ExoMol molecular line lists: IX The spectrum of AlO

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ABSTRACT

Accurate line lists are calculated for aluminium monoxide covering the pure rotation, rotation-vibration and electronic (B – X blue-green and A – X infrared bands) spectrum. Line lists are presented for the main isotopologue, $^{27}$Al$^{16}$O, as well as for $^{27}$Al$^{17}$O, $^{27}$Al$^{18}$O and $^{26}$Al$^{16}$O. These line lists are suitable for high temperatures (up to 8000 K) including those relevant to exoplanetary atmospheres and cool stars. A combination of empirical and ab initio methods is used: the potential energy curves were previously determined to high accuracy by fitting to extensive data from analysis of laboratory spectra; a high quality ab initio dipole moment curve is calculated using quadruple zeta basis set and the multi-reference configuration interaction (MRCI) method. Partition functions plus full line lists of transitions are made available in an electronic form as supplementary data to this article and at www.exomol.com.

Key words: molecular data; opacity; astronomical data bases: miscellaneous; planets and satellites: atmospheres; stars: low-mass

1 INTRODUCTION

Aluminium monoxide (AlO) is an interesting astronomical species whose spectrum is prominent in a new class of Nova-stars first discovered by Tenenbaum & Ziurys (2009) of which the most prominent examples are probably V838 Mon and V4332 Sgr (Merrill et al. 1962; Bernard & Gravina 1984; Banerjee et al. 2005; Tylenda et al. 2003; Banerjee et al. 2012). These two objects defined a new type of eruptive variables called intermediate luminosity red transients and the observational data showed the intense presence of the near-infrared A – X system of the AlO radical. Indeed this A – X band is also found to be fairly prominent in a variety of cool, oxygen rich stars (Bernard & Gravina 1984; Banerjee et al. 2012); besides the Mira variables discussed above AlO emissions were also observed in the OH/IR stars and two bright infrared sources (Banerjee et al. 2012).

Transitions in the blue-green B – X system have been observed in sunspots (Sriramachandran et al. 2013) and the red supergiant VY Canis Majoris (Kaminski et al. 2013), in which millimeter-wave rotational transitions have also been observed (Tenenbaum & Ziurys 2009). Finally, AlO spectra have been used to try and determine abundance of the long-lived, radioactive $^{26}$Al isotope (Banerjee et al. 2004).

Terrestrially AlO emissions arise from rocket exhausts in the atmosphere (Johnson 1965; Knecht et al. 1994). Its spectrum is also extensively used in the laboratory to monitor AlO in plasmas and other applications (Bescos et al. 1994; Naulin & Costes 1999; Glumac et al. 2001; Zhang & Li 2003; Bai et al. 2014; Surmick & Parigger 2014).

These applications, combined with technological uses of AlO spectra, have motivated a number of laboratory studies which have produced molecular constants characterising the lowest three states of AlO $X^2\Sigma^+$, $A^2\Pi$ and $B^2\Sigma^+$. There have also been attempts to produce line lists. Parigger & Hornkohl (2011) constructed a comprehensive line list for the X – B system for temperatures up to 6000 K but did not provide a transition dipole, so all their transition intensities are only relative. Launila & Berg (2011) performed a combined analysis of the A – X and B – X band systems involving 21 500 lines; we compare with some of their results below. There is, however, no single line list that combines a comprehensive set of transition frequencies with an accurate model for the transition intensities. It is this that we aim to do here as part of the ExoMol project. ExoMol aims to provide line lists of spectroscopic transitions for key molecular species which are likely to be important in the atmospheres of extrasolar planets and cool stars; its aims, scope and methodology have been summarised by Tennyson & Yurchenko (2012). Line lists for $^{2}\Sigma^+$ XH molecules, X = Be, Mg, Ca, have already been published (Yadin et al. 2012), as well as for a number of closed-shell diatomics (Barton et al. 2013, 2014; Yorke et al. 2014). In the present paper, we present rotation-vibration transition lists and associated spectra for AlO. These line lists are particularly comprehensive and should be valid for temperatures up to 8000 K.
2 METHOD

