RAS Techniques and Instruments

RASTAI **1,** 43–47 (2022)
Advance Access publication 2022 July 26

https://doi.org/10.1093/rasti/rzac004

Simple semiclassical model of pressure-broadened infrared/microwave linewidths in the temperature range 200–3000 K

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Accepted 2022 July 6. Received 2022 June 26; in original form 2022 March 30

ABSTRACT

There is a need for line-broadening parameters for molecules found in exoplanetary atmospheres for a variety of broadeners and a range of temperatures. The use of an easily handled semiclassical theoretical expression is suggested for the calculation of pressure-broadened linewidths for (vib)rotational transitions over a large temperature range (200–3000 K) starting from a minimal set of input parameters: kinetic molecular properties and the character of the leading term in the intermolecular interaction potential. Applications to NO and OH colliding with rare-gas atoms and non-polar molecules demonstrate good consistency with available measurements over the full temperature range indicated. The procedure therefore can be expected to provide realistic estimates for line broadening of 'exotic' molecules and molecular ions present in hot planetary atmospheres.

Key words: line profiles.

1 INTRODUCTION

The characterization and modelling of exoplanetary atmospheres require large volumes of laboratory spectroscopic data (Hedges & Madhusudhan 2016; Tennyson & Yurchenko 2018; Gandhi et al. 2020; Grimm et al. 2021). While there are a number of projects dedicated to the production of extensive line lists of molecular line positions and transition probabilities (Rey et al. 2016; Bernath 2020; Tennyson et al. 2020; Huang et al. 2021), the provision of the associated parameters to quantify the effects of line broadening is much less well developed. Simulations have demonstrated the need to deal correctly with line broadening in the atmospheres of exoplanets (Tinetti et al. 2012; Amundsen et al. 2014; Anisman et al. 2022). The provision of these line-broadening parameters was identified as the most important requirement by Fortney et al. (2019) in their review of needs for laboratory measurements and ab initio studies to aid understanding of exoplanetary atmospheres. While some crude attempts have been made to provide general procedures to produce the volume of line broadening data required, such as that by Barton et al. (2017), there is an outstanding need for these data for a wide range of molecules, temperatures and broadeners.

Current spectroscopic data need for studies of hot atmospheres include at least qualitative estimates of pressure-broadening parameters for many 'exotic' molecules and molecular ions, including those forming solely at very elevated temperatures. The variety of exoplanet atmospheres being probed suggest that while in gas giants the main perturbing partners are hydrogen (H_2) and helium (He), a whole range of other broadeners including carbon dioxide (CO_2), nitrogen (N_2), oxygen (O_2), water vapour (H_2O), carbon monoxide (CO), nitric monoxide (NO), methane (CH_4), and ammonia (NH_3) are of interest too. Laboratory studies of line-shape parameters are very scarce or totally missing for transitions at a both infrared/microwave (IR/MW) and visible/ultraviolet (UV) for the many spectroscopically active species that occur in the hot atmospheres found in many exoplanets. These species are being probed by instruments on-board space missions and ground-based telescopes.

In this paper, we suggest and test the use of a simple theoretical expression as the means of providing reasonable estimates of pressure-broadened linewidths of vibration–rotation and pure rotation transitions which largely lie in the IR/MW frequency domain.

2 WORKING FORMULA

The line shapes of exoplanet vibration–rotation spectra are generally modelled using Voigt profiles, which assume statistical independence of two main broadening mechanisms: Doppler broadening due to the thermal motion of the spectroscopically active species and pressure broadening induced by collisions with surrounding particles. Consequently, the Voigt profile is a convolution of a Gaussian profile characterized by a Doppler width (straightforward to compute) and of a Lorentzian profile having a pressure-broadening width which depends on the active molecule (a), the perturber (p), and the temperature (T). In principle, this pressure-broadening width also varies between individual transitions. Here, we simply consider means of estimating its value and temperature dependence for different collision pairs.

Unlike electronic absorption bands, line shapes of vibration–rotation and pure rotation transitions are mostly influenced by inelastic collisions, i.e. those inducing non-radiative transitions among the internal states of the active molecule. This key feature was first noted by Anderson (1949), who included 'on-resonance' exchange of energy quanta between pairs of levels in the identical active and

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Table 1. Tabulated kinetic diameters (or Lennard–Jones parameters) used in calculations, taken from ‘12Ba’ (Baker 2012), ‘82KhBo’ (Khayar & Bonamy 1982), and ‘14JaMi’ (Jasper & Miller 2014).

