Collisional excitation of doubly deuterated ammonia ND$_2$H by para-H$_2$

L. Wiesenfeld 1, E. Scifoni 1,2, A. Faure 1, and E. Roueff 3

1 Laboratoire d’Astrophysique de Grenoble, CNRS/Université Joseph-Fourier, Grenoble, France.
2 Department of Biophysics, Gesellschaft für Schwerionenforschung, Darmstadt, Germany.
3 LUTH, CNRS/Observatoire de Paris, Meudon, France

30 December 2010

ABSTRACT

Collisional de-excitation rates of partially deuterated molecules are different from the fully hydrogenated species because of lowering of symmetry. We compute the collisional (de)excitation rates of ND$_2$H by ground state para-H$_2$, extending the previous results for Helium. We describe the changes in the potential energy surface of NH$_3$ - H$_2$ involved by the presence of two deuterium nuclei. Cross sections are calculated within the full close-coupling approach and augmented with coupled-state calculations. Collisional rate coefficients are given between 5 and 35 K, a range of temperatures which is relevant to cold interstellar conditions. We find that the collisional rates of ND$_2$H by H$_2$ are about one order of magnitude higher than those obtained with Helium as perturber. These results are essential to radiative transfer modelling and will allow to interpret the millimeter and submillimeter detections of ND$_2$H with better constraints than previously.

1 INTRODUCTION

Doubly deuterated ammonia has been detected for the first time by Roueff et al. (2000) towards the dark cloud L134N via its $1_{00} - 1_{01}$ ortho and para transitions at 110 GHz and subsequently in the protostellar environment L1689N by Loinard et al. (2001). The submillimeter fundamental transitions have then been detected at the Caltech Sub-millimeter Observatory by Roueff et al. (2005); Lis et al. (2006) and on the APEX antenna in Chile by Gerin et al. (2006) towards the Barnard 1 molecular cloud and L1689N. ND$_2$H was shown to be a sensitive tracer of the physical conditions of this star forming region. In a previous paper [Machin & Roueff 2007] some of us have presented the collisional formalism and computed the collisional excitation cross-sections and rate coefficients of ND$_2$H by He by introducing the appropriate changes in the potential energy surface of NH$_3$ - He, computed by Hedges & Wheatley (2001). This new accurate intermolecular potential energy surface (PES) for NH$_3$-He has also been previously reevaluated by Maret et al. (2009). This PES was taken at its ground-state average value of 1.4488 Bohr. Simultaneously with the (de)excitation rates of ND$_2$H in collision with para-H$_2$, H$_2$ is the main constituent of dark clouds environment where ND$_2$H has been detected. Collisional excitation is dominated by interaction with low temperature H$_2$; this motivated our present study, aimed particularly at the low temperature excitation schemes of ND$_2$H.

The paper is organized as follows. In section 2 we briefly describe the changes introduced by the presence of two deuterons in the PES of NH$_3$ - H$_2$, published recently (Maret et al. 2009). We present in section 3 the collisional equations for the ND$_2$H - H$_2$ system. The cross sections and the corresponding reaction rate coefficients of the ND$_2$H - H$_2$ system are given in section 4. We present our conclusions in Section 5.

2 POTENTIAL ENERGY SURFACE

We have recently put forward a potential energy surface (PES) of NH$_3$ in interaction with H$_2$. This rigid rotor PES is reported in full details in Maret et al. (2009). Here we need to transform this PES from the triple H isotopologue of ammonia to the doubly deuterated one, ND$_2$H. For a given inter-molecular geometry, the interaction between the molecules of ammonia and H$_2$ depends on the various electronic charges (electrons and nuclei) as well as of the intra-molecular geometries of ammonia and molecular hydrogen. For the two isotopologues NH$_3$ and ND$_2$H the charge structure is identical, as long as we remain in the Born-Oppenheimer approximation. However, the geometries are different in two aspects: (i) the intra-molecular distances change slightly and (ii) the position of the centre of mass of ND$_2$H is shifted with respect to the centre of mass of NH$_3$ and the principal axes of inertia are rotated. Let us treat both points in succession.