Rotation-vibration line lists for the three lower electronic states of AlO were obtained by direct solution of the nuclear motion Schrödinger equation using program Duo (Yurchenko et al. 2013). The calculations require both a potential energy curve (PEC) for each of the three states considered and also couplings between these curves. These curves were taken from our previous study (Patrascu et al. 2014), which computed ab initio potential energies, spin-orbit and electronic angular momenta couplings, and refined them using available experimental data. Nuclear motion calculations using these refined curves showed that the observed transition frequencies and energy levels could be reproduced with root mean square error of only 0.07 cm⁻¹. In order to cover all vibrational excitations below 35,000 cm⁻¹, we have increased the sizes of the vibrational basis set to 90 for each of the X, A, and B states from those used by Patrascu et al. (2014). The ranges of rotational excitations are listed in Table 2.

2.1 Dipole moments

There appears to be no experimental measurements of any AlO transition dipoles. For this reason we constructed new dipole moment curves (DMC) using high level ab initio calculations. These are compared to previous, high-level ab initio determinations (Zenouda et al. 1999) below. The ab initio calculations were performed using MOLPRO (Werner et al. 2010); we used multi-reference configuration interaction (MRCI) methods with different choices of basis sets. Our optimal basis choice was aug-cc-pVQZ; the active space used in MOLPRO representation was (9,4,4). Electronic dipole moments as function of bondlength, R, were computed as the expectation value

$$\mu(R) = e \langle \Psi_M | \sum_i \mathbf{r}_i | \Psi_N \rangle,$$

where the integral and the summation run over the electron coordinates, denoted by \( \mathbf{r}_i \), and \( e \) is the charge of the electron. For permanent dipole moments, the electronic wave-functions in the bra and ket are the same, ie \( M = N \), and the dipole moment, which is denoted \( \mu(M) \) below, also contains a term due to permanent nuclear charge. For transition dipole moments, \( M \neq N \), and the dipole is denoted \( \mu(M - N) \) below. For transition dipole moments, care must be taken to ensure that the dipole phases are consistent as a function of \( R \) (Tennyson 2014; Patrascu et al. 2014).

Our calculations produce the values for the dipole at equilibrium given in Table 1, which compare well to the previous results obtained by Zenouda et al. (1999). Our ground state value of the dipole and that of Zenouda et al. (1999) are both slightly smaller than the value 4.60 D used in the JPL database (Pickett et al. 1998), which was taken from the earlier calculations of Lengsfield & Liu (1982).

Figures 1 and 2 compare our calculated diagonal and off-diagonal DMCs, respectively, with those of Zenouda et al. (1999). The agreement is good. Our calculations suggest that the \( \mu(B-A) \) DMC is small at all geometries meaning that the B – A band will be very weak; a similar conclusion was reached by Partridge et al. (1983). The ab initio DMC grid points were used directly in Duo to produce a line list for AlO.

There is a lack of experimental data on AlO transition dipoles or transition intensities. Table 2 therefore compares the lifetime for the \( \text{B} \rightarrow \text{X} \) state with experimental data available from Johnson et al. (1972); Dagdigian et al. (1977) and two ab initio estimates from Partridge et al. (1983). For Partridge et al. (1983) we have taken their figures which include the small contribution from the weak \( \text{B} \rightarrow \text{A} \) decay channel since this contribution is also included in our estimate. Our lifetimes were computed by summing over all decays from a given \( \text{B} \rightarrow \text{X} \) state in Debye at \( R = 1.76 \text{ Å} \).

