Supporting Information for

Microwave spectra of dinitrotoluene isomers: a new step towards the detection of explosive vapors

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S1 Theoretical determination of χ_2,θ_2,ϕ_2 for 2,4-DNT

These three Eulerian-type angles are involved in the rotational dependence of the tunneling splitting. They should be determined using the procedure outlined in Section 5 of Hougen.[1] Atom positions in the xyz molecule fixed axis system, $\mathbf{a}_i(\eta)$, with $1 \leq i \leq 19$, are parameterized in terms of a path coordinate η, with $-1 \leq \eta \leq +1$, such that $\eta = -1$ at the beginning of the tunneling path, at Configuration 1, and $\eta = +1$ at the end of the tunneling path, at Configuration 2. Atom positions can be obtained with the help of Fig. S1. As emphasized by this figure, positions of all atoms, except the three methyl group hydrogen atoms, do not depend on η and satisfy $a(\eta)_{iy} = 0$. The methyl group hydrogen atoms position are parameterized by the torsional angle α introduced in the paper. Taking $\alpha(\eta) = (1+\eta)\pi/3$, ensures that the methyl group is rotated through $2\pi/3$ when η goes from -1 to $+1$.

In agreement with Hougen,[1] the rotational angular momentum $\mathbf{L}(\eta)$ generated by the large amplitude motion along the tunneling path and the molecule inertia tensor $\mathbf{I}(\eta)$ need to be evaluated. The former is given by:

$$\mathbf{L}(\eta) = \sum_{i=1}^{19} m_i\, \mathbf{a}_i(\eta) \times \frac{\mathrm{d}\mathbf{a}_i(\eta)}{\mathrm{d}\eta} \tag{1}$$

where m_i is the mass of atom i. It is found in the case of 2,4-DNT that $\mathbf{L}(\eta)$ does not depend on η and reduces to:

$$\mathbf{L} = \frac{I\pi}{3}\begin{pmatrix}\sin\delta\\ 0\\ \cos\delta\end{pmatrix} \tag{2}$$

where I is the diagonal component of the methyl group inertia tensor along its three fold axis of symmetry and δ is the angle between the axis of internal rotation and the molecule fixed z axis. This equation shows that the tunneling angular momentum is η-independent and lies in the xz plane. Similarly, it is found that the inertia tensor does not depend on η and that the y axis is the c principal axis of inertia.

The next step is solving the three coupled ordinary, nonlinear, differential equations in Eqs. (49) of Hougen.[1] In the present case, In the present case, these equations reduces to:

$$\begin{pmatrix}\mathrm{d}\gamma\\ \mathrm{d}\beta\\ \mathrm{d}\alpha\end{pmatrix} = \begin{pmatrix}+\cos\alpha/\cos\beta & -\sin\alpha/\cos\beta & 0\\ +\sin\alpha & +\cos\alpha & 0\\ -\cos\alpha\sin\beta/\cos\beta & +\sin\alpha\sin\beta/\cos\beta & 1\end{pmatrix}\boldsymbol{\mu}\cdot\mathbf{L} \tag{3}$$

where $\boldsymbol{\mu}$ is the inverse inertia tensor and α, β, γ are shorthand notations for $\alpha_{Pp}, \beta_{Pp}, \gamma_{Pp}$. The latter parameterize the 3×3 rotation matrix $T^{-1}(\alpha,\beta,\gamma)$ introduced in Eq. (30) of Hougen.[1] Equation (3) is solved numerically using the `DERKF` subroutine from the `SLATEC` library.[2] This yields values for $\alpha_{Pp}, \beta_{Pp}, \gamma_{Pp}$ at Configuration 2 which are denoted $\alpha_{P2}, \beta_{P2}, \gamma_{P2}$. The angles χ_2, θ_2, ϕ_2 are then obtained solving Eq. (4) of Coudert and Hougen[3] rewritten below:

$$T^{-1}(\alpha_{P2}, \beta_{P2}, \gamma_{P2}) = S^{-1}(\chi_2, \theta_2, \phi_2) \tag{4}$$

where S^{-1} is the usual 3×3 rotation matrix depending on the Eulerian angles. It can be found in many textbooks and in Eq. (18) of Hougen.[1]

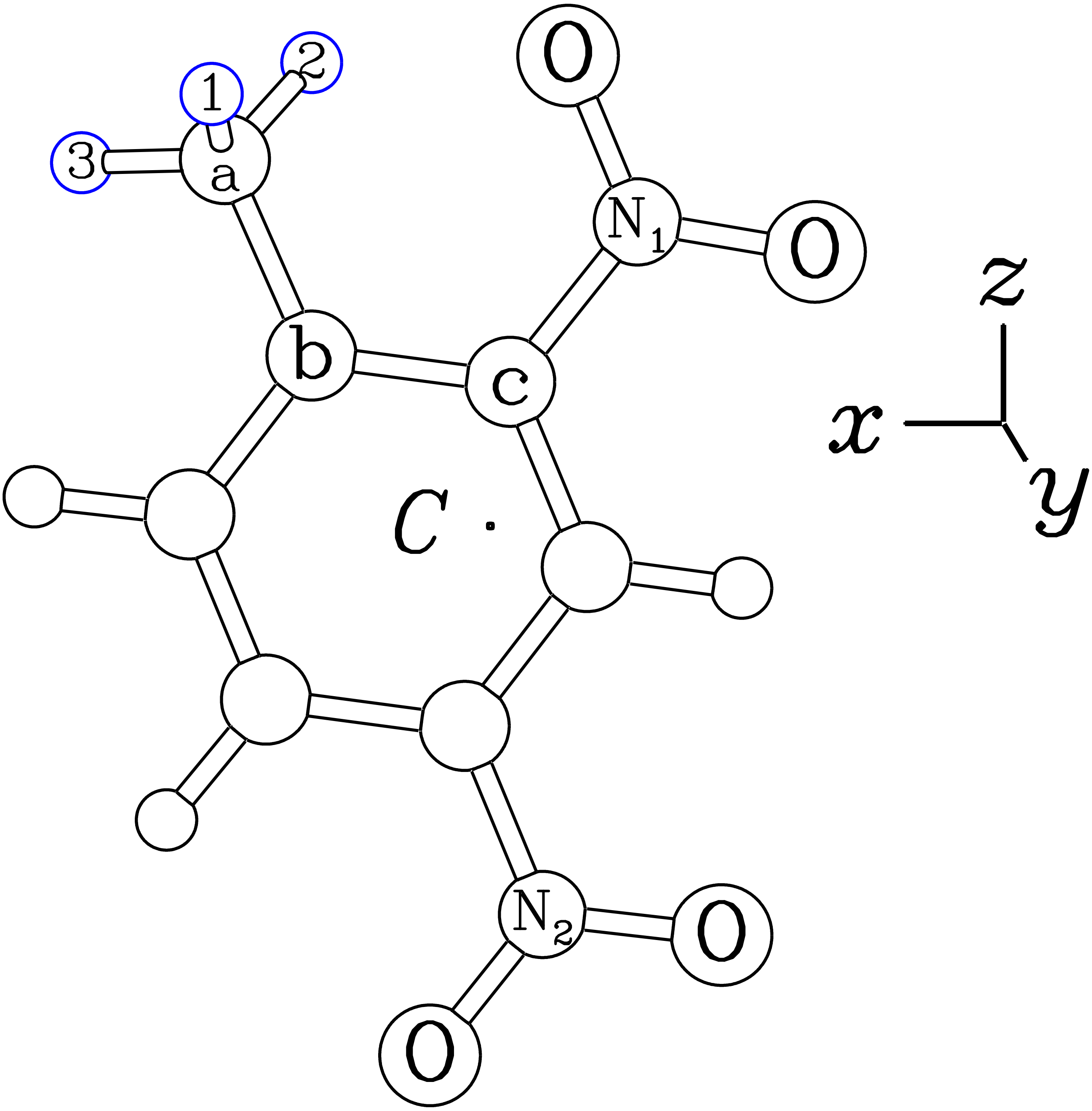

Figure S1: The molecular model used for 2,4-DNT is illustrated. It consists of a rigid planar $C_6H_3N_2O_4$ frame and a C_{3v} methyl group. Numbers 1, 2, and 3 identify the three hydrogen atoms of this group, the letter a its carbon atom, the letters b and c two carbon atoms of the phenyl ring, N_1 and N_2 the two nitrogen atoms, and the letter C the molecular center of mass. The methyl group rotates about an axis parallel to the C_aC_b bond. In agreement with the paper, the torsional angle α is the dihedral angle $\angle H_1C_aC_bC_c$. The molecular fixed xyz axis system coincides with the principal axis system and the I^r representation is used. The molecule fixed xyz axis system is not drawn at the molecular center of mass for clarity.

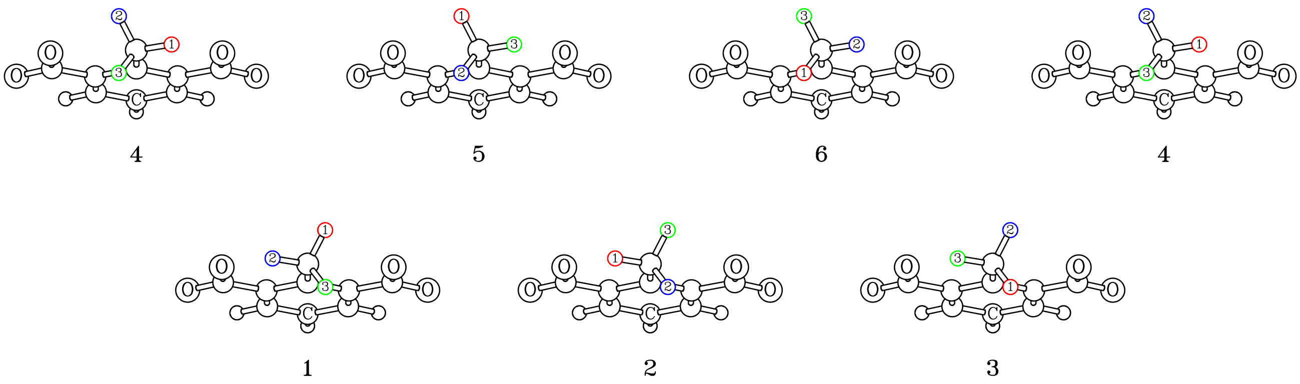

Figure S2: The geometry of the 6 minima of the 2,6-DNT isomer 2-dimensional potential energy surface drawn in the upper panel of Fig. 3 and corresponding to methyl group torsion in the weak steric hindrance limit. The numbering of the 6 minima is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and drawn respectively in red, blue, and green.