	NO	OH	N_2	O_2	H_2	He	Ar
d (pm)	317 [12Ba]	336[a] [82KhBo]	368 [14JaMi]	346 [14JaMi]	292 [14JaMi]	258 [14JaMi]	333 [14JaMi]
$m_{a/p}$ (amu)	30	17	28	32	2	4	40

[a] Deduced from OH–N_2 (Khayar & Bonamy 1982) and N_2 (Jasper & Miller 2014) data by combination rules.

perturbing molecules. Later, Anderson’s theory was systematized and extended to non-resonant interactions by Tsao & Curnutte (1962) to give what is now called the ATC approach. In their analysis of the close-collisions contribution to the second-order scattering matrix S_2 responsible for line broadening, these authors derived an approximate expression for γ, the collisional half-width-at-half-maximum (HWHM) of intensity, as a sum of two terms.

The first term comes from ‘strong’ collisions corresponding to small values of the impact parameter b. As such collisions interrupt the radiation completely as the active molecule leaves its initial state, here S_2 is set to 1 and the critical (‘cut-off’) value b_0 for the impact parameter is defined by the condition $S_2(b_0) = 1$. Assuming the same b_0 for all rotational states of the perturber, calculation of the cross-section $\sigma = \int S_2(b)\, 2\pi b db$ for b ranging from 0 to b_0 gives $\gamma = nv\sigma/(2\pi c)$ in cm^{-1} which leads to

$$\gamma_{0\to b_0} = \frac{nv}{2c} b_0^2, \tag{1}$$

where n is the number density of perturbing particles, v is the mean relative speed, and c is the speed of light. The second term, the contribution from ‘weak’ (distant) collisions corresponding to $b > b_0$, can be estimated from the $S_2(b)$ dependence of the leading interaction in the anisotropic intermolecular potential, which typically varies as b^{-m} (m = 4, 6, 8, 10 for dipole–dipole, dipole–quadrupole, quadrupole–quadrupole, and dipole-‘induced dipole’ interactions, respectively), so that

$$\gamma_{b_0\to\infty} = \frac{nv}{(m-2)c} b_0^2. \tag{2}$$

We emphasize that the m-value should not be confused with the power q of the inverse intermolecular-distance dependence in the interaction-potential R^{-q}: for the straight-line trajectories used by Anderson they are related by $m = 2(q - 1)$. Taking account of the full b-range results in

$$\gamma = \frac{m}{(m-2)} \frac{nv}{2c} b_0^2. \tag{3}$$

This expression can be made more explicit by using n corresponding to 1 atm and the dependence of v on the absolute temperature T (in K) and on the masses of the active (m_a) and perturbing (m_p) molecules (in Dalton):

$$n = \frac{N_a}{V_{1\text{mole}}} = 7.3385 \times 10^{21} \frac{1}{T}\ \text{cm}^{-3}, \tag{4}$$

$$v = \sqrt{\frac{8kT}{\pi m^*}} = 1.455 \times 10^4 \sqrt{T} \sqrt{\frac{m_a + m_p}{m_a m_p}}\ \text{cm s}^{-1}, \tag{5}$$

where the standard notations are employed for the Avogadro number N_A, one-mole volume $V_{1\text{mole}}$, and Boltzmann’s constant k. Substituting the above formulae in equation (3) and assuming b_0 is given in picometres, we get the half-width in the commonly used units of $\text{cm}^{-1}\ \text{atm}^{-1}$:

$$\gamma = 1.7796 \times 10^{-5} \frac{m}{(m-2)} \frac{1}{\sqrt{T}} \sqrt{\frac{m_a + m_p}{m_a m_p}} b_0^2. \tag{6}$$

The remaining point concerns the choice of a reasonable estimate for b_0. Tsao & Curnutte (1962) suggested using the kinetic diameter d as b_0. Although d is a characteristic averaged over all collisions, in the following we test this choice for various kinds of molecular pairs.