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Table 2. Radiative lifetimes (nsec) for B$^2\Sigma^+$ state of AlO, compared to the measurements of Johnson et al. (1972) and Dagdigian et al. (1973), and the two separate calculations of Partridge et al. (1983).

| Vibrational Level | This work | Partridge et al. (1983) I | Partridge et al. (1983) II | Johnson et al. (1972) | Dagdigian et al. (1975) |
|-------------------|-----------|---------------------------|---------------------------|----------------------|------------------------|
| 0                 | 92.4      | 88.1                      | 109.4 ± 6                 | 128 ± 6              | 1060 ± 7               |
| 1                 | 94.5      | 90.5                      | 112.6 ± 7                | 125 ± 3              | 102 ± 7                |
| 2                 | 96.7      | 93.0                      | 115.2 ± 7                | 130 ± 7              | 102 ± 4                |

Figure 2. Ab initio transition dipole moment curves for AlO linking the lowest three electronic states. The previous calculations by Zenouda et al. (1999) are represented by crosses.

Figure 3. Computed spectra of $^{27}\text{Al}^{16}\text{O}$ at $T=298$ K given as sticks with the intensity (cm molecule$^{-1}$) represented by their height. Upper panel: rotational region; lower panel: vibrational fundamental.

2.2 Partition function

Partition functions for AlO were calculated by summing all the calculated energy levels below using DuO (Yurchenko et al. 2013). When summing these levels it is necessary to multiply by the appropriate degeneracy factors. Since we follow HITRAN (Fischer et al. 2003) and use the full nuclear spin degeneracy, the degeneracy factor, $q$, is given by $(2J+1)(2I_A+1)(2I_O+1)$ where $J$ is the total angular momentum quantum number obtained by adding the rotational and spin angular momenta. $I_A$ and $I_O$ are the nuclear spins of the isotopes of Al and O in the given isotopologue. Explicit inclusion of these nuclear spin factors accounts for hyperfine effects which we make no attempt to resolve. These factors are 11, 6, 1, 6 and 1 for $^{26}\text{Al}$, $^{27}\text{Al}$, $^{16}\text{O}$, $^{17}\text{O}$ and $^{18}\text{O}$, respectively.

Table 3 compares our results for $^{27}\text{Al}^{16}\text{O}$ with those of Sauval & Tatum (1984). We have multiplied the results of Sauval & Tatum (1984) by the appropriate nuclear spin factors to bring their results into line with our convention outlined above. Table 3 shows good agreement between our $^{27}\text{Al}^{16}\text{O}$ partition function and that given by Sauval & Tatum (1984) at temperatures above 1000 K for which their results are valid. At lower temperatures we also agree well with the partition function given by JPL (Picknett et al. 1994) who, for example, give $Q(300) = 3966.43$ which is slightly lower than our value of 3966.90, probably due to neglect of the contribution of excited vibrational states.

As we use all ro-vibrational energy levels there are no issues with convergence of this sum. We follow Vidler & Tennyson (2000) and represent our partition function using the following functional form

$$\log_{10} Q(T) = \sum_{n=0}^{8} a_n [\log_{10} T]^n$$

where the fitting parameters $a_n$ are given in Table 2. These fits reproduce the partition functions for the entire region below 9000 K with a relative root-mean-square (rms) errors of better than 1.6%.

2.3 Line list calculations

Line lists were calculated for the four isotopologues $^{27}\text{Al}^{16}\text{O}$, $^{27}\text{Al}^{18}\text{O}$, $^{27}\text{Al}^{17}\text{O}$, and $^{26}\text{Al}^{18}\text{O}$. All rotation-vibration states were considered and transitions satisfying the dipole selection rule $\Delta J = 0, \pm 1$. These line lists span frequencies up to 35 000 cm$^{-1}$ ($\lambda > 0.286$ $\mu$m). The procedure described above was used to produce line lists, i.e. catalogues of transition frequencies $\nu_{ij}$ and Einstein coefficients $A_{ij}$, for four Aluminium oxide isotopologues $^{27}\text{Al}^{16}\text{O}$, $^{27}\text{Al}^{18}\text{O}$, $^{27}\text{Al}^{17}\text{O}$, $^{26}\text{Al}^{18}\text{O}$.
Table 4. Partition function parameters for various isotopologues, see Eq. (2)