The original PES for NH$_3$-H$_2$ was computed with both monomer geometries taken at their average value in the ground vibrational state (Maret et al. 2009). This has been demonstrated to be a much better approximation than taking equilibrium geometries: in the case of the similar H$_2$O-H$_2$ system, Faure et al. (2005), Valiron et al. (2008) have found that employing state-averaged geometries is a very good approximation for including vibrational effects within a rigid rotor PES. We note that the importance of the zero-point vibrational correction was discussed earlier by Meuwly & Bemish (1997), in the N$_2$H$^+$ - He system.

In particular the $r$(HH) distance for molecular hydrogen was shown to provide the largest vibrational correction. It was taken by Maret et al. (2009) at its average value of 1.4488 Bohr. Similarly, the NH$_3$ molecule was taken at its ground-state average geometry with the following parameter: $r$(NH) = 1.9512 Bohr.
The relevant rotation of the new centre of mass in the old coordinate system, then perform

\[ \begin{align*}
x_H &= x'_H \cos \gamma - z'_H \sin \gamma \\
y_H &= y'_H \\
z_H &= x'_H \sin \gamma + z'_H \cos \gamma
\end{align*} \]

(3)

Eventually, the functional form we take is identical to the one for water-hydrogen \cite{Phillips1994, Valiron2008}. The spherical angles, all primed, refer to the new frames \(O'x'y'z'\) and \(O_Hx'_H y'_H z'_H\):

\[ V(R', \theta', \phi', \theta_H', \phi_H') = \sum_l V_{l_1 l_2 l_3}(R) t_{l_1 l_2 l_3}(\theta',\phi', \theta_H',\phi_H') \]

(4)

where the function \( t_{l_1 l_2 l_3} \) are explicitly given in \cite{Phillips1994, Valiron2008}. As previously \cite{Valiron2008, Maret2009}, we selected iteratively all statistically significant terms \( v_{l_1 l_2 l_3}(R) \) using the procedure described in \cite{Valiron2008}. The final expansion includes anisotropies up to \( l_1=10 \) for ND\textsubscript{3}H and \( l_2=4 \) for H\textsubscript{2}, resulting in 197 \( t_{l_1 l_2 l_3} \) functions.

3 COLLISIONAL TREATMENT

In the low temperature environments where ND\textsubscript{3}H has been detected the kinetic temperature is below 20 K \cite{Roueff2000} and the main constituent, H\textsubscript{2}, is expected to lie in its ground rotational (para) state, \( J = 0 \) \cite{Troscompt2009}. The calculations presented below were restricted to collisions between ND\textsubscript{3}H and para-H\textsubscript{2}(\( J = 0 \)), i.e. by neglecting the \( J = 2 \) (closed) channel. This latter was actually found to change the cross-sections, at very low energies, by up to a factor of 3, as observed for NH\textsubscript{3}H\textsubscript{2} (see references in \cite{Maret2009}). Its effect on the average cross-sections and rate coefficients is however much smaller, typically 30 \%, which is therefore the typical accuracy of the rates below. The rotational constants of ND\textsubscript{3}H were taken from \cite{Couplet1986}. The resulting rotational energy levels in are given Table I. The reduced collisional mass is \( \mu = 1.822684 \)amu.

Full quantum close coupling (CC) scattering calculations were performed with help of the Molscat program \cite{Hudson1995} which computes scattering matrices (S matrices) and combines these in order to determine elastic and inelastic cross sections, at defined total energies \( E \). The convergence of the inelastic cross sections was checked to be better than 5\%, for the different rotational transitions investigated here. The different collision parameters defined in Molscat are given the default ones. We used the following values: \( \text{RMIN} = 3.0 \), \( \text{INTFLG} = 0 \), \( \text{STEPS} = 10.0 - 30.0 \). Calculations have been performed for total energies between 10 cm\textsuperscript{-1} and 430 cm\textsuperscript{-1}. The energy step has been varied with increasing collision energy. It was 0.25 cm\textsuperscript{-1} for a total energy between 10 cm\textsuperscript{-1} and 40 cm\textsuperscript{-1}, 1 cm\textsuperscript{-1} between 40 cm\textsuperscript{-1} and 80 cm\textsuperscript{-1}, 5 cm\textsuperscript{-1} between 80 cm\textsuperscript{-1} and 100 cm\textsuperscript{-1} and 20 cm\textsuperscript{-1} above 100 cm\textsuperscript{-1}. The size of the rotational basis set of ND\textsubscript{3}H was also varied with energy. For \( E \leq 100 \text{cm}^{-1} \), \( \text{J(ND}_{3}\text{H)} \leq 10 \); at \( E = 120 \text{cm}^{-1} \), \( \text{J(ND}_{3}\text{H)} \leq 12 \). For the CS calculations at \( E \geq 150 \text{cm}^{-1} \), \( \text{J(ND}_{3}\text{H)} \leq 16 \).