3 APPLICATION TO NEUTRAL MOLECULES

Line lists for open-shell diatomics NO (Qu et al. 2021) and OH (Bernath 2020) are included in the ExoMol database (Tennyson et al. 2020); these species were chosen as active molecules. Their permanent electric dipole moments differ by an order of magnitude: μ_{NO} = 0.158 D (Stogryn & Stogryn 1966) and μ_{OH} = 1.668 D (Meerts & Dymanus 1973). This allows us to test both cases of weakly polar and strongly polar active molecules. Moreover, experimental linewidths are available for these species perturbed by different partners over wide temperature ranges which allows comparisons with our predictions. Here, we consider N_2, O_2, H_2 (with the quadrupole moments $Q_{N_2} = -1.52$ DÅ, $Q_{O_2} = -0.39$ DÅ, $Q_{H_2} = 0.66$ DÅ (Stogryn & Stogryn 1966)) but also He and Ar [polarizabilities $\alpha_{\text{He}} = 0.208$ Å^3, $\alpha_{\text{Ar}} = 1.662$ Å^3 (Olney et al. 1997)] as representative perturbers for astrophysical applications. Additionally, this choice of species also provides a check on the influence of the perturber/radiator mass ratio. We need to consider two types of leading interactions: dipole–quadrupole (m = 6) for perturbation by N_2, O_2, H_2, and dipole-‘induced dipole’ (m = 10) for perturbation by He and Ar. The corresponding half-widths follow from equation (6):

$$\gamma = 2.6694 \times 10^{-5} \frac{1}{\sqrt{T}} \sqrt{\frac{m_a + m_p}{m_a m_p}} d^2 \quad \text{for} \quad m = 6, \tag{7}$$

$$\gamma = 2.2245 \times 10^{-5} \frac{1}{\sqrt{T}} \sqrt{\frac{m_a + m_p}{m_a m_p}} d^2 \quad \text{for} \quad m = 10. \tag{8}$$

For our case of different active and perturbing molecules, the kinetic diameter should be taken as a sum of kinetic radii of collision partners: $d = (d_a + d_p)/2$. The values of d_a and d_p used in our calculations are gathered in Table 1. In the cases, where kinetic diameters were unavailable, Lennard–Jones parameters σ_{LJ} were used instead.

Theoretical estimates obtained with equations (7, 8) and the data of Table 1 are compared to experimental values in Table 2. It is worth mentioning that experimental data for (vib)rotational transitions in the IR/MW regions generally demonstrate quite pronounced dependence on the rotational quantum number (except when the perturber is very light, such as He and H_2), so we selected ‘mean’ experimental results (corresponding to intermediate values of the rotational quantum number or averaged on the rotational numbers). For almost all the molecular pairs considered and all temperatures, very satisfactory agreement is found. The one exception is the NO–He case, where the theoretical estimate is double the measured value. This discrepancy can be ascribed to the small values of the NO dipole moment and He polarizability as well as to the small He mass: the dipole-

Table 2. Comparison of estimated collisional half-widths γ (in cm^{-1} atm^{-1}) with measurements. Experimental data are taken as averaged or characteristic values for mid-range rotational quantum numbers. Calculated values between parentheses correspond to the kinetic 'hard-sphere' model. The experimental data are from '83HoBo' (Houdeau et al. 1983), '19AlSu' (Almodovar et al. 2019), '99AlDaMa' (Allout et al. 1999), '91LiLiLi' (Liu et al. 1991), '99PaZiCh' (Park et al. 1999), '96PaZi' (Park et al. 1996), '91ChJe' (Chance et al. 1991), '79BaBr' (Bastard et al. 1979), '79BuCl' (Burrows et al. 1979), and '17Da' (Dagdigian 2017).

		N_2		O_2		H_2		He		Ar	
		calc.	expt	calc.	expt	calc.	expt	calc.	expt	calc.	expt
NO	163 K	0.065 (0.043)	0.080 [83HoBo]	0.058 (0.039)	0.095[a]						
	296 K	0.048 (0.032)	0.055 [19AlSu]	0.043 (0.029)	0.050 [99AlDa]			0.057 (0.046)	0.024[c] [91LiLi]	0.033 (0.026)	0.040 [19AlSu]
	802 K	0.029 (0.019)	0.024 [19AlSu]							0.020 (0.016)	0.017 [19AlSu]
	1000 K	0.026 (0.017)	0.025 [19AlSu]							0.018 (0.014)	0.015 [19AlSu]
OH	194 K	0.073 (0.049)	0.112[b] [99PaZ]i	0.055 (0.037)	0.067 [99PaZi]	0.141 (0.094)	0.108 [99PaZi]	0.078 (0.062)	0.019 [99PaZi]	0.052 (0.042)	0.070 [96PaZi]
	296 K	0.059 (0.039)	0.068 99PaZi	0.045 (0.030)	0.050 [91ChJe] 0.035 [99PaZi]	0.114 (0.076)	0.104 [79BaBr] 0.089 [99PaZi]	0.063 (0.050)	0.076 [79BaBr] 0.015 [99PaZi]	0.042 (0.034)	0.050 [79BuCl]
	500 K									0.032 (0.026)	0.045[d] [17Da]