|                        | $^{27}$Al$^{16}$O | $^{27}$Al$^{18}$O | $^{26}$Al$^{16}$O | $^{26}$Al$^{17}$O |
|------------------------|-------------------|-------------------|-------------------|-------------------|
| $a_0$                  | -1.0409381038     | -1.59727184392    | -0.677569296333   | -0.54167387448    |
| $a_1$                  | 9.6408607554      | 11.9848644854     | 9.21909968136     | 10.8157290731     |
| $a_2$                  | -14.3512337912    | -18.295471026     | -13.6457740234    | -16.3230021925    |
| $a_3$                  | 13.0627960677     | 16.7055086746     | 12.4154930773     | 14.8789580625     |
| $a_4$                  | -7.20103828655    | -9.21814194734    | -6.84559240132    | -8.20306751046    |
| $a_5$                  | 2.49431683028     | 3.17902318889     | 2.37492955521     | 2.83289571369     |
| $a_6$                  | -0.538890191754   | -0.67795876234    | -0.514966111414   | -0.607255974396   |
| $a_7$                  | 0.0673568508718   | 0.0828183310157   | 0.0647424233238   | 0.074909373167    |
| $a_8$                  | -0.00372906050126 | -0.004450320873   | -0.00360977781061 | -0.00407761291349 |

Table 5. Summary of our AlO linelists.

|                  | $^{27}$Al$^{16}$O | $^{27}$Al$^{18}$O | $^{26}$Al$^{16}$O | $^{26}$Al$^{17}$O |
|------------------|-------------------|-------------------|-------------------|-------------------|
| $X^2\Sigma^+$    |                   |                   |                   |                   |
| Maximum $v$      | 66                | 69                | 66                | 68                |
| Maximum $J$      | 300.5             | 300.5             | 300.5             | 300.5             |
| $A^2\Pi$         |                   |                   |                   |                   |
| Maximum $v$      | 63                | 65                | 62                | 64                |
| Maximum $J$      | 300.5             | 300.5             | 300.5             | 300.5             |
| $B^2\Sigma^+$    |                   |                   |                   |                   |
| Maximum $v$      | 40                | 41                | 39                | 40                |
| Maximum $J$      | 232.5             | 241.5             | 230.5             | 237.5             |
| Number of lines  | 4945580           | 5365592           | 4866540           | 5148996           |

Table 3. Partition function, $Q(T)$, for $^{27}$Al$^{16}$O, as a function of temperature.

| $T$ / K | Q(T) | $T$ | Q(T) | Sauval & Tatum (1984) |
|---------|------|-----|------|-----------------------|
| 10      | 134.73 | 1000 | 17595.69 | 17693.4 |
| 20      | 265.35 | 2000 | 57302.56 | 57060.6 |
| 30      | 396.01 | 3000 | 138649.47 | 135168 |
| 40      | 526.68 | 4000 | 283031.72 | 274740 |
| 50      | 657.37 | 5000 | 508066.61 | 487708 |
| 60      | 788.07 | 6000 | 828224.93 | 793980 |
| 70      | 918.78 | 7000 | 1254881.70 | 1216536 |
| 80      | 1049.50 | 8000 | 1795616.84 | 1781718 |
| 100     | 1310.96 |       |        |           |
| 200     | 2621.45 |       |        |           |
| 300     | 3966.90 |       |        |           |
| 400     | 5407.40 |       |        |           |
| 500     | 6988.27 |       |        |           |
| 600     | 8754.58 |       |        |           |
| 750     | 11692.87 |       |        |           |

and $^{26}$Al$^{16}$O. The full line list for each of the studied isotopologues are summarised in Table 5.

3 RESULTS

The line lists contain about 5 million transitions each and, therefore, for compactness and ease of use, are divided into separate energy level and transitions file. This is done using standard ExoMol format (Tennyson et al. 2013) which is based on a method originally developed for the BT2 line list (Barber et al. 2006). Extracts for the start of the $^{26}$Al$^{16}$O files are given in Tables 6 and 7. The full line list for each of these isotopologues can be downloaded from the CDS, via ftp://cdsarc.u-strasbg.fr/pub/cats/J/MNRAS/xxx/yy or http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/MNRAS//xxx/yy.