In order to limit the time of computation needed for a scattering calculation, some customary approximations of the collisional treatment are implemented in the Molscat program such as the Coupled State (CS) approximation introduced by McGuire & Kouri \cite{McGuire1974}. In this approximation, scattering equations are written in the body-fixed frame which is rotating. Then the projection of the

\[ x_{y'} = x' \cos \gamma - z' \sin \gamma + x_{y'}' \]

\[ y = y' \]

\[ z = z' \sin \gamma + z' \cos \gamma + z_{y'}' \]

(2)
Collisional excitation of doubly deuterated ammonia ND$_2$H by para-H$_2$

Table 1. Rotational level energies for ND$_2$H, as used in our computation.

| $J_aK_c$ | Energy (cm$^{-1}$) |
|----------|--------------------|
| 0$0_0$  | 0                  |
| 1$1_1$  | 9.03939            |
| 1$1_1$  | 11.19743           |
| 1$1_0$  | 12.87456           |
| 2$0_2$  | 26.65954           |
| 2$1_2$  | 27.79543           |
| 2$1_1$  | 32.55350           |
| 2$1_0$  | 38.86400           |
| 2$2_0$  | 39.48154           |

orbital angular momentum $l$ is restricted to the value $m_l = 0$. The accuracy of this method is questionable but it was shown to agree with CC calculations within typically ~ 30% for the present system, as shown below. Here we resorted to the CS approximation for two problems are identical, differing by a much shallower potential well. Even if the symmetry of the CS level, from Machin & Roue (2000). For comparison, also cross sections with He computed at the CS level, from Machin & Roue (2000), are shown. A complex resonance structure is seen for energies smaller than about 100 cm$^{-1}$ with broad and narrow features, resulting in large variations of the cross sections. The sharp maxima are due to the opening of new collision channels and correspond to both Feshbach and shape resonances. This is in contrast with the He-NH$_2$D$_2$ collision case, with a much shallower potential well. Even if the symmetry of the two problems are identical, differences arise in their cross-section structures and cross section values. A similar effect was found recently at much higher energies, for the differential inelastic cross section of water-H$_2$, $J = 0$ compared with water-He (Yang 2010).

As is always been observed, the resonances quickly disappear with increasing energy. The cross sections relative to Helium are significantly smaller in the energy range displayed in Figure 2. However, they converge to those involving para-H$_2$ at collision energies above ~80 cm$^{-1}$.

Knowing the importance of the hyperfine quadrupolar effect for $^{14}$N, nuclear spin $I = 1$, extending those cross section calculations to include explicitly the hyperfine structure could be of interest. Hyperfine structure has indeed been observed with some precision in the lower transitions (Gerin et al. 2006). However, because of the low symmetry of NH$_2$D$_2$ (asymmetric top), no close formula exist in the literature that could connect state to state hyperfine rates to state to state global rotational rates. One should resort to a full summation of $\Delta$ matrix elements in order to get all detailed hyperfine rates. Also, because of the small column density of NH$_2$D$_2$, the differential effects on the various hyperfine lines should remain small (Daniel et al. 2006).

