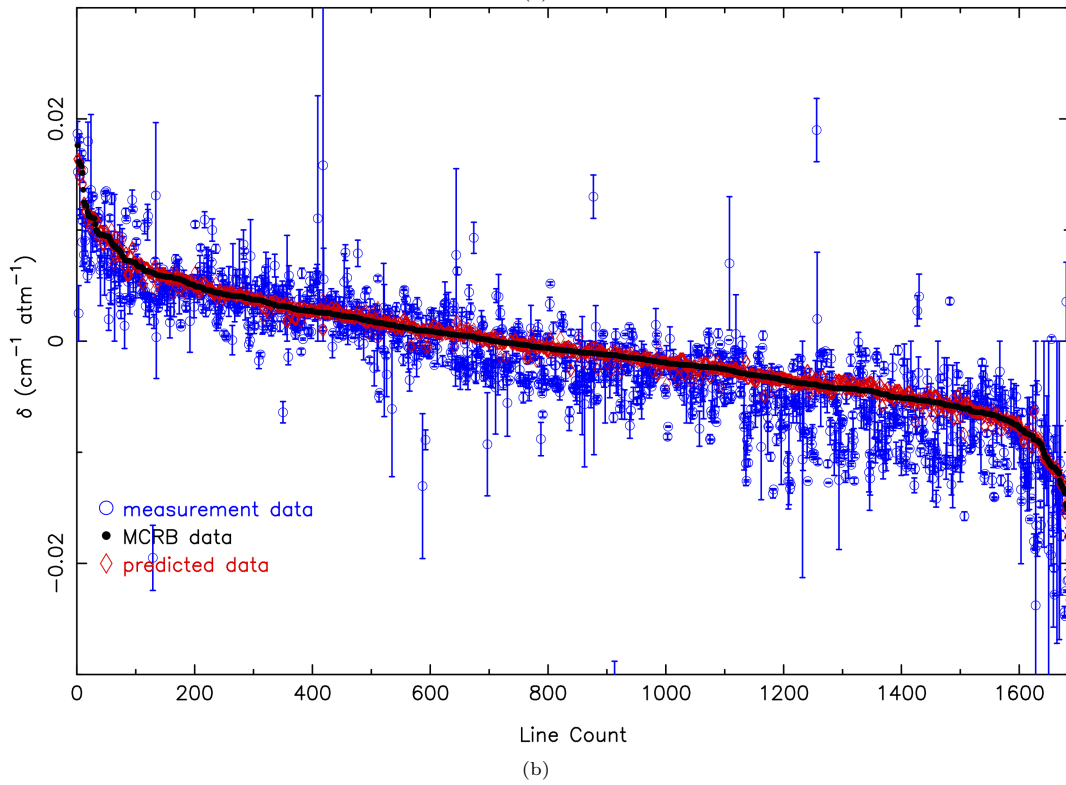
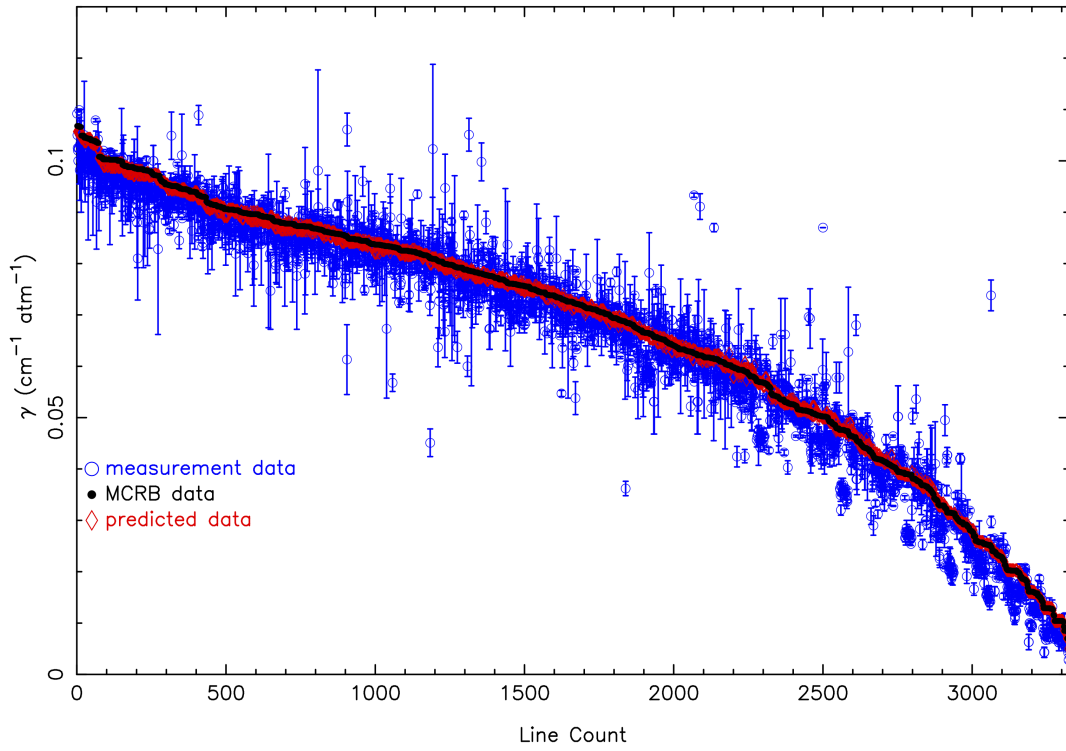