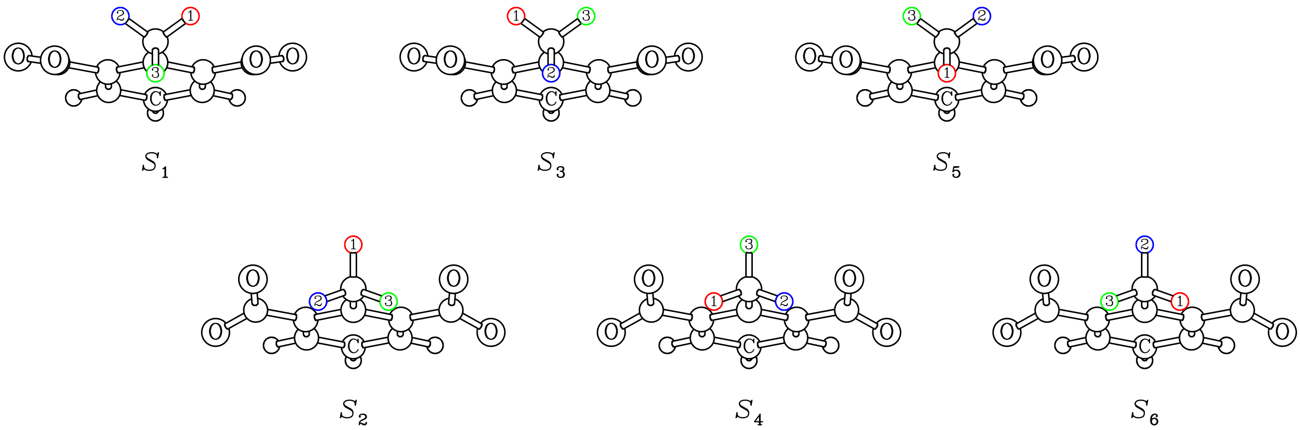

Figure S3: The geometry of the 6 stationary points of the 2,6-DNT isomer 2-dimensional potential energy surface drawn in the upper panel of Fig. 3 and corresponding to methyl group torsion in the weak steric hindrance limit. The labeling of the 6 stationary points is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and drawn respectively in red, blue, and green.

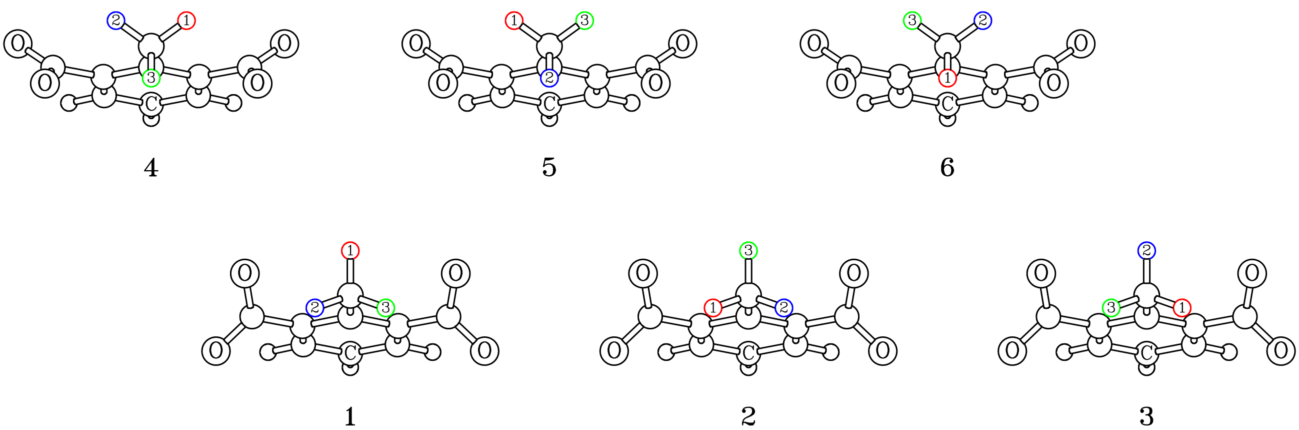

Figure S4: The geometry of the 6 minima of the 2,6-DNT isomer 2-dimensional potential energy surface drawn in the lower panel of Fig. 3 and corresponding to methyl group torsion in the strong steric hindrance limit. The numbering of the 6 minima is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and drawn respectively in red, blue, and green.

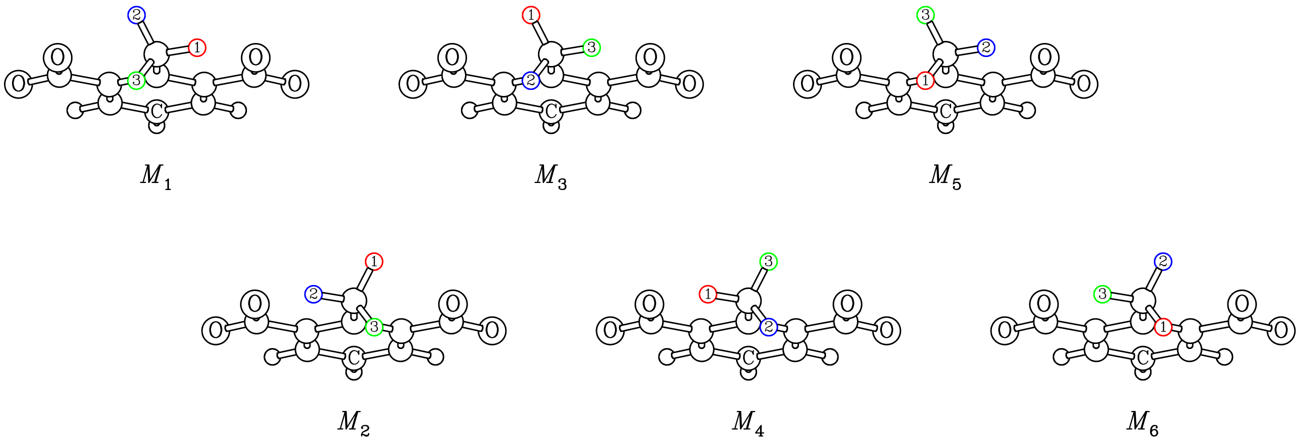

Figure S5: The geometry of the 6 maxima of the 2,6-DNT isomer 2-dimensional potential energy surface drawn in the lower panel of Fig. 3 and corresponding to methyl group torsion in the strong steric hindrance limit. The numbering of the 6 maxima is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and are drawn respectively in red, blue, and green.

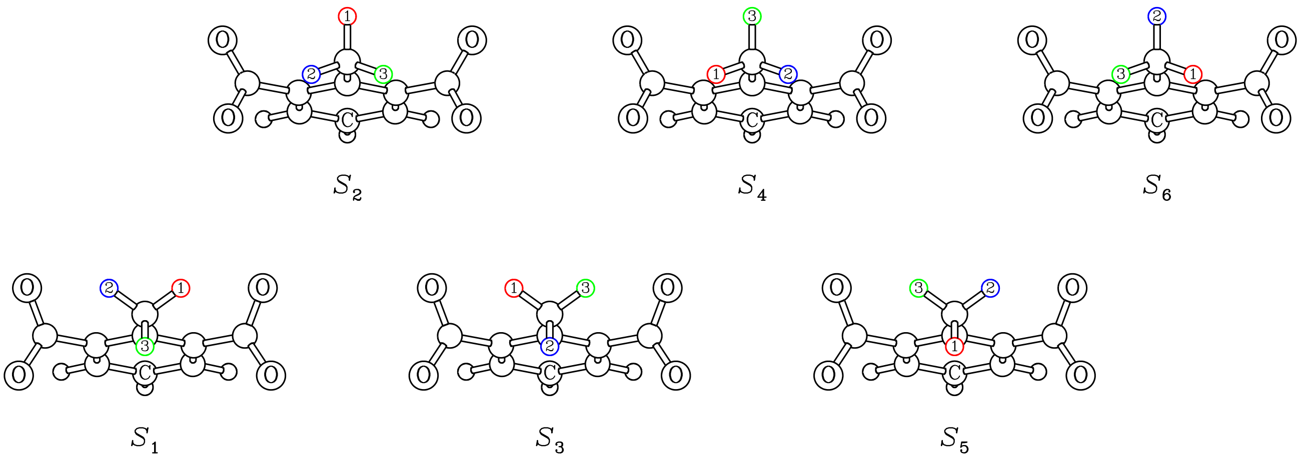

Figure S6: The geometry of the 6 stationary points of the 2,6-DNT isomer 2-dimensional potential energy surface drawn in the lower panel of Fig. 3 and corresponding to methyl group torsion in the strong steric hindrance limit. The numbering of the 6 stationary points is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and are drawn respectively in red, blue, and green.

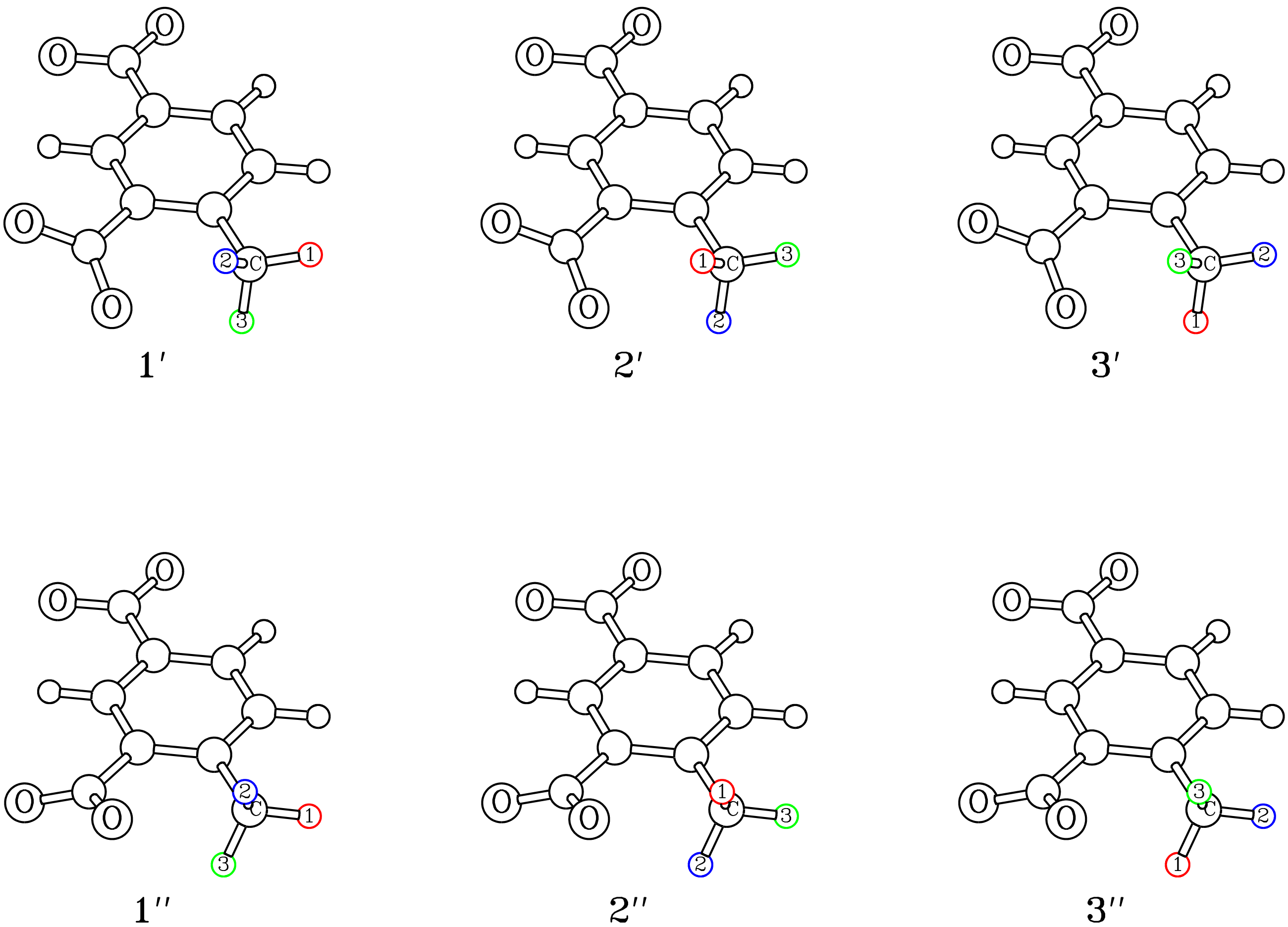

Figure S7: The geometry of the 6 minima of the 2,4-DNT isomer 2-dimensional potential energy surface drawn in Fig. 6. The minima are labeled using the pair identifier with a prime sign (′) or double prime sign (″). The hydrogen atoms of the methyl group are numbered 1 through 3 and drawn respectively in red, blue, and green.