The collisional (de)excitation rates $R$ as a function of temperature $T$ were obtained by a Maxwell-Boltzmann averaging of the cross sections times the relative velocity. In the equation below, $E_{\text{kin}}$ is the relative kinetic energy:

$$R_{J_aK_c \rightarrow J_bK_c'}(T) = \left( \frac{8k_B T}{\pi \mu} \right)^{\frac{3}{2}} \left( \frac{1}{k_B T} \right)^{\frac{1}{2}} \int_0^\infty \sigma_{J_aK_c \rightarrow J_bK_c'}(E_{\text{kin}}) \exp \left( -\frac{E_{\text{kin}}}{k_B T} \right) E_{\text{kin}} dE_{\text{kin}}$$

$k_B$ is the Boltzmann constant and $\mu$ is the reduced mass of the ND$_2$H - H$_2$ system. Cross sections having been computed for collision energies up to above 390 cm$^{-1}$, the rate coefficients may be calculated very safely for temperatures between 5 K and 35 K which are relevant for cold prestellar cores. Table 2 gives the de-excitation rate coefficients for the 9 first rotational levels as well as the fitting parameters allowing to display the rate coefficients for any temperature between 5 and 35 K via the following expression (Faure, Gorfinkiel, & Tennyson 2004), with $R$ in $10^{-11}$ cm$^3$ s$^{-1}$:

$$\log_{10} R(T) = \sum_{i=1}^3 a_i T^{-\alpha_i/6}$$

All fits have been verified to be precise to better than 1%. It should be noted that the following inelastic transitions are strictly forbidden in the CS approximation (owing to spurious selection rules): $J_{1 \downarrow 1} \rightarrow 0_0$, $J_{2 \downarrow 1} \rightarrow 0_0$ and $J_{2 \downarrow 1} \rightarrow 0_0$. We see that the corresponding CC rates are not negligible, although about one order of magnitude smaller than the largest rates. There is therefore no obvious collisional propensity rules for the presented transitions. We note that since the dipole moment has two non-zero projections ($\mu_a$ and $\mu_c$), the corresponding radiative selection rules are $\Delta J = 0$, 1 and $\Delta K_a = \pm 1$, $\Delta K_c = \pm 1$ for transitions along $\mu_a$ and $\Delta K_a = 0$, $\pm 2$ for transitions along $\mu_c$. The Einstein coefficients have been computed by Coudert and Roue (2006) and recalled in Machin & Roue (2007).

5 DISCUSSION AND CONCLUSIONS

The comparison of the present rates with the values obtained by Machin & Roue (2007) where Helium is the collider is informative. The collision rates obtained in the present work when para-H$_2$ ($J=0$) is the perturber are typically one order of magnitude larger than those obtained with Helium. The origin of this discrepancy lies in the significantly different potential wells of the NH$_3$-H$_2$ and NH$_3$-He PES, as discussed by Maret et al. (2009). The usual scaling between the collision rates obtained from the ratio of the reduced masses is clearly not accurate and the calculations have to be performed explicitly in order to obtain the appropriate rates with molecular hydrogen. We display in Table 3 the resulting critical densities for the para and ortho transitions. These were obtained by simply dividing the Einstein coefficient of a given transition by the corresponding de-excitation rate coefficient at 10 K. Note that other definitions are possible (Maret et al. 2009). These values set the limit of the perturber density above which the transitions become thermalized. We see that the critical densities corresponding to the two transitions $1_{1 \downarrow 1} \rightarrow 0_0$ and $1_{1 \downarrow 0} \rightarrow 0_0$ are different by about one order of magnitude at 10 K, which is about a factor of 3 less than the ratio of the Einstein coefficients. Such differences may have profound consequences on the interpretation of these two transitions which are both observable from the ground (Lis et al. 2006; Gerin et al. 2006) at 335 and 389 GHz respectively, as the
Figure 2. Collisional de-excitation cross sections as a function of the relative kinetic energy. Left: transition $1_{11} \rightarrow 0_{00}$ of ND$_2$H with Helium in CS approximation (red) ([Machin & Roueff 2007]) and para H$_2$ (present work) in CC (blue) and CS (green) approximations. Right: transition $1_{10} \rightarrow 1_{01}$ of ND$_2$H with Helium in CS approximation (red) ([Machin & Roueff 2007]) and para H$_2$ (present work) in CC (blue) and CS (green) approximations.