[a] Theoretical result (Buldyreva et al. 2001) giving a good agreement with room-temperature measurements (Allout et al. 1999).
[b] Data for very low rotational quantum number.
[c] Obtained for ^{15}NO.
[d] Quantum scattering calculations for MW transitions averaged over rotational quantum numbers.

'induced dipole' term is unable to mimic the NO-He interaction within the classical-path approximation. However, with increasing temperature the use of classical trajectories becomes better justified, so even for perturbation by He equations (7) and (8) as well as the general expression of equation (6) are expected to yield predictions of accuracy better than 50 per cent. We note that for the strongly polar OH radical the use of equation (8), even for the light collision partner He, leads to a reliable approximation of the intermolecular interaction by the leading term judged by comparison with the experimental data (Bastard et al. 1979) at 296 K. The measurements provided for OH by Park et al. (1999) are significantly lower than the results of other authors, so we consider the factor of 4, difference found between their measurements for OH–He and our theoretical value at 194 K to be questionable. Finally, the power -0.5 for the T-dependence given by equation (6) is confirmed for NO–N_2 and NO–Ar by the measurements of Almodovar et al. (2017) over the temperature interval 1000–3000 K.

For completeness, we note that in the absence of measured and/or calculated line-broadening data some authors use a formula arising from the kinetic gas theory (Dodge et al. 1980; Murzyn et al. 2022). Indeed, the mean frequency of molecular collisions, i.e. the average number of collisions per second or the inverse of the free path time τ, can be written as

$$\tau^{-1} = \pi \varnothing^2 n v, \tag{9}$$

where $\varnothing$ denotes the collision diameter (called also optical diameter) and the other variables have the same meaning as in equation (1). equation (9) assumes that the foreign-gas pressure is much higher than the pressure of the active gas, so that no collisions occur between pairs of active molecules. τ^{-1} gives the collisional line half-width in angular frequency units. Converting this half-width into cm^{-1} at 1 atm pressure, we get

$$\begin{aligned}\gamma_{\text{kin}} &= \frac{\tau^{-1}}{2\pi c} = \frac{n}{2c}\sqrt{\frac{8kT}{\pi m^*}}\varnothing^2 \\ &= 1.7796\times 10^{-5}\frac{1}{\sqrt{T}}\sqrt{\frac{m_{\text{a}}+m_{\text{p}}}{m_{\text{a}}m_{\text{p}}}}\varnothing^2.\end{aligned} \tag{10}$$

As mentioned by Weisskopf (1933), the collision diameter $\varnothing$ is much larger than the kinetic diameter d. For example, the use of equation (10) in fits of Lorentzian lines in the $\gamma(0, 0)$ band of NO perturbed by N_2, CO_2, CO, CH_4, and Ar (Dodge et al. 1980) resulted in the optical collisions diameters about three times bigger than literature values obtained from viscosity measurements. However, the current point of view (Kunze et al. 2022) is rather that different kinds of 'molecular diameters' manifest themselves in different physical processes and are probed by different experimental techniques, so that the term 'collision diameter' is also used as an equivalent of 'kinetic diameter' (Albrecht et al. 2003). Assuming the equivalence of d and $\varnothing$, equations (6) and (10) differ solely by the ratio $m/(m-2)$ which 'corrects' the kinetic ('hard-sphere') approach by accounting for the leading intermolecular interaction term. The line half-widths obtained by equation (10) are given in parentheses as calculated values in Table 2. They demonstrate less good agreement with the measurements, therefore the use of equation (6) is clearly preferable.