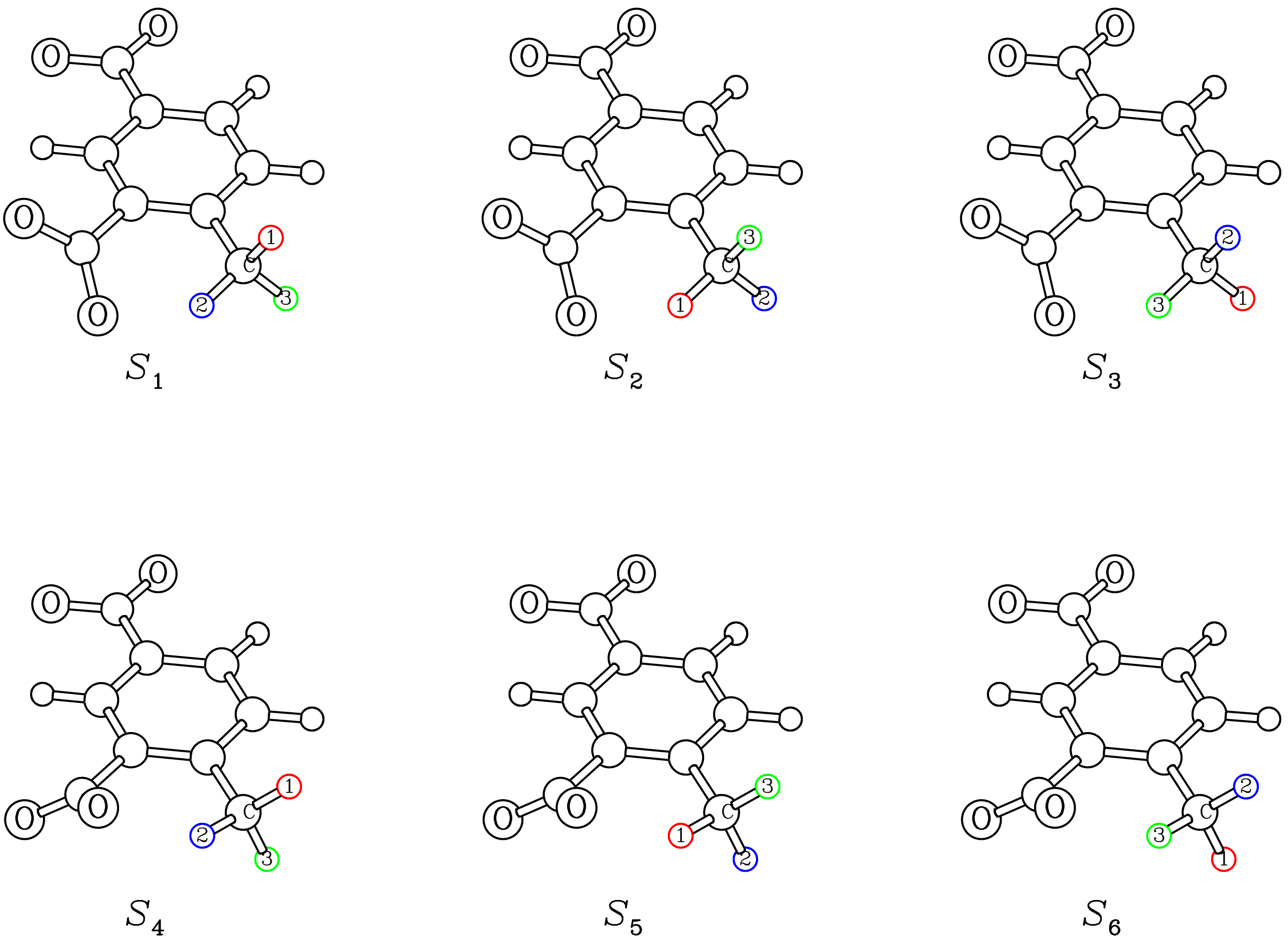

Figure S8: The geometry of the 6 stationary points of the 2,4-DNT isomer 2-dimensional potential energy surface drawn in Fig. 6. The labeling of the stationary points is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and are drawn respectively in red, blue, and green.

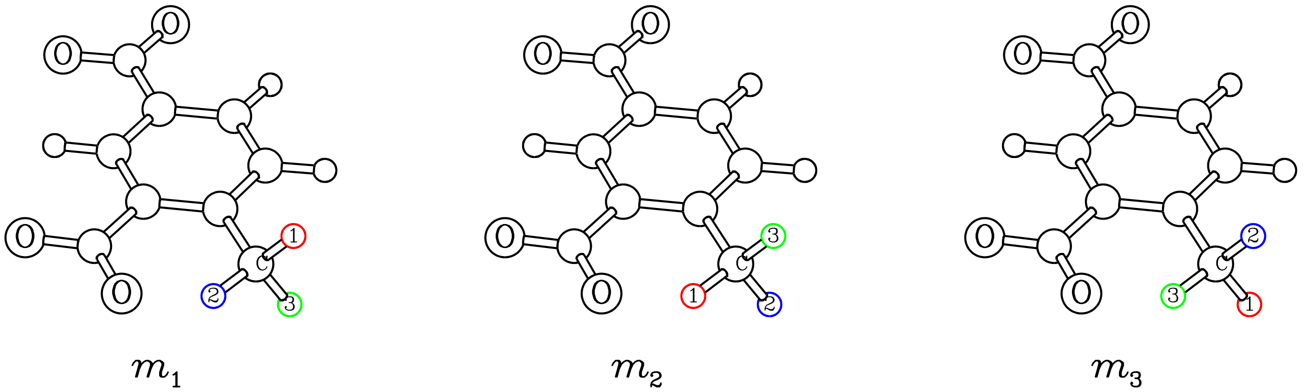

Figure S9: The geometry of the 3 local minima of the 2,4-DNT isomer 2-dimensional potential energy surface drawn in Fig. 6. The labeling of the local minima is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and are drawn respectively in red, blue, and green.

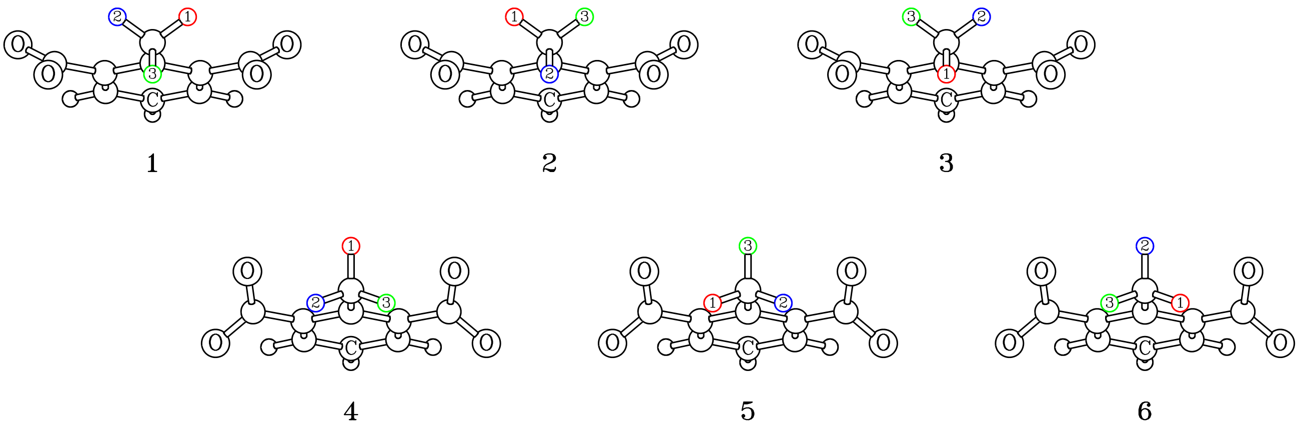

Figure S10: The geometry of the 6 minima of the 2,6-DNT isomer 2-dimensional potential energy surface drawn in Fig. 8. The numbering of the 6 minima is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and drawn respectively in red, blue, and green.

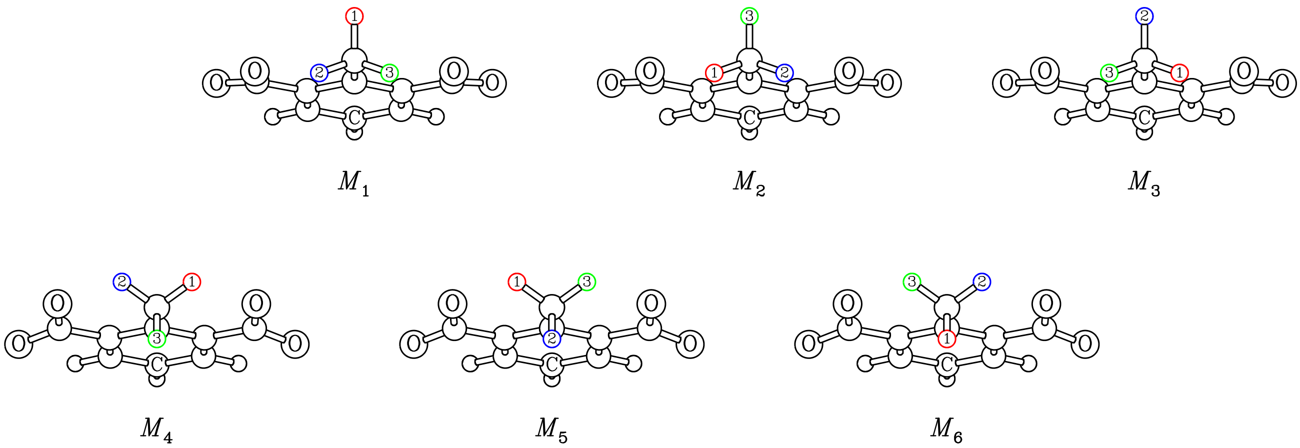

Figure S11: The geometry of the 6 maxima of the 2,6-DNT isomer 2-dimensional potential energy surface drawn in Fig. 8. The numbering of the 6 maxima is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and drawn respectively in red, blue, and green.