Table 3. Calculated critical densities for the first ortho and para transitions of ND$_2$H with H$_2$ at 10 K.

| Transition | Critical density (cm$^{-3}$) |
|------------|-------------------------------|
|            | ortho                         | para                         |
| $1_{11} \rightarrow 0_{00}$ | $1.17 \times 10^6$ | $1.34 \times 10^6$ |
| $1_{11} \rightarrow 1_{01}$ | $3.48 \times 10^4$ | $6.63 \times 10^4$ |
| $1_{10} \rightarrow 0_{00}$ | $1.10 \times 10^7$ | $1.01 \times 10^7$ |
| $1_{10} \rightarrow 1_{01}$ | $5.19 \times 10^4$ | $5.94 \times 10^4$ |
| $2_{00} \rightarrow 1_{11}$ | $6.34 \times 10^5$ | $6.76 \times 10^5$ |
| $2_{00} \rightarrow 1_{01}$ | $5.33 \times 10^5$ | $5.66 \times 10^5$ |
| $2_{12} \rightarrow 1_{01}$ | $2.31 \times 10^5$ | $9.26 \times 10^5$ |
| $2_{11} \rightarrow 1_{10}$ | $1.14 \times 10^5$ | $1.18 \times 10^5$ |
| $2_{11} \rightarrow 1_{01}$ | $1.33 \times 10^5$ | $1.45 \times 10^5$ |
| $2_{11} \rightarrow 2_{02}$ | $7.59 \times 10^4$ | $7.12 \times 10^4$ |
| $2_{21} \rightarrow 1_{11}$ | $1.80 \times 10^5$ | $1.79 \times 10^5$ |
| $2_{21} \rightarrow 1_{01}$ | $4.17 \times 10^5$ | $1.77 \times 10^5$ |
| $2_{21} \rightarrow 2_{02}$ | $2.70 \times 10^5$ | $1.94 \times 10^5$ |
| $2_{21} \rightarrow 2_{11}$ | $1.39 \times 10^5$ | $1.23 \times 10^5$ |
| $2_{20} \rightarrow 1_{11}$ | $5.78 \times 10^4$ | $2.26 \times 10^4$ |
| $2_{20} \rightarrow 1_{01}$ | $1.47 \times 10^5$ | $1.49 \times 10^5$ |
| $2_{20} \rightarrow 2_{12}$ | $5.65 \times 10^4$ | $6.44 \times 10^4$ |
| $2_{20} \rightarrow 2_{11}$ | $3.96 \times 10^5$ | $2.48 \times 10^5$ |

corresponding upper levels may not be accounted for by a single excitation temperature.

ACKNOWLEDGEMENTS

We are deeply indebted to Pierre Valiron, who gave impetus and ideas throughout the inception of this work. ES was supported by a grant of the “Molecular Universe” FP6 Marie Curie network. We acknowledge support from the French Institut National des Sciences de l’Univers, through its program “Physique et Chimie du Milieu Interstellaire”. LAOG is a joint laboratory Université Joseph-Fourier/CNRS under the name UMR 5571.