The line lists and partition function together with auxiliary data including the potential parameters and dipole moment functions, as well as the absorption spectrum given in cross section format (Hill et al. 2013), can all be obtained from there as well as at www.exomol.com.

Figure 3 shows the rotational component, and the P- and weaker R-branches of the vibrational fundamental ($v = 0 - 1$) obtained at $T=298$ K. As has been noted before (Lengsfield & Liu 1982), the X-state dipole is very flat in the equilibrium region. As the strength of a $\Delta v = 1$ vibration-rotation transition depends on the slope of the dipole in this region, this causes the vibrational fundamental to be particularly weak. Therefore this feature, which lies between 10 and 11 $\mu$m, is unlikely to be astronomically important. Our calculations suggest that the overtones ($\Delta v > 1$) are also weak so the entire AlO vibration-rotation spectrum is unlikely to feature strongly in astronomical objects.

Much more significant at infrared wavelengths is the A – X electronic band. Figure 4 shows an overview of the A – X and B – X electronic transitions which are presented as absorption spectra generated at $T = 2000$ K. Our spectra are compared to available experimental data (Launila & Jonsson 1994; Saksena et al. 2008): we note that these measurements do not give absolute intensities, so have been scaled by us. A more detailed comparison of a portion of the A – X spectrum with the experimental results of Launila & Berg (2011) is presented in Fig. 5. Figure 6 compares the theoretical spectrum obtained here with an astronomical spectrum of Kaminski et al. (2013). The agreement is remarkable. The calculation performed using the vi-
mental (Launila & Jonsson 1994; Saksena et al. 2008) spectra of Figure 4. Overview of the theoretical (ExoMol) and experimental (Launila & Jonsson 1994; Saksena et al. 2008) spectra of \( ^{27}\text{Al}\,^{16}\text{O} \). The theoretical spectra were obtained as cross sections convolved with a Gaussian line profile of width 1 cm\(^{-1}\) assuming the local thermal equilibrium at \( T = 2000 \) K. The experimental \( A – X \) and \( B – X \) spectra were scaled by \( 1 \times \) \( 10^{-17} \) and \( 5 \times \) \( 10^{-18} \), respectively.

Finally, Fig. 8 compares our calculated spectra \( B – X \) for the two isotopologues of \( ^{20}\text{Al}\,^{16}\text{O} \) and \( ^{27}\text{Al}\,^{16}\text{O} \). The shift in \( \Delta \nu = 0 \) emission spectrum at \( T_{\text{rot}}=700 \) K and \( T_{\text{rot}}=2200 \) K compared with an astronomical spectrum obtained by Kaminski et al. (2013). Cross sections (lower part) were obtained by convolving with a Gaussian profile of width 0.3 cm\(^{-1}\).

Figure 6. \( B – X \) \( \Delta \nu = 0 \) emission spectrum at \( T_{\text{rot}}=700 \) K and \( T_{\text{rot}}=2200 \) K compared with an astronomical spectrum obtained by Kaminski et al. (2013) for VY Canis Majoris (\( T_{\text{rot}} \) and \( T_{\text{vib}} \) in Kaminski et al. 2013). Cross sections (lower part) were obtained by convolving with a Gaussian profile of width 0.3 cm\(^{-1}\).