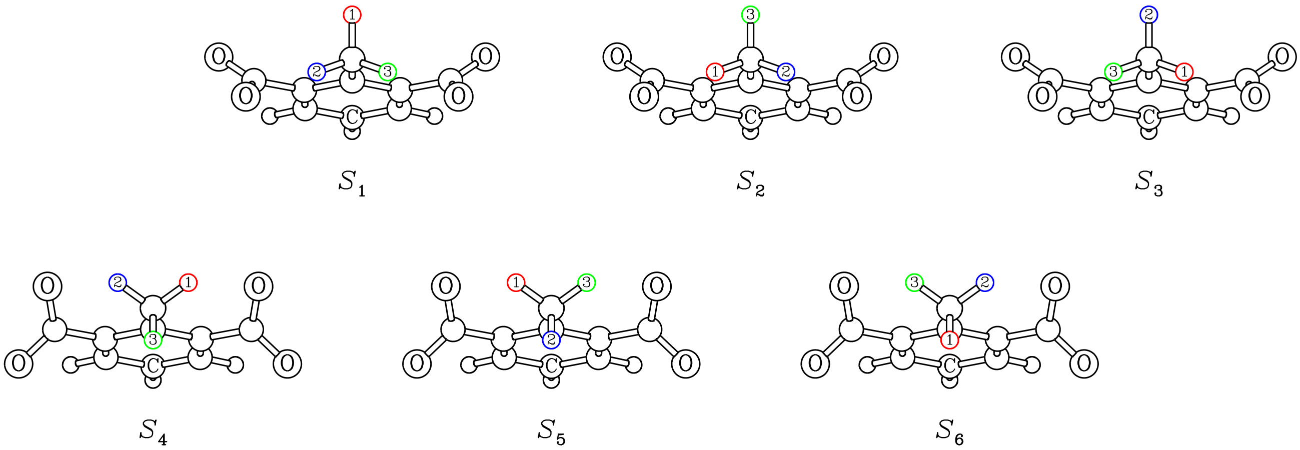

Figure S12: The geometry of the 6 stationary points of the 2,6-DNT isomer 2-dimensional potential energy surface drawn in Fig. 8. The numbering of the 6 stationary points is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and drawn respectively in red, blue, and green.

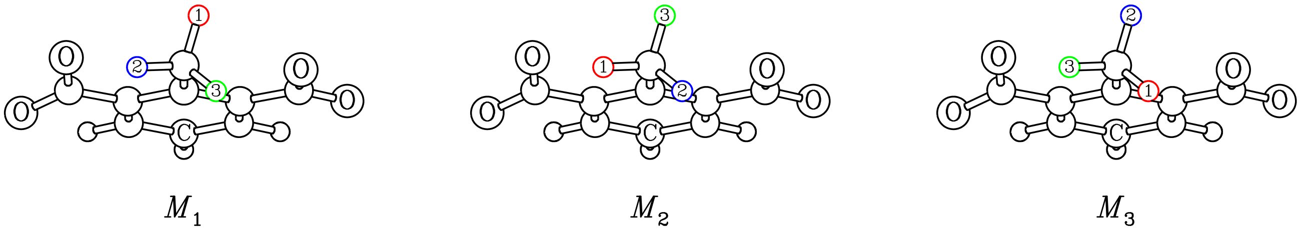

Figure S13: The geometry of the 3 maxima of the 2,6-DNT isomer 2-dimensional potential energy surface drawn in Fig. 10. The numbering of the 3 maxima is the same as in this figure. The hydrogen atoms of the methyl group are numbered 1 through 3 and drawn respectively in red, blue, and green.

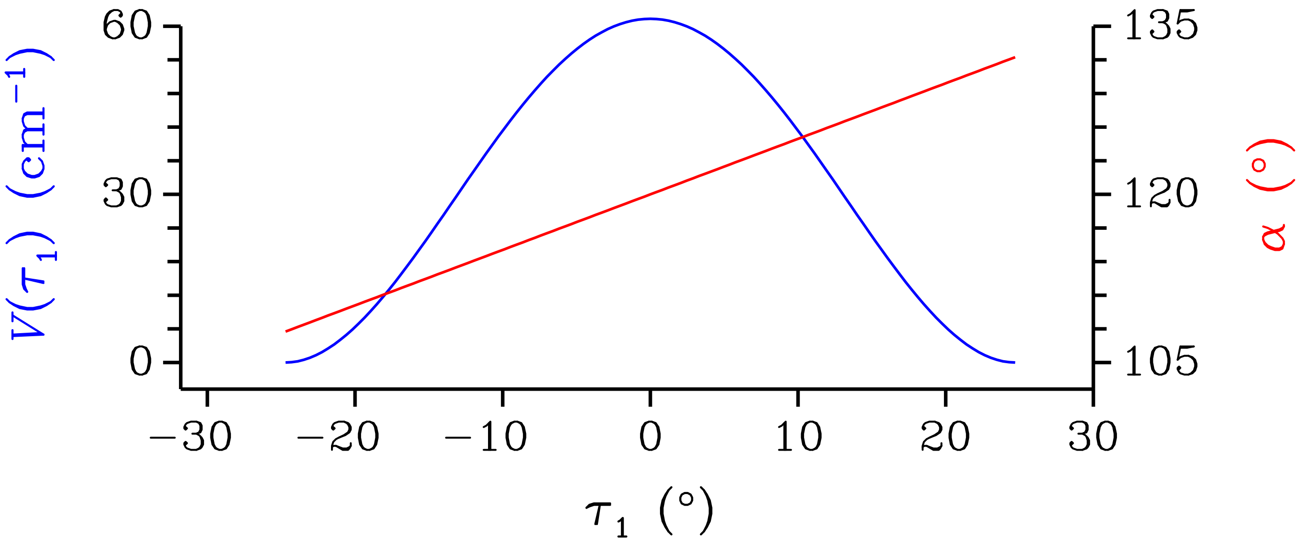

Figure S14: A cut of the 2-D potential energy surface of 2,4-DNT, as calculated at the B98/cc-pVTZ level of theory in the paper and shown in Fig. 6. The cut corresponds to a tunneling path allowing us to connect the two minima belonging to Pair 1. The potential energy, in cm^{-1}, blue curve, and the angle α, in degrees, red curve, are plotted as a function of the angle τ. The y-axes on the left and on the right should be used for the potential energy and the angle α, respectively.

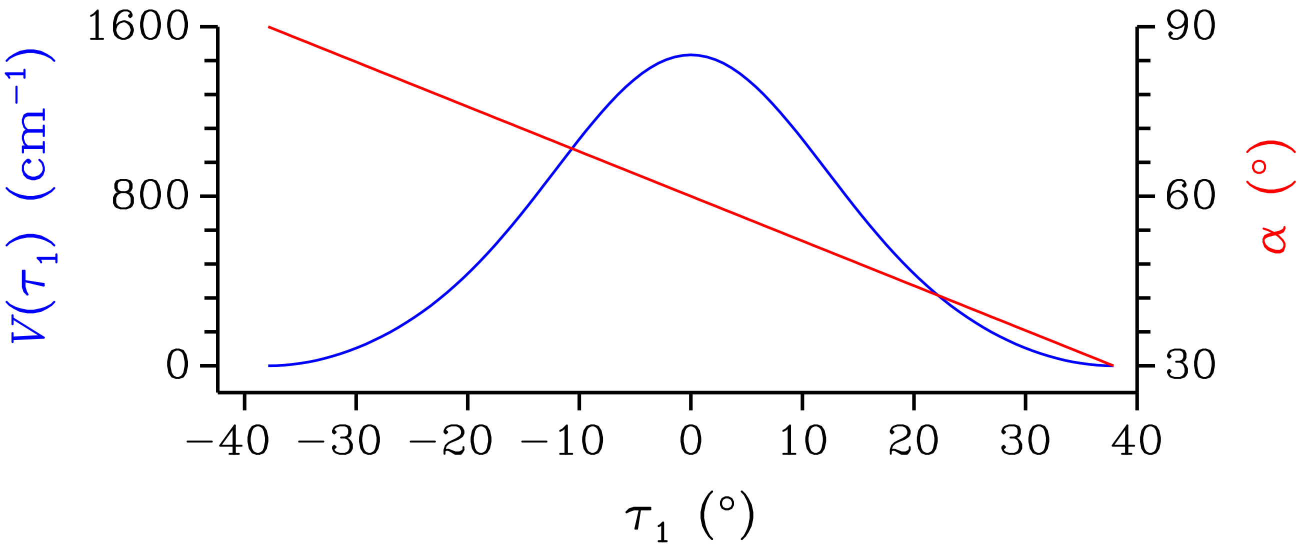

Figure S15: A cut of the 2-D potential energy surface of 2,6-DNT, as calculated at the B98/cc-pVTZ level of theory in the paper and shown in Fig. 8. The cut corresponds to the $1 \rightarrow 4$ tunneling path allowing us to go from equilibrium configuration 1 to equilibrium configuration 4. The potential energy, in cm^{-1}, blue curve, and the angle α, in degrees, red curve, are plotted as a function of the angle τ. The y-axes on the left and on the right should be used for the potential energy and the angle α, respectively.

References

[1] J. T. Hougen, *J. Mol. Spectrosc.*, 1985, **114**, 395–426.

[2] R. Brent, *ACM Transactions on Mathematical Software*, 1978, **4**, 71–81.

[3] L. H. Coudert and J. T. Hougen, *J. Mol. Spectrosc.*, 1988, **130**, 86–119.