REFERENCES

Benedict W. S., Gailar N. & Plyler E. K., 1957, Can. J. Phys., 35, 1235
Cohen A. E. & Pickett H. M., 1982, J. Mol. Spectrosc., 93, 83
Coudert L., Valentin A., & Henry L., 1986, J. Mol. Spectrosc., 120, 185
Coudert L., Roueff E., 2006, Astron. & Astrophys., 449, 855
Daniel F., Cernicharo J., Dubernet M.L. 2006, ApJ, 648, 461
Dubernet M.L. et al., 2006, A&A, 460, 323
Garrison B. J., Lester W. A., Miller W. H., 1976, J. Chem. Phys., 65, 2193
Faure A., Gorfinkel J. D., Tennyson J., 2004, MNRAS, 347, 323
Faure A., Valiron P., Wernli M., Wiesenfeld L., Rist C., Noga J., Tennyson J., 2005, J. Chem. Phys., 122, 1102
Garrison B. J. & Lester W. A., 1977 J.Chem.Phys., 66, 531
Gerin, M., Lis, D. C., Phillip, S., Guesten, R., Roueff, E., and Reveret, V., 2006, A&A, 454, L63
Phillips, T.R., Maluendes, S., McLean, A. D. and Green, S., 1994, J. Chem. Phys., 101, 5824
Hodges M. P. and Wheatley R. J., 2001, J. Chem.Phys., 114, 8836
Larsson B., Liseau R., Bergman P. et al., 2003, A&A, 402, L69
Lis, D. C., Gerin, M., Roueff, E., Vastel, C., Phillips, T.G., 2006, ApJ, 636, 916
Loinard, L., Castets, A., Ceccarelli, C., Caux, E., Tielens, A.G.G.M., 2001, ApJ, 552, L163
Machin L., Roueff E., 2005, J. Phys. B: At. Mol. Opt. Phys., 38, 1519
Machin L., Roueff E., 2006, A&A, 460, 953
Machin L., Roueff E., 2007, A&A, 465, 647
Maret S., Faure A., Scifoni E., Wiesenfeld L., 2009, Mon. Not. R. Astr. Soc., 399, 425
Table 2. Deexcitation rate coefficients for ND$_2$H para-H$_2$ ($J = 0$) collisions. Fits to formula (6) are given in the last 4 columns.