It should be also noted that for kinetic/collision diameters not measured experimentally, Loukhovitski & Sharipov (2021) suggested a semi-empirical formula for their calculation from electronic polarizabilities: $d = p_1 + p_2\alpha^{1/3}$, where $p_1 = 0.768$ Å and $p_2 = 2.168$ (d here is obtained in Å and should be multiplied by 100 to be expressed in pm). This formula gives a d-estimate coinciding with the value of Table 1 for Ar, slightly different results for N_2, O_2, H_2, and a nearly 20 per cent lower value for He. However, for small-

Table 3. Comparison of estimated collisional half-widths γ (in $\mathrm{cm^{-1}\ atm^{-1}}$) with measurements or independent calculations for ionic active molecules in collision with H_2, He, and Ar.

	Calculation with equations (7) or (11)	expt/other
NO^+-H_2 300K	0.078 ($d = 264$ pm)	0.05^a (López-Puertas et al. 2006)
	0.083 ($d = 271$ pm)	
HCO^+-H_2 100 K	0.180 ($d = 304$ pm)	0.750^b (Anderson et al. 1980)
HCO^+-H_2 300 K	0.104 ($d = 304$ pm)	0.310 (Liao & Herbst 1996)
HCO^+-He 88 K	0.111 ($d = 287$ pm)	0.313^c (Buffa et al. 2008)
HCO^+-Ar 77 K	0.069 ($d = 324.5$ pm)	0.369^c (Buffa et al. 1994)

[a] Rough estimate from fig. 2 of López-Puertas et al. (2006).
[b] $J = 1 - 0$ line.
[c] $J = 4 - 3$ line,

size collision partners considered here, the diameters are generally available from measurements, so that the semi-empirical formula given above can be more useful for considering large polyatomic collision partners.

4 IONIC MOLECULES

It is also important to consider molecular ions whose spectra and hence line broadening are thought to become important at the top of exoplanetary atmospheres (Bourgalais et al. 2020). Observation of rotational spectra of molecular ions (Woods 1983, and references therein) demonstrates that their pressure-broadened linewidths are similar or slightly larger than those of corresponding neutral molecules.

Most semiclassical theories published in the literature deal with neutral species. However, Buffa et al. (1994) extended semiclassical Anderson–Tsao–Curnutte (ATC) theory to the case of molecular ions colliding with neutral perturbers. They argued that the interaction between the ion charge and the multipole moments (permanent or induced) of the perturber does not contribute to collisional broadening but affects the trajectory (if curved trajectories are used instead of the straight-line paths) and induces a polarization on the neutral collision partner. This is the dipole moment induced on the perturber by the ionic monopole which interacts with the dipole moment of the ionic monopole and gives the dominant contribution to the collisional broadening in the case of HCO^+ colliding with Ar, for example. The dipole-‘monopole-induced dipole’ interaction varies as R^{-5}, and we get

$$\gamma = 2.3728 \times 10^{-5} \frac{1}{\sqrt{T}} \sqrt{\frac{m_{\mathrm{a}} + m_{\mathrm{p}}}{m_{\mathrm{a}} m_{\mathrm{p}}}} d^2 \quad \text{for } m = 8. \tag{11}$$

If the collision partner is a non-polar diatomic (e.g. H_2), equation (7) for dipole–quadrupole interactions applies.

We have attempted some linewidth estimates (Table 3) for ionic active molecules interacting with homonuclear diatomics (H_2) and rare gases (He and Ar). Molecular ions NO^+ and HCO^+ with permanent dipole moments absorbing in the IR/MW regions were chosen. However, for these molecular systems measurements and advanced calculations published in the literature correspond to low temperatures (typically far below room temperature), where semiclassical approaches lose their validity. In particular, orbiting collisions (capture effects) not accounted for by the ATC approach occur, so that our estimates are already expected to be lower than measurements. A possible criterion to check the applicability of semiclassical treatment for a given temperature is the isotropic potential depth ε (in K). For temperatures higher than ε, the relative kinetic energy is large enough for capture effects to be negligible. If the temperature becomes close to or even smaller than ε, an increasing number of molecular complexes is formed and the ATC linewidth is (strongly) underestimated. When available in the literature, we indicated the ε values for the molecular pairs considered, which allows one to evaluate the applicability of semiclassical treatments.