Table S1: Measured frequencies ($\nu_{obs.}$) and residuals ($\nu_{obs.} - \nu_{calc.}$) in MHz of the 2,4 dinitrotoluene isomer

J'	K'_a	K'_c	I'	F'	←	J''	K''_a	K''_c	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
5	1	5	1	6	←	4	0	4	1	5	4871.7010	0.0044	0.002
5	1	5	1	4	←	4	0	4	1	3	4871.7010	0.0060	0.002
3	2	1	2	5	←	2	1	2	2	4	6182.3274	−0.0029	0.001
3	2	1	1	4	←	2	1	2	1	3	6182.4987	−0.0002	0.001
7	1	7	2	7	←	6	0	6	2	6	6293.7429	0.0001	0.002
7	1	7	2	9	←	6	0	6	2	8	6293.8170	0.0016	0.002
8	4	4	2	8	←	8	3	5	2	8	6683.1789	0.0041	0.005
8	0	8	2	7	←	7	1	7	2	6	6838.8531	−0.0007	0.005
8	0	8	2	6	←	7	1	7	2	5	6838.8587	−0.0020	0.005
8	0	8	2	8	←	7	1	7	2	7	6838.8587	−0.0017	0.005
8	0	8	0	8	←	7	1	7	0	7	6838.8668	0.0000	0.005
8	0	8	1	7	←	7	1	7	1	6	6838.8668	−0.0021	0.005
8	0	8	1	9	←	7	1	7	1	8	6838.8668	0.0037	0.005
8	0	8	1	8	←	7	1	7	1	7	6838.8668	−0.0017	0.005
8	0	8	2	9	←	7	1	7	2	8	6838.8739	0.0019	0.005
8	0	8	2	10	←	7	1	7	2	9	6838.8739	0.0008	0.005
7	2	5	1	6	←	6	2	4	1	5	7137.5173	−0.0001	0.002
7	2	5	2	8	←	6	2	4	2	7	7137.5173	−0.0001	0.002
7	2	5	2	6	←	6	2	4	2	5	7137.5246	0.0003	0.002
7	2	5	1	8	←	6	2	4	1	7	7137.5246	−0.0005	0.002
7	2	5	2	5	←	6	2	4	2	4	7137.5246	−0.0017	0.002
7	2	5	0	7	←	6	2	4	0	6	7137.5246	−0.0018	0.002
7	2	5	1	7	←	6	2	4	1	6	7137.5246	−0.0026	0.002
7	2	5	2	9	←	6	2	4	2	8	7137.5246	−0.0026	0.002
9	0	9	2	8	←	8	1	8	2	7	7700.3406	−0.0001	0.002
9	0	9	1	10	←	8	1	8	1	9	7700.3487	0.0010	0.002
9	0	9	2	10	←	8	1	8	2	9	7700.3534	−0.0003	0.002
9	0	9	2	11	←	8	1	8	2	10	7700.3588	0.0010	0.002
6	2	5	2	8	←	5	1	4	2	7	7736.6670	−0.0034	0.001
6	2	5	0	6	←	5	1	4	0	5	7736.6757	0.0010	0.001
6	2	5	1	6	←	5	1	4	1	5	7736.6867	0.0013	0.001
6	2	5	2	4	←	5	1	4	2	3	7736.6936	0.0022	0.001
10	2	9	2	10	←	9	2	8	2	9	9248.9131	0.0008	0.002
10	2	9	2	9	←	9	2	8	2	8	9248.9296	0.0021	0.005
10	2	9	1	11	←	9	2	8	1	10	9248.9296	0.0005	0.005
10	2	9	1	10	←	9	2	8	1	9	9248.9461	−0.0009	0.005
10	2	9	2	8	←	9	2	8	2	7	9248.9461	0.0004	0.005
10	2	9	2	12	←	9	2	8	2	11	9248.9461	−0.0014	0.005
10	2	9	0	10	←	9	2	8	0	9	9248.9461	−0.0004	0.005
9	2	8	2	9	←	8	1	7	2	8	9399.8607	−0.0018	0.005
9	2	8	1	8	←	8	1	7	2	7	9399.8689	0.0005	0.002
5	3	2	2	5	←	4	2	3	2	4	9948.9115	0.0025	0.002
12	0	12	2	12	←	11	1	11	2	11	10 204.5764	−0.0038	0.002
6	2	4	2	4	←	5	1	5	2	3	10 654.4884	−0.0001	0.001
6	2	4	2	6	←	5	1	5	2	5	10 655.1736	−0.0001	0.001

J'	K_a'	K_c'	I'	F'	←	J''	K_a''	K_c''	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
11	4	8	2	11	←	10	4	7	2	10	10 723.8987	−0.0001	0.002
11	4	8	2	12	←	10	4	7	2	11	10 723.9135	0.0022	0.002
11	4	8	1	10	←	10	4	7	1	9	10 723.9135	0.0017	0.002
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13	0	13	1	12	←	12	1	12	1	11	11 027.7532	0.0023	0.005
13	0	13	2	14	←	12	1	12	2	13	11 027.7532	0.0008	0.005
13	0	13	2	11	←	12	1	12	2	10	11 027.7532	0.0004	0.005
13	0	13	1	14	←	12	1	12	1	13	11 027.7532	0.0026	0.005
13	0	13	0	13	←	12	1	12	0	12	11 027.7568	0.0017	0.005
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13	1	12	1	14	←	12	2	11	1	13	11 669.4847	−0.0010	0.005
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13	2	12	2	15	←	12	1	11	2	14	11 982.2055	0.0005	0.002
13	2	12	0	13	←	12	1	11	0	12	11 982.2055	0.0004	0.002
13	2	12	1	13	←	12	1	11	1	12	11 982.2055	0.0002	0.002
13	2	12	2	11	←	12	1	11	2	10	11 982.2055	0.0002	0.002

J'	K'_a	K'_c	I'	F'	←	J''	K''_a	K''_c	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
7	2	5	2	9	←	6	1	6	2	8	12 552.7794	0.0021	0.001
7	2	5	2	7	←	6	1	6	2	6	12 553.3680	−0.0005	0.001
15	0	15	2	15	←	14	1	14	2	14	12 668.7943	0.0001	0.005
15	0	15	2	14	←	14	1	14	2	13	12 668.7943	−0.0020	0.005
15	0	15	1	14	←	14	1	14	1	13	12 668.8022	0.0038	0.005
15	0	15	2	16	←	14	1	14	2	15	12 668.8022	0.0025	0.005
15	0	15	2	13	←	14	1	14	2	12	12 668.8022	0.0019	0.005
15	0	15	0	15	←	14	1	14	0	14	12 668.8022	0.0001	0.005
15	0	15	1	16	←	14	1	14	1	15	12 668.8022	0.0036	0.005
15	0	15	1	15	←	14	1	14	1	14	12 668.8022	−0.0001	0.005
15	0	15	2	17	←	14	1	14	2	16	12 668.8022	−0.0015	0.005
14	2	13	2	14	←	13	1	12	2	13	12 734.6503	−0.0043	0.005
14	2	13	2	13	←	13	1	12	2	12	12 734.6706	−0.0033	0.005
14	2	13	2	15	←	13	1	12	2	14	12 734.6706	−0.0029	0.005
14	2	13	1	13	←	13	1	12	1	12	12 734.6706	−0.0029	0.005
14	2	13	1	15	←	13	1	12	1	14	12 734.6706	−0.0038	0.005
14	2	13	0	14	←	13	1	12	0	13	12 734.6952	0.0021	0.005
14	2	13	2	12	←	13	1	12	2	11	12 734.6952	0.0025	0.005
14	2	13	2	16	←	13	1	12	2	15	12 734.6952	0.0020	0.005
14	2	13	1	14	←	13	1	12	1	13	12 734.6952	0.0022	0.005
15	1	14	2	15	←	14	2	13	2	14	13 403.0512	−0.0018	0.002
15	1	14	2	14	←	14	2	13	2	13	13 403.0609	0.0001	0.002
15	1	14	1	16	←	14	2	13	1	15	13 403.0609	−0.0010	0.002
15	1	14	1	14	←	14	2	13	1	13	13 403.0609	−0.0012	0.002
15	1	14	2	16	←	14	2	13	2	15	13 403.0609	−0.0018	0.002
15	1	14	2	13	←	14	2	13	2	12	13 403.0716	0.0019	0.002
15	1	14	0	15	←	14	2	13	0	14	13 403.0716	0.0010	0.002
15	1	14	1	15	←	14	2	13	1	14	13 403.0716	0.0009	0.002
16	0	16	2	16	←	15	1	15	2	15	13 488.1457	0.0053	0.005
16	0	16	2	15	←	15	1	15	2	14	13 488.1457	0.0033	0.005
16	0	16	1	15	←	15	1	15	1	14	13 488.1457	0.0016	0.005
16	0	16	2	14	←	15	1	15	2	13	13 488.1457	−0.0001	0.005
16	0	16	0	16	←	15	1	15	0	15	13 488.1457	−0.0016	0.005
16	0	16	1	16	←	15	1	15	1	15	13 488.1457	−0.0018	0.005
16	1	16	2	16	←	15	1	15	2	15	13 488.6970	0.0050	0.005
16	1	16	2	15	←	15	1	15	2	14	13 488.6970	0.0030	0.005
16	1	16	1	15	←	15	1	15	1	14	13 488.6970	0.0013	0.005
16	1	16	2	14	←	15	1	15	2	13	13 488.6970	−0.0004	0.005
16	1	16	0	16	←	15	1	15	0	15	13 488.6970	−0.0019	0.005
16	1	16	1	16	←	15	1	15	1	15	13 488.6970	−0.0022	0.005
16	1	16	2	16	←	15	0	15	2	15	13 489.7573	0.0054	0.005
16	1	16	2	15	←	15	0	15	2	14	13 489.7573	0.0033	0.005
16	1	16	1	15	←	15	0	15	1	14	13 489.7573	0.0017	0.005
16	1	16	2	14	←	15	0	15	2	13	13 489.7573	−0.0002	0.005
16	1	16	0	16	←	15	0	15	0	15	13 489.7573	−0.0017	0.005
16	1	16	1	16	←	15	0	15	1	15	13 489.7573	−0.0019	0.005