| Temperature | Rate coefficients $R_J$ ($10^{-11}$ cm$^3$ s$^{-1}$) | Fit coefficients |
|-------------|---------------------------------------------------|------------------|
|             | $a_0$ 1 2 3                                        |                  |
| $1_0$ $\rightarrow$ $0_0$ | 0.572 0.436 0.351 0.29 0.245 0.211 0.183 | 19.71 -46.57 37.81 -10.74 |
| $1_1$ $\rightarrow$ $0_0$ | 1.14 1.10 1.03 0.938 0.854 0.781 0.717 | 22.53 -51.13 38.73 -9.74 |
| $1_1$ $\rightarrow$ $1_0$ | 7.57 6.79 6.14 5.62 5.21 4.89 4.63 | 0.00 -3.51 5.63 -1.38 |
| $1_0$ $\rightarrow$ $0_0$ | 4.75 4.39 4.05 3.74 3.49 3.29 3.13 | 1.89 -7.36 8.07 -2.04 |
| $1_0$ $\rightarrow$ $1_1$ | 1.49 1.34 1.23 1.12 1.03 0.953 0.887 | 15.74 -35.56 27.24 -6.91 |
| $1_0$ $\rightarrow$ $1_1$ | 1.37 1.25 1.14 1.05 0.959 0.887 0.826 | 14.76 -33.90 26.31 -6.76 |
| $2_0$ $\rightarrow$ $0_0$ | 0.824 0.782 0.71 0.64 0.581 0.532 0.493 | 6.58 -19.33 17.89 -5.40 |
| $2_0$ $\rightarrow$ $1_0$ | 1.13 0.842 0.709 0.613 0.537 0.476 0.425 | 30.13 -63.93 46.67 -11.72 |
| $2_0$ $\rightarrow$ $1_1$ | 3.19 3.06 2.97 2.90 2.83 2.77 2.73 | 2.52 -5.88 4.76 -0.82 |
| $2_0$ $\rightarrow$ $1_0$ | 1.29 1.12 1.00 0.904 0.821 0.752 0.694 | 15.98 -36.13 27.88 -7.23 |
| $2_1$ $\rightarrow$ $0_0$ | 0.275 0.272 0.234 0.199 0.171 0.148 0.13 | 6.25 -24.01 24.97 -8.41 |
| $2_1$ $\rightarrow$ $1_0$ | 3.95 3.84 3.73 3.61 3.52 3.44 3.37 | 1.09 -3.63 3.67 -0.58 |
| $2_1$ $\rightarrow$ $1_1$ | 0.808 0.868 0.823 0.753 0.684 0.623 0.569 | 15.88 -40.31 32.97 -8.84 |
| $2_1$ $\rightarrow$ $2_0$ | 0.739 0.787 0.744 0.683 0.621 0.565 0.516 | 17.41 -43.09 34.66 -9.22 |
| $2_1$ $\rightarrow$ $2_1$ | 3.40 3.77 3.97 4.03 4.03 4.01 3.99 | 11.93 -25.60 17.74 -3.40 |
| $2_1$ $\rightarrow$ $0_0$ | 0.104 0.116 0.102 0.0875 0.0749 0.0647 0.0564 | 2.64 -19.41 23.36 -8.68 |
| $2_1$ $\rightarrow$ $1_0$ | 1.95 2.22 2.36 2.40 2.40 2.38 2.35 | 16.14 -34.63 24.05 -5.07 |
| $2_1$ $\rightarrow$ $1_1$ | 3.72 4.02 4.14 4.14 4.08 3.98 3.88 | 18.59 -39.65 27.74 -5.77 |
| $2_1$ $\rightarrow$ $1_1$ | 0.464 0.489 0.464 0.428 0.393 0.362 0.336 | 10.75 -28.86 24.57 -7.06 |
| $2_1$ $\rightarrow$ $2_0$ | 2.78 2.99 3.00 2.96 2.90 2.85 2.81 | -1.02 -0.82 2.40 -0.45 |
| $2_1$ $\rightarrow$ $2_1$ | 1.08 1.25 1.23 1.15 1.07 1.00 0.943 | 2.38 -13.06 14.38 -4.38 |
| $2_1$ $\rightarrow$ $0_0$ | 0.341 0.346 0.342 0.334 0.325 0.317 0.311 | 4.09 -10.33 8.44 -2.71 |
| $2_1$ $\rightarrow$ $1_1$ | 3.41 3.86 3.98 3.93 3.82 3.69 3.57 | 15.47 -35.32 26.13 -5.71 |
| $2_1$ $\rightarrow$ $1_1$ | 2.21 2.33 2.43 2.48 2.50 2.50 2.50 | 13.36 -26.93 17.69 -3.41 |
| $2_1$ $\rightarrow$ $1_1$ | 0.616 0.593 0.577 0.554 0.529 0.506 0.486 | 17.15 -36.63 26.22 -6.52 |
| $2_1$ $\rightarrow$ $1_1$ | 1.55 1.34 1.20 1.10 1.01 0.947 0.896 | 3.52 -9.97 9.64 -2.92 |
| $2_1$ $\rightarrow$ $1_1$ | 3.50 3.02 2.75 2.56 2.41 2.29 2.19 | 4.43 -10.36 8.80 -2.11 |
| $2_1$ $\rightarrow$ $1_1$ | 1.93 2.07 2.10 2.09 2.05 2.00 1.96 | 10.90 -24.41 17.82 -3.94 |
| $2_0$ $\rightarrow$ $0_0$ | 2.43 2.39 2.31 2.20 2.11 2.02 1.95 | 6.54 -16.01 12.96 -3.09 |
| $2_0$ $\rightarrow$ $1_1$ | 0.631 0.649 0.649 0.638 0.625 0.612 0.600 | 6.85 -15.70 11.80 -3.10 |
| $2_0$ $\rightarrow$ $1_1$ | 0.441 0.408 0.399 0.367 0.346 0.327 0.309 | 21.50 -45.57 32.53 -8.20 |
| $2_0$ $\rightarrow$ $1_0$ | 2.98 3.00 3.03 3.04 3.03 3.02 3.00 | 7.58 -15.32 10.22 -1.77 |
| $2_0$ $\rightarrow$ $2_0$ | 1.86 1.66 1.56 1.47 1.40 1.33 1.27 | 14.77 -31.02 22.26 -5.22 |
| $2_0$ $\rightarrow$ $2_1$ | 1.09 1.02 0.998 0.97 0.938 0.906 0.876 | 20.42 -41.66 28.53 -6.55 |
| $2_0$ $\rightarrow$ $2_1$ | 0.897 0.992 1.03 1.03 1.02 1.00 0.989 | 10.70 -24.06 17.45 -4.11 |
| $2_0$ $\rightarrow$ $2_1$ | 0.405 0.379 0.365 0.346 0.324 0.303 0.284 | 32.14 -67.28 47.18 -11.49 |