For the NO^+–H_2 pair the diameter was taken as $d = 264$ pm (estimated from fig. 6 of Cabrera-González et al. 2020) as the intermolecular distance corresponding to zero isotropic potential). A more recent study by Orek et al. (2021) of the NO^+–H_2 potential energy surface gives a slightly different value $d = 271$ pm (estimated from their fig. 5). With respect to a visual estimation 0.05 $\mathrm{cm^{-1}\ atm^{-1}}$ from atmospheric spectra (López-Puertas et al. 2006), our estimates with both diameters have the same order of magnitude. We note that the isotropic potential depth for the NO^+–H_2 complex is about 400 $\mathrm{cm^{-1}}$ (Cabrera-González et al. 2020), i.e. about 575 K, meaning that the condition for the applicability of semiclassical approaches is not obeyed at 300 K.

In the HCO^+–H_2 case, $d = 316$ pm was deduced for HCO^+ from the intermolecular distance of 287 pm corresponding to the zero isotropic potential of the HCO^+–He system (Buffa et al. 2009) and $d = 258$ pm for He (Table 1); the diameter for the HCO^+–H_2 pair was found therefore to be $d = 304$ pm. For this system, the linewidth $\gamma = 29.6\ \mathrm{MHz\ Torr^{-1}} = 0.750\ \mathrm{cm^{-1}\ atm^{-1}}$ of the $J = 1$–0 transition was measured at 100 K (Anderson et al. 1980), which is four times bigger than $\gamma = 0.180\ \mathrm{cm^{-1}\ atm^{-1}}$ calculated by equation (7). γ’s measured by Liao & Herbst (1996) unexpectedly gave values three times larger than those found for neutral targets; however, their ATC calculations with more terms in the anisotropic potential finally gave satisfactory agreement with experiment (Anderson et al. 1980). The ATC result of Liao & Herbst (1996) for 300 K (0.310 $\mathrm{cm^{-1}atm^{-1}}$ deduced from their Fig. 2a) is also three times bigger than our estimate with equation (7) of 0.104 $\mathrm{cm^{-1}atm^{-1}}$.

Collisional broadening of HCO^+–He rotational lines at 88 K was measured by Buffa et al. (2008). Their linewidth for the $J = 4$–3 transition (0.313 $\mathrm{cm^{-1}atm^{-1}}$) is again three times larger than the value calculated by equation (11) with $d = 287$ pm (Buffa et al. 2009). The isotropic-potential depth (Buffa et al. 2009) is 277.4 $\mathrm{cm^{-1}}$ or 399 K, so that the applicability of semiclassical treatment is strongly violated. With Ar as the collision partner, the experimental value for the same transition at 77 K is 14.56(7) $\mathrm{MHz\ Torr^{-1}} = 0.369\ \mathrm{cm^{-1}atm^{-1}}$ (Buffa et al. 1994), whereas our calculation with $d = (316 + 333)/2$ pm $= 324.5$ pm yields 0.069 $\mathrm{cm^{-1}atm^{-1}}$, underestimated by a factor of 5. For HCO^+–Ar at 77 K, Buffa et al. (1999) communicated the average capture radius value of 8.7 Å, which explains this underestimation.

These comparisons with low-temperature measurements demonstrating regular underestimates of line broadening for ionic active molecules confirm the internal coherence of the model: It does not work for temperatures where it is not expected to work. At high temperatures characteristic of hot planetary atmospheres the conditions of applicability of semiclassical approaches are amply satisfied, and linewidth estimates provided by equation (11) for He, Ar or by equation (7) for H_2 are believed to be quite realistic.

5 CONCLUSION

We propose the use of a simple semiclassical formula for rough estimates of collisional broadening for (vib)rotational molecular transitions occurring at infrared and microwave wavelengths when neither measurements nor calculations are available. Only kinetic molecular diameters and the type of the leading intermolecular interaction are required to get the correct order of magnitude for pressure-broadened linewidths, as demonstrated for neutral active species NO and OH colliding with rare gases and non-polar diatomics in a wide temperature range relevant to hot planetary atmospheres. A theoretical basis is also presented to extend the use of the model to ionic molecules. This approach will be incorporated into an updated ExoMol diet (Barton et al. 2017) to providing default line-broadening parameters when none are available from other sources.

ACKNOWLEDGEMENTS

This work was supported by the European Research Council under Advanced Investigator Project 883830. JB acknowledges the mobility grant provided by the Region Bourgogne-Franche-Comté for her visit to UCL.

DATA AVAILABILITY

All data are included in the article

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