J'	K_a'	K_c'	I'	F'	←	J''	K_a''	K_c''	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
15	2	14	2	15	←	14	1	13	2	14	13 511.9023	−0.0029	0.002
15	2	14	2	14	←	14	1	13	2	13	13 511.9194	−0.0009	0.002
15	2	14	1	16	←	14	1	13	1	15	13 511.9194	−0.0016	0.002
15	2	14	1	14	←	14	1	13	1	13	13 511.9194	−0.0004	0.002
15	2	14	2	16	←	14	1	13	2	15	13 511.9194	−0.0006	0.002
15	2	14	2	13	←	14	1	13	2	12	13 511.9378	0.0030	0.002
15	2	14	0	15	←	14	1	13	0	14	13 511.9378	0.0024	0.002
15	2	14	1	15	←	14	1	13	1	14	13 511.9378	0.0025	0.002
15	2	14	2	17	←	14	1	13	2	16	13 511.9378	0.0020	0.002
7	4	3	2	9	←	6	3	4	2	8	13 809.1542	0.0021	0.002
16	1	15	2	16	←	15	2	14	2	15	14 242.9662	−0.0017	0.002
16	1	15	2	15	←	15	2	14	2	14	14 242.9756	−0.0004	0.002
16	1	15	1	15	←	15	2	14	1	14	14 242.9756	−0.0011	0.002
16	1	15	2	14	←	15	2	14	2	13	14 242.9864	0.0018	0.002
16	1	15	0	16	←	15	2	14	0	15	14 242.9864	0.0009	0.002
16	1	15	1	16	←	15	2	14	1	15	14 242.9864	0.0009	0.002
16	2	15	2	16	←	15	2	14	2	15	14 265.5461	−0.0011	0.002
16	2	15	2	15	←	15	2	14	2	14	14 265.5566	−0.0001	0.002
16	2	15	1	17	←	15	2	14	1	16	14 265.5566	−0.0011	0.002
16	2	15	1	15	←	15	2	14	1	14	14 265.5566	−0.0004	0.002
16	2	15	2	17	←	15	2	14	2	16	14 265.5566	−0.0009	0.002
16	2	15	2	14	←	15	2	14	2	13	14 265.5680	0.0015	0.002
16	2	15	0	16	←	15	2	14	0	15	14 265.5680	0.0007	0.002
16	2	15	1	16	←	15	2	14	1	15	14 265.5680	0.0007	0.002
16	2	15	2	18	←	15	2	14	2	17	14 265.5680	0.0001	0.002
16	2	15	2	16	←	15	1	14	2	15	14 305.3471	−0.0031	0.002
16	2	15	2	15	←	15	1	14	2	14	14 305.3617	−0.0007	0.002
16	2	15	1	17	←	15	1	14	1	16	14 305.3617	−0.0015	0.002
16	2	15	1	15	←	15	1	14	1	14	14 305.3617	−0.0002	0.002
16	2	15	2	17	←	15	1	14	2	16	14 305.3617	−0.0006	0.002
16	2	15	2	14	←	15	1	14	2	13	14 305.3773	0.0032	0.002
16	2	15	0	16	←	15	1	14	0	15	14 305.3773	0.0025	0.002
16	2	15	1	16	←	15	1	14	1	15	14 305.3773	0.0026	0.002
16	2	15	2	18	←	15	1	14	2	17	14 305.3773	0.0021	0.002
17	0	17	2	16	←	16	1	16	2	15	14 307.1694	0.0024	0.002
17	0	17	1	16	←	16	1	16	1	15	14 307.1694	0.0011	0.002
17	0	17	2	15	←	16	1	16	2	14	14 307.1694	−0.0005	0.002
17	1	17	2	16	←	16	1	16	2	15	14 307.4537	0.0015	0.002
17	1	17	1	16	←	16	1	16	1	15	14 307.4537	0.0001	0.002
17	1	17	2	15	←	16	1	16	2	14	14 307.4537	−0.0014	0.002
17	1	17	2	16	←	16	0	16	2	15	14 308.0061	0.0023	0.002
17	1	17	1	16	←	16	0	16	1	15	14 308.0061	0.0010	0.002
17	1	17	2	15	←	16	0	16	2	14	14 308.0061	−0.0007	0.002
8	2	6	2	8	←	7	1	7	2	7	14 651.5694	−0.0002	0.001
8	4	4	2	6	←	7	3	5	2	5	14 809.2848	−0.0015	0.001
8	4	4	1	8	←	7	3	5	1	7	14 809.2953	0.0001	0.001
8	4	4	2	7	←	7	3	5	2	6	14 809.3342	−0.0008	0.001
6	5	2	2	4	←	5	4	1	2	3	14 836.0507	0.0015	0.002
6	5	1	2	6	←	5	4	2	2	5	14 836.6131	−0.0018	0.002

J'	K_a'	K_c'	I'	F'	←	J''	K_a''	K_c''	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
17	1	16	2	16	←	16	2	15	2	15	15 073.7179	−0.0004	0.002
17	1	16	1	16	←	16	2	15	1	15	15 073.7179	−0.0006	0.002
17	1	16	2	15	←	16	2	15	2	14	15 073.7281	0.0017	0.002
17	2	16	2	17	←	16	1	15	2	16	15 108.9249	−0.0015	0.002
17	2	16	2	16	←	16	1	15	2	15	15 108.9364	−0.0002	0.002
17	2	16	1	16	←	16	1	15	1	15	15 108.9364	0.0002	0.002
17	2	16	1	18	←	16	1	15	1	17	15 108.9364	−0.0010	0.002
17	2	16	2	18	←	16	1	15	2	17	15 108.9364	−0.0001	0.002
17	2	16	2	15	←	16	1	15	2	14	15 108.9487	0.0024	0.002
17	2	16	0	17	←	16	1	15	0	16	15 108.9487	0.0017	0.002
17	2	16	1	17	←	16	1	15	1	16	15 108.9487	0.0018	0.002
17	2	16	2	19	←	16	1	15	2	18	15 108.9487	0.0012	0.002
18	0	18	2	16	←	17	1	17	2	15	15 126.0276	−0.0006	0.002
18	1	18	2	16	←	17	0	17	2	15	15 126.4594	−0.0008	0.002
7	5	3	2	9	←	6	4	2	2	8	15 795.5887	0.0012	0.002
7	5	3	2	7	←	6	4	2	2	6	15 795.6666	−0.0006	0.002
7	5	2	2	5	←	6	4	3	2	4	15 797.9939	−0.0016	0.002
7	5	2	2	8	←	6	4	3	2	7	15 798.0536	0.0028	0.002
7	5	2	2	7	←	6	4	3	2	6	15 798.0865	0.0001	0.002
18	1	17	1	17	←	17	2	16	1	16	15 899.0273	−0.0010	0.002
18	1	17	2	17	←	17	2	16	2	16	15 899.0273	−0.0011	0.002
18	1	17	2	19	←	17	2	16	2	18	15 899.0273	−0.0015	0.002
18	1	17	1	19	←	17	2	16	1	18	15 899.0273	−0.0019	0.002
18	1	17	2	16	←	17	2	16	2	15	15 899.0369	0.0011	0.002
18	1	17	0	18	←	17	2	16	0	17	15 899.0369	0.0004	0.002
18	1	17	1	18	←	17	2	16	1	17	15 899.0369	0.0004	0.002
18	1	17	2	20	←	17	2	16	2	19	15 899.0369	−0.0002	0.002
18	2	17	2	18	←	17	1	16	2	17	15 918.6462	−0.0020	0.002
18	2	17	2	17	←	17	1	16	2	16	15 918.6568	−0.0002	0.002
18	2	17	1	17	←	17	1	16	1	16	15 918.6568	0.0002	0.002
18	2	17	1	19	←	17	1	16	1	18	15 918.6568	−0.0010	0.002
18	2	17	2	19	←	17	1	16	2	18	15 918.6568	−0.0002	0.002
18	2	17	2	16	←	17	1	16	2	15	15 918.6682	0.0029	0.002
18	2	17	0	18	←	17	1	16	0	17	15 918.6682	0.0022	0.002
18	2	17	1	18	←	17	1	16	1	17	15 918.6682	0.0023	0.002
18	2	17	2	20	←	17	1	16	2	19	15 918.6692	0.0027	0.002
19	2	18	2	19	←	18	1	17	2	18	16 732.0200	−0.0002	0.100
19	2	18	2	18	←	18	1	17	2	17	16 732.0288	0.0009	0.005
19	2	18	1	18	←	18	1	17	1	17	16 732.0288	0.0013	0.005
19	2	18	1	20	←	18	1	17	1	19	16 732.0288	0.0001	0.005
19	2	18	2	20	←	18	1	17	2	19	16 732.0288	0.0009	0.005
19	2	18	2	17	←	18	1	17	2	16	16 732.0375	0.0024	0.002
19	2	18	0	19	←	18	1	17	0	18	16 732.0375	0.0018	0.002
19	2	18	1	19	←	18	1	17	1	18	16 732.0375	0.0018	0.002
19	2	18	2	21	←	18	1	17	2	20	16 732.0375	0.0012	0.002

Table S2: Measured frequencies ($\nu_{\mathrm{obs.}}$) and residuals ($\nu_{\mathrm{obs.}} - \nu_{\mathrm{calc.}}$) in MHz of the 2,6 dinitrotoluene isomer

J'	K_a'	K_c'	I'	F'	←	J''	K_a''	K_c''	I''	F''	$\nu_{\mathrm{obs.}}$	$\nu_{\mathrm{obs.}} - \nu_{\mathrm{calc.}}$	exp. error
4	0	4	1	5	←	3	1	3	1	4	3310.7904	−0.0020	0.002
4	0	4	2	6	←	3	1	3	2	5	3310.8243	0.0019	0.002
7	2	6	2	9	←	7	1	7	2	9	5111.5202	−0.0021	0.002
7	1	6	2	9	←	6	2	5	2	8	5633.4364	0.0016	0.002
3	2	2	1	2	←	2	1	1	1	1	6022.9959	−0.0017	0.002
4	2	3	1	4	←	3	1	2	1	3	6851.4975	−0.0009	0.002
7	1	7	2	7	←	6	0	6	2	6	6870.0577	0.0008	0.005
7	1	7	2	6	←	6	0	6	2	5	6870.0700	0.0000	0.005
7	1	7	0	7	←	6	0	6	0	6	6870.0988	−0.0001	0.000
7	4	3	2	8	←	7	3	4	2	8	7110.6056	0.0014	0.001
7	4	3	2	7	←	7	3	4	2	7	7110.6715	−0.0002	0.001
6	4	2	2	6	←	6	3	3	2	6	7199.4768	−0.0003	0.005
9	4	6	2	9	←	9	3	7	2	9	7309.1867	−0.0004	0.002
8	1	8	2	8	←	7	0	7	2	7	7693.2749	−0.0002	0.002
8	1	8	2	10	←	7	0	7	2	9	7693.3115	0.0016	0.005
3	3	1	2	5	←	2	2	0	2	4	8305.3468	−0.0020	0.002
4	3	1	2	2	←	3	2	2	2	1	9379.9997	−0.0011	0.002
4	3	1	0	4	←	3	2	2	0	3	9380.0237	−0.0011	0.002
4	3	1	1	4	←	3	2	2	1	3	9380.0313	0.0009	0.002
4	3	1	2	6	←	3	2	2	2	5	9380.0485	−0.0007	0.002
4	3	1	1	5	←	3	2	2	1	4	9380.1235	−0.0009	0.002
4	3	1	1	3	←	3	2	2	1	2	9380.1482	−0.0004	0.002
4	3	1	2	4	←	3	2	2	2	3	9380.2311	−0.0010	0.002
11	0	11	2	11	←	10	1	10	2	10	10 237.6080	−0.0006	0.002
11	1	11	2	11	←	10	0	10	2	10	10 285.9167	−0.0011	0.002
11	1	11	2	11	←	10	0	10	2	10	10 285.9169	−0.0009	0.002
5	3	2	2	3	←	4	2	3	2	2	10 475.8484	−0.0017	0.001
5	3	2	2	7	←	4	2	3	2	6	10 475.8958	−0.0013	0.002
5	3	2	1	4	←	4	2	3	1	3	10 475.9905	−0.0007	0.001
5	3	2	2	5	←	4	2	3	2	4	10 476.0700	0.0003	0.002
11	1	10	2	9	←	10	2	9	2	8	10 568.2988	0.0032	0.002
11	1	10	0	11	←	10	2	9	0	10	10 568.2988	0.0009	0.002
11	1	10	1	11	←	10	2	9	1	10	10 568.2988	0.0005	0.002
11	1	10	2	10	←	10	2	9	2	9	10 568.2988	0.0050	0.002
11	1	10	2	13	←	10	2	9	2	12	10 568.2988	−0.0013	0.002
11	1	10	1	10	←	10	2	9	1	9	10 568.2988	−0.0004	0.002
11	1	10	1	12	←	10	2	9	1	11	10 568.2988	0.0018	0.002
11	1	10	2	12	←	10	2	9	2	11	10 568.2988	−0.0019	0.002
11	1	10	2	11	←	10	2	9	2	10	10 568.2988	0.0017	0.002
10	2	9	1	11	←	9	1	8	1	10	10 857.9832	−0.0007	0.005
10	2	9	2	9	←	9	1	8	2	8	10 857.9832	−0.0011	0.005
10	2	9	2	11	←	9	1	8	2	10	10 857.9832	0.0011	0.005
10	2	9	1	9	←	9	1	8	1	8	10 857.9832	0.0001	0.005
10	2	9	2	12	←	9	1	8	2	11	10 858.0166	0.0001	0.005
10	2	9	0	10	←	9	1	8	0	9	10 858.0166	−0.0007	0.005
10	2	9	1	10	←	9	1	8	1	9	10 858.0166	−0.0009	0.005
10	2	9	2	8	←	9	1	8	2	7	10 858.0166	−0.0015	0.005
12	0	12	2	12	←	11	1	11	2	11	11 145.2931	−0.0002	0.002
12	1	12	2	12	←	11	0	11	2	11	11 172.3284	−0.0001	0.002