Figure 1: (a) half-widths and (b) line shifts in  $\text{cm}^{-1}\text{atm}^{-1}$  for transitions in the  $\nu_2$  band from the measurement database (blue open circle symbols with measurement error bars), the MCRB calculated values (black solid circle symbols), and values from the prediction algorithm (red open diamond symbols) versus a line count ordered on the magnitude of the MCRB half-widths.

Table S1: Summary of line-shape data for water vapor used for HITRAN2020.

$\gamma$ (H <sub>2</sub> O-air)	H <sub>2</sub> <sup>16</sup> O	H <sub>2</sub> <sup>18</sup> O	H <sub>2</sub> <sup>17</sup> O	HD <sup>16</sup> O	HD <sup>18</sup> O	HD <sup>17</sup> O	D <sub>2</sub> <sup>16</sup> O
Priority data	4681	4414	3391	3 172	919	722	
Intercomparison data	2629	2579	2076	16	16	16	
Single measured datum	5407	4477	2699	566	541	452	222
MCRB data	24 453	7116	3418	23 266	6599	4093	
Predicted data	133 123	18 446	7679	13 892	1215	456	
$J''$ Average values	145 593	5146	8281	15 518	1374	627	22 973
$\delta$ (H <sub>2</sub> O-air)							
Priority data	3600	3379	2553	2947	697	500	
Intercomparison data	701	700	678				
Single measured datum	3271	2795	1743				116
MCRB data	25 695	8282	4304	37 956	8590	5237	0
Predicted data	133 992	21 868	9983				
PL $n$ (H <sub>2</sub> O-air)*							
Priority data	4359	4100	3135	3025	772	575	
Intercomparison data	250	250	245	3	3	3	
Single measured datum	33	23	20				
MCRB data	26 167	8744	4605				
Predicted data	139 445	23 915	11 258				
$J''$ Average values	149 632	5146	8281	53 402	9889	5788	23 195
DPL $\gamma$ T dep (H <sub>2</sub> O-air)**							
MCRB data	29 207	11 706	6945				
Predicted data	140 778	25 265	12 280				
PL $\delta$ T dep (H <sub>2</sub> O-air)*							
MCRB data	25 286	9792	5753				
Predicted data	119 145	20 927	10 107				
DPL $\delta$ T dep (H <sub>2</sub> O-air)**							
MCRB data	29 229	11 714	6949				
Predicted data	140 771	25 256	12 289				
$\gamma$ (H <sub>2</sub> O-H <sub>2</sub> O)							
Intercomparison data	5358	5100	3661	118	90	24	
Single measured datum	16 859	11 703	5651	4533	1119	938	
MCRB data	1607	1526	1234	3741	3300	2200	1531
Rotation band data							15 853
Average values	296 062	23 849	16 998	48 038	6155	3404	5811

\* power law data

\*\* Gamache–Vispoel temperature dependence model. Not included in the official release of HITRAN2020, but will be evaluated for future updates. See Ref. [1] for parametrization of temperature dependencies.