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| n  | E     | g | J  | +/− | e/f   | State         | v | |\(|\Lambda|\) | |\(|\Sigma|\) | |\(|\Omega|\) |
|----|-------|---|----|-----|-------|---------------|---|---|---|---|---|---|---|---|
| 1  | 0.0000000 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 0 | 0 | 0.5 | 0.5 | 0.5 |
| 2  | 965.435497 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 1 | 0 | 0.5 | 0.5 | 0.5 |
| 3  | 1916.845371 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 2 | 0 | 0.5 | 0.5 | 0.5 |
| 4  | 2854.206196 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 3 | 0 | 0.5 | 0.5 | 0.5 |
| 5  | 3777.503929 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 4 | 0 | 0.5 | 0.5 | 0.5 |
| 6  | 4686.660386 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 5 | 0 | 0.5 | 0.5 | 0.5 |
| 7  | 5581.906844 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 6 | 0 | 0.5 | 0.5 | 0.5 |
| 8  | 6066.934830 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 7 | 0 | 0.5 | 0.5 | 0.5 |
| 9  | 6463.039443 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 8 | 0 | 0.5 | 0.5 | 0.5 |
| 10 | 6778.997803 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 9 | 0 | 0.5 | 0.5 | 0.5 |
| 11 | 7086.327188 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 10 | 0 | 0.5 | 0.5 | 0.5 |
| 12 | 7392.427637 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 11 | 0 | 0.5 | 0.5 | 0.5 |
| 13 | 7698.528105 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 12 | 0 | 0.5 | 0.5 | 0.5 |
| 14 | 7904.628571 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 13 | 0 | 0.5 | 0.5 | 0.5 |
| 15 | 8210.729038 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 14 | 0 | 0.5 | 0.5 | 0.5 |
| 16 | 8516.829494 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 15 | 0 | 0.5 | 0.5 | 0.5 |
| 17 | 8822.930961 | 12 | 0.5 | +   | e     | $X_2\Sigma^+$ | 16 | 0 | 0.5 | 0.5 | 0.5 |

$n$: State counting number.

$E$: State energy in cm$^{-1}$.

$J$: Total angular momentum quantum number.

g: State degeneracy.

+/−: Total parity.

e/f: Rotationless-parity (Brown et al. 1975).

$\Lambda$: Absolute value of $\Lambda$ (projection of the electronic angular momentum).

$\Sigma$: Absolute value of $\Sigma$ (projection of the electronic spin).

$\Omega$: Absolute value of $\Omega = \Lambda + \Sigma$ (projection of the total angular momentum).

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Figure 7. Emission spectra of three sub-bands within the X – B band at 1700 K compared to the experiment of Saksena et al. (2008) (up). Top panel: $\Delta v = 1$, middle panel: $\Delta v = 0$, lower panel: $\Delta v = -1$. The experimental data is in arbitrary units; calculated cross sections were obtained by convolving with a Doppler profile at 1700 K.

Figure 8. Calculated B – X $v' - v'' = 0 - 1$ absorption spectrum at 1700 K for $^{26}$Al$^{16}$O and $^{27}$Al$^{16}$O obtained by convolving with a Doppler profile at 1700 K.

Table 7. Extracts from the transitions file for $^{27}$Al$^{16}$O. Full tables are available from http://cdsarc.u-strasbg.fr/cgi-bin/VizieR?-source=J/MNRAS/xxx/yy.

$$
\begin{array}{ccc}
 f & i & A_{f_i} \\
 47156 & 47355 & 1.1598E-04 \\
 9373 & 8773 & 5.0797E-02 \\
 10989 & 10389 & 1.5734E-02 \\
 10789 & 10589 & 1.5455E-02 \\
 9755 & 9155 & 6.3206E-03 \\
 12788 & 13387 & 2.7204E-06 \\
 10178 & 9578 & 2.3282E-02 \\
 9555 & 9355 & 6.7365E-03 \\
 9187 & 8987 & 5.4969E-02 \\
 9587 & 9387 & 5.4633E-02 \\
 7360 & 7159 & 9.1545E-06 \\
 9184 & 9384 & 4.8954E-05 \\
 9751 & 9151 & 5.9125E-03 \\
 9551 & 9351 & 5.9229E-03 \\
 10166 & 9566 & 8.9220E-03 \\
 10985 & 10385 & 1.4584E-02 \\
 10785 & 10585 & 1.4584E-02 \\
 8548 & 7948 & 5.1842E-02 \\
 20975 & 20775 & 5.7037E-05 \\
 8148 & 7548 & 5.2229E-02 \\
 2966 & 9766 & 9.1712E-03 \\
\end{array}
$$

$f$: Upper state counting number; $i$: Lower state counting number; $A_{f_i}$: Einstein-A coefficient in s$^{-1}$.

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