J'	K_a'	K_c'	I'	F'	$\leftarrow$	J''	K_a''	K_c''	I''	F''	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error
9	6	4	2	7	←	9	5	5	2	7	11 394.5838	−0.0033	0.002
9	6	4	0	9	←	9	5	5	0	9	11 394.5975	0.0002	0.002
9	6	4	1	9	←	9	5	5	1	9	11 394.5975	−0.0008	0.002
9	6	4	2	11	←	9	5	5	2	11	11 394.6094	0.0019	0.002
9	6	4	2	9	←	9	5	5	2	9	11 394.7885	0.0001	0.002
8	6	2	0	8	←	8	5	3	0	8	11 414.5720	0.0001	0.002
4	4	1	2	6	←	3	3	0	2	5	11 429.9707	−0.0001	0.005
4	4	1	1	4	←	3	3	0	1	3	11 429.9787	0.0013	0.005
4	4	1	1	3	←	3	3	0	1	2	11 430.0062	0.0030	0.005
4	4	1	2	4	←	3	3	0	2	3	11 430.0658	−0.0005	0.001
4	4	0	2	6	←	3	3	1	2	5	11 430.8027	0.0007	0.002
4	4	0	1	4	←	3	3	1	1	3	11 430.8103	0.0018	0.002
4	4	0	1	5	←	3	3	1	1	4	11 430.8527	0.0009	0.002
4	4	0	2	3	←	3	3	1	2	2	11 430.8860	−0.0038	0.002
4	4	0	2	4	←	3	3	1	2	3	11 430.8979	−0.0003	0.002
11	2	10	2	11	←	10	1	9	2	10	11 539.0618	0.0022	0.002
11	2	10	2	12	←	10	1	9	2	11	11 539.0882	0.0012	0.002
11	2	10	1	10	←	10	1	9	1	9	11 539.0882	0.0006	0.002
11	2	10	2	10	←	10	1	9	2	9	11 539.0882	0.0005	0.002
11	2	10	1	12	←	10	1	9	1	11	11 539.0882	0.0004	0.002
11	2	10	2	13	←	10	1	9	2	12	11 539.1152	0.0002	0.002
11	2	10	0	11	←	10	1	9	0	10	11 539.1152	0.0001	0.002
11	2	10	1	11	←	10	1	9	1	10	11 539.1152	−0.0001	0.002
11	2	10	2	9	←	10	1	9	2	8	11 539.1152	−0.0001	0.002
6	3	3	2	4	←	5	2	4	2	3	11 631.1382	0.0010	0.002
6	3	3	0	6	←	5	2	4	0	5	11 631.1571	0.0004	0.002
6	3	3	1	6	←	5	2	4	1	5	11 631.1571	−0.0036	0.002
6	3	3	2	8	←	5	2	4	2	7	11 631.1765	0.0001	0.002
6	3	3	2	7	←	5	2	4	2	6	11 631.2771	−0.0002	0.002
6	3	3	2	6	←	5	2	4	2	5	11 631.3436	0.0007	0.002
13	0	13	2	13	←	12	1	12	2	12	12 048.5090	−0.0011	0.005
13	0	13	2	12	←	12	1	12	2	11	12 048.5090	−0.0012	0.005
13	0	13	2	15	←	12	1	12	2	14	12 048.5179	−0.0013	0.005
12	2	11	2	12	←	11	1	10	2	11	12 269.6952	0.0017	0.005
12	2	11	2	13	←	11	1	10	2	12	12 269.7158	0.0003	0.005
12	2	11	1	11	←	11	1	10	1	10	12 269.7158	0.0001	0.005
12	2	11	1	13	←	11	1	10	1	12	12 269.7158	0.0003	0.005
12	2	11	2	11	←	11	1	10	2	10	12 269.7158	0.0009	0.005
12	2	11	2	14	←	11	1	10	2	13	12 269.7371	−0.0001	0.005
12	2	11	0	12	←	11	1	10	0	11	12 269.7371	0.0001	0.005
12	2	11	1	12	←	11	1	10	1	11	12 269.7371	−0.0001	0.005
12	2	11	2	10	←	11	1	10	2	9	12 269.7371	0.0002	0.005
5	4	2	2	3	←	4	3	1	2	2	12 462.6350	0.0053	0.005
5	4	2	1	6	←	4	3	1	1	5	12 462.7023	0.0033	0.002
5	4	2	2	6	←	4	3	1	2	5	12 462.7132	0.0001	0.005
5	4	2	2	5	←	4	3	1	2	4	12 462.7665	−0.0004	0.002
13	1	12	2	11	←	12	2	11	2	10	12 646.9768	0.0025	0.005
13	1	12	0	13	←	12	2	11	0	12	12 646.9768	0.0011	0.005
13	1	12	1	13	←	12	2	11	1	12	12 646.9768	0.0008	0.005
13	1	12	2	15	←	12	2	11	2	14	12 646.9768	−0.0003	0.005

J'	K_a'	K_c'	I'	F'	←	J''	K_a''	K_c''	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
7	3	4	2	8	←	6	2	5	2	7	12 878.3608	0.0007	0.002
13	2	12	2	13	←	12	1	11	2	12	13 047.8113	−0.0068	0.005
13	2	12	2	12	←	12	1	11	2	11	13 047.8345	0.0003	0.005
13	2	12	1	14	←	12	1	11	1	13	13 047.8345	−0.0005	0.005
13	2	12	2	14	←	12	1	11	2	13	13 047.8345	−0.0012	0.005
13	2	12	1	12	←	12	1	11	1	11	13 047.8345	−0.0010	0.005
13	2	12	0	13	←	12	1	11	0	12	13 047.8532	0.0012	0.005
13	2	12	2	11	←	12	1	11	2	10	13 047.8532	0.0017	0.005
13	2	12	2	15	←	12	1	11	2	14	13 047.8532	0.0007	0.005
13	2	12	1	13	←	12	1	11	1	12	13 047.8578	0.0057	0.005
6	4	3	2	4	←	5	3	2	2	3	13 485.4292	0.0018	0.005
6	4	3	1	7	←	5	3	2	1	6	13 485.5000	0.0061	0.002
6	4	3	2	7	←	5	3	2	2	6	13 485.5107	−0.0002	0.005
6	4	3	2	6	←	5	3	2	2	5	13 485.5571	−0.0001	0.002
6	4	2	0	6	←	5	3	3	0	5	13 509.0249	−0.0003	0.002
6	4	2	1	6	←	5	3	3	1	5	13 509.0387	0.0116	0.005
6	4	2	2	5	←	5	3	3	2	4	13 509.0737	0.0002	0.002
6	4	2	1	5	←	5	3	3	1	4	13 509.0936	−0.0047	0.005
6	4	2	2	7	←	5	3	3	2	6	13 509.1060	0.0002	0.002
6	4	2	2	6	←	5	3	3	2	5	13 509.1559	0.0002	0.002
8	7	2	1	7	←	8	6	3	1	7	13 512.4050	−0.0026	0.002
8	7	1	2	9	←	8	6	2	2	9	13 512.4133	−0.0005	0.002
8	7	2	2	9	←	8	6	3	2	9	13 512.4215	0.0007	0.002
8	7	1	2	8	←	8	6	2	2	8	13 512.5314	−0.0016	0.002
8	7	2	2	8	←	8	6	3	2	8	13 512.5410	0.0010	0.002
14	1	13	2	14	←	13	2	12	2	13	13 618.6712	−0.0013	0.002
14	1	13	2	13	←	13	2	12	2	12	13 618.6780	0.0014	0.002
14	1	13	1	15	←	13	2	12	1	14	13 618.6780	−0.0001	0.002
14	1	13	1	13	←	13	2	12	1	12	13 618.6780	−0.0012	0.002
14	1	13	2	15	←	13	2	12	2	14	13 618.6780	−0.0020	0.002
14	1	13	2	12	←	13	2	12	2	11	13 618.6851	0.0020	0.002
14	1	13	0	14	←	13	2	12	0	13	13 618.6851	0.0008	0.002
14	1	13	1	14	←	13	2	12	1	13	13 618.6851	0.0006	0.002
14	1	13	2	16	←	13	2	12	2	15	13 618.6851	−0.0003	0.002
10	3	8	2	8	←	9	2	7	2	7	13 811.8180	−0.0026	0.002
14	2	13	2	14	←	13	1	12	2	13	13 864.7702	−0.0040	0.005
14	2	13	2	13	←	13	1	12	2	12	13 864.7867	0.0003	0.002
14	2	13	1	15	←	13	1	12	1	14	13 864.7867	−0.0006	0.002
14	2	13	1	13	←	13	1	12	1	12	13 864.7867	−0.0012	0.002
14	2	13	2	15	←	13	1	12	2	14	13 864.7867	−0.0016	0.002
14	2	13	2	12	←	13	1	12	2	11	13 864.8023	0.0023	0.002
14	2	13	0	14	←	13	1	12	0	13	13 864.8023	0.0017	0.002
14	2	13	1	14	←	13	1	12	1	13	13 864.8023	0.0015	0.002
14	2	13	2	16	←	13	1	12	2	15	13 864.8023	0.0010	0.002
11	3	9	2	9	←	10	2	8	2	8	14 310.4236	−0.0022	0.002
7	4	4	2	6	←	6	3	3	2	5	14 486.8579	0.0006	0.002
7	4	4	2	8	←	6	3	3	2	7	14 486.8821	0.0001	0.002
7	4	4	2	7	←	6	3	3	2	6	14 486.9197	0.0010	0.005

J'	K_a'	K_c'	I'	F'	←	J''	K_a''	K_c''	I''	F''	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error
5	5	1	2	7	←	4	4	0	2	6	14 548.2413	−0.0005	0.002
5	5	1	1	5	←	4	4	0	1	4	14 548.2492	0.0008	0.002
5	5	1	1	6	←	4	4	0	1	5	14 548.2840	0.0057	0.002
5	5	0	2	7	←	4	4	1	2	6	14 548.2916	0.0081	0.002
5	5	0	1	6	←	4	4	1	1	5	14 548.3172	−0.0027	0.002
5	5	0	2	4	←	4	4	1	2	3	14 548.3421	−0.0020	0.002
5	5	0	2	5	←	4	4	1	2	4	14 548.3495	0.0006	0.002
7	4	3	2	5	←	6	3	4	2	4	14 557.4945	0.0033	0.001
7	4	3	0	7	←	6	3	4	0	6	14 557.5002	−0.0007	0.002
7	4	3	1	7	←	6	3	4	1	6	14 557.5002	−0.0024	0.002
7	4	3	2	9	←	6	3	4	2	8	14 557.5124	0.0015	0.002
7	4	3	2	6	←	6	3	4	2	5	14 557.5449	0.0005	0.002
7	4	3	1	6	←	6	3	4	1	5	14 557.5642	−0.0030	0.002
7	4	3	2	8	←	6	3	4	2	7	14 557.5746	0.0007	0.002
7	4	3	2	7	←	6	3	4	2	6	14 557.6184	−0.0003	0.001
15	2	14	2	15	←	14	1	13	2	14	14 710.2163	−0.0033	0.002
15	2	14	2	14	←	14	1	13	2	13	14 710.2300	0.0010	0.002
15	2	14	1	16	←	14	1	13	1	15	14 710.2300	−0.0001	0.002
15	2	14	1	14	←	14	1	13	1	13	14 710.2300	−0.0007	0.002
15	2	14	2	16	←	14	1	13	2	15	14 710.2300	−0.0011	0.002
15	2	14	2	13	←	14	1	13	2	12	14 710.2437	0.0037	0.002
15	2	14	0	15	←	14	1	13	0	14	14 710.2437	0.0030	0.002
15	2	14	1	15	←	14	1	13	1	14	14 710.2437	0.0029	0.002
15	2	14	2	17	←	14	1	13	2	16	14 710.2437	0.0023	0.002
16	1	16	2	16	←	15	0	15	2	15	14 749.0651	0.0057	0.005
16	1	16	2	15	←	15	0	15	2	14	14 749.0651	0.0054	0.005
16	1	16	1	15	←	15	0	15	1	14	14 749.0651	0.0021	0.005
16	1	16	2	17	←	15	0	15	2	16	14 749.0651	0.0010	0.005
16	1	16	1	17	←	15	0	15	1	16	14 749.0651	0.0036	0.005
16	1	16	2	14	←	15	0	15	2	13	14 749.0651	0.0020	0.005
16	1	16	0	16	←	15	0	15	0	15	14 749.0651	0.0005	0.005
16	1	16	1	16	←	15	0	15	1	15	14 749.0651	0.0004	0.005
16	1	16	2	18	←	15	0	15	2	17	14 749.0651	−0.0008	0.005
12	3	10	2	14	←	11	2	9	2	13	14 782.2136	0.0035	0.002
8	4	5	2	6	←	7	3	4	2	5	15 449.0900	−0.0022	0.001
8	4	5	0	8	←	7	3	4	0	7	15 449.0983	0.0001	0.002
8	4	5	1	8	←	7	3	4	1	7	15 449.0983	−0.0008	0.002
8	4	5	1	9	←	7	3	4	1	8	15 449.1303	−0.0005	0.002
8	4	5	1	7	←	7	3	4	1	6	15 449.1367	0.0000	0.002
8	4	5	2	9	←	7	3	4	2	8	15 449.1422	0.0012	0.002
8	4	5	2	8	←	7	3	4	2	7	15 449.1642	−0.0024	0.002
6	5	2	2	6	←	5	4	1	2	5	15 584.1038	−0.0008	0.002
6	5	1	2	7	←	5	4	2	2	6	15 584.4373	0.0002	0.002
6	5	1	2	6	←	5	4	2	2	5	15 584.4818	−0.0002	0.002
8	4	4	0	8	←	7	3	5	0	7	15 623.8881	−0.0005	0.005
8	4	4	1	8	←	7	3	5	1	7	15 623.8881	−0.0016	0.005
8	4	4	2	10	←	7	3	5	2	9	15 623.8997	0.0020	0.005
8	4	4	2	7	←	7	3	5	2	6	15 623.9276	−0.0015	0.002
8	4	4	1	7	←	7	3	5	1	6	15 623.9404	−0.0072	0.005
8	4	4	2	9	←	7	3	5	2	8	15 623.9486	−0.0061	0.004
8	4	4	2	8	←	7	3	5	2	7	15 623.9972	0.0018	0.002

J'	K_a'	K_c'	I'	F'	$\leftarrow$	J''	K_a''	K_c''	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
17	1	16	2	17	←	16	2	15	2	16	16 402.0520	−0.0006	0.005
17	1	16	1	16	←	16	2	15	1	15	16 402.0584	−0.0006	0.005
17	1	16	2	18	←	16	2	15	2	17	16 402.0584	−0.0012	0.005
17	1	16	2	16	←	16	2	15	2	15	16 402.0584	0.0012	0.005
17	1	16	1	18	←	16	2	15	1	17	16 402.0584	0.0001	0.005
17	1	16	2	15	←	16	2	15	2	14	16 402.0648	0.0013	0.005
17	1	16	0	17	←	16	2	15	0	16	16 402.0648	0.0004	0.005
17	1	16	1	17	←	16	2	15	1	16	16 402.0648	0.0003	0.005
17	1	16	2	19	←	16	2	15	2	18	16 402.0648	−0.0003	0.005
18	0	18	2	18	←	17	1	17	2	17	16 542.3129	0.0010	0.005
18	0	18	2	17	←	17	1	17	2	16	16 542.3129	0.0008	0.005
18	0	18	1	17	←	17	1	17	1	16	16 542.3129	−0.0017	0.005
18	0	18	2	19	←	17	1	17	2	18	16 542.3129	−0.0026	0.005
18	0	18	1	19	←	17	1	17	1	18	16 542.3129	−0.0005	0.005
18	0	18	2	16	←	17	1	17	2	15	16 542.3129	−0.0017	0.005
18	0	18	0	18	←	17	1	17	0	17	16 542.3129	−0.0029	0.005
18	0	18	1	18	←	17	1	17	1	17	16 542.3129	−0.0030	0.005
18	0	18	2	20	←	17	1	17	2	19	16 542.3129	−0.0041	0.005
18	1	18	2	18	←	17	0	17	2	17	16 542.9855	0.0052	0.005
18	1	18	2	17	←	17	0	17	2	16	16 542.9855	0.0051	0.005
18	1	18	1	17	←	17	0	17	1	16	16 542.9855	0.0024	0.005
18	1	18	2	19	←	17	0	17	2	18	16 542.9855	0.0015	0.005
18	1	18	1	19	←	17	0	17	1	18	16 542.9855	0.0036	0.005
18	1	18	2	16	←	17	0	17	2	15	16 542.9855	0.0024	0.005
18	1	18	0	18	←	17	0	17	0	17	16 542.9855	0.0012	0.005
18	1	18	1	18	←	17	0	17	1	17	16 542.9855	0.0011	0.005
18	1	18	2	20	←	17	0	17	2	19	16 542.9855	0.0000	0.005
7	5	3	2	5	←	6	4	2	2	4	16 617.4494	−0.0019	0.002
7	5	3	0	7	←	6	4	2	0	6	16 617.4572	−0.0001	0.002
7	5	3	1	7	←	6	4	2	1	6	16 617.4572	−0.0007	0.002
7	5	3	2	9	←	6	4	2	2	8	16 617.4650	0.0016	0.002
7	5	3	2	6	←	6	4	2	2	5	16 617.4975	−0.0019	0.002
7	5	3	1	8	←	6	4	2	1	7	16 617.5067	−0.0003	0.002
7	5	3	1	6	←	6	4	2	1	5	16 617.5122	−0.0007	0.002
7	5	3	2	8	←	6	4	2	2	7	16 617.5192	0.0018	0.002
7	5	3	2	7	←	6	4	2	2	6	16 617.5595	−0.0007	0.002
7	5	2	2	5	←	6	4	3	2	4	16 619.3431	−0.0029	0.002
7	5	2	0	7	←	6	4	3	0	6	16 619.3518	−0.0005	0.002
7	5	2	1	7	←	6	4	3	1	6	16 619.3518	−0.0009	0.002
7	5	2	2	9	←	6	4	3	2	8	16 619.3600	0.0015	0.002
7	5	2	2	6	←	6	4	3	2	5	16 619.3921	−0.0023	0.002
7	5	2	1	8	←	6	4	3	1	7	16 619.4031	0.0002	0.002
7	5	2	1	6	←	6	4	3	1	5	16 619.4085	−0.0002	0.002
7	5	2	2	8	←	6	4	3	2	7	16 619.4150	0.0020	0.002
7	5	2	2	7	←	6	4	3	2	6	16 619.4562	0.0001	0.002
9	4	5	2	10	←	8	3	6	2	9	16 724.6097	0.0024	0.002
9	4	5	2	9	←	8	3	6	2	8	16 724.6481	0.0005	0.002
6	6	1	2	8	←	5	5	0	2	7	17 666.0686	−0.0007	0.002

J'	K_a'	K_c'	I'	F'	$\leftarrow$	J''	K_a''	K_c''	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
7	6	2	1	7	$\leftarrow$	6	5	1	1	6	18 702.2867	0.0008	0.002
7	6	2	2	5	$\leftarrow$	6	5	1	2	4	18 702.2867	0.0005	0.002
7	6	2	0	7	$\leftarrow$	6	5	1	0	6	18 702.2867	0.0001	0.002
7	6	2	2	9	$\leftarrow$	6	5	1	2	8	18 702.2867	−0.0002	0.002
7	6	1	1	7	$\leftarrow$	6	5	2	1	6	18 702.3092	0.0024	0.002
7	6	1	2	5	$\leftarrow$	6	5	2	2	4	18 702.3092	0.0021	0.002
7	6	1	0	7	$\leftarrow$	6	5	2	0	6	18 702.3092	0.0017	0.002
7	6	1	2	9	$\leftarrow$	6	5	2	2	8	18 702.3092	0.0013	0.002
7	6	1	2	7	$\leftarrow$	6	5	2	2	6	18 702.3840	0.0006	0.002

Table S3: Observed minus calculated table for the analysis reported in Section 4.1 for 2,4-DNT. Transitions are assigned with the rotational quantum numbers $J_{K_aK_c}$ and the torsional symmetry species S of the upper and lower levels. For transitions with resolved hyperfine splittings, the total angular momentum F and the total nuclear spin angular momentum I are given. Columns headed obs, $\nu_{\text{obs.}} - \nu_{\text{calc.}}$, and exp. error list observed frequencies, observed minus calculated residuals, and uncertainties in MHz, respectively.

J'	K_a'	K_c'	S	I'	F'	←	J''	K_a''	K_c''	S	I''	F''	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error
2	2	1	A2	2	4	←	2	1	2	A1	2	4	3235.8047	−0.0093	0.0020
2	2	1	A2	1	3	←	2	1	2	A1	1	3	3236.0600	−0.0260	0.1000
5	1	5	A2	2	5	←	4	0	4	A1	2	4	4871.6228	−0.0046	0.0050
5	1	5	A2	1	4	←	4	0	4	A1	1	3	4871.7010	0.0081	0.0020
5	1	5	A2	1	6	←	4	0	4	A1	1	5	4871.7010	0.0023	0.0020
5	1	5	A2	1	5	←	4	0	4	A1	1	4	4871.7626	0.0074	0.0020
3	2	1	A2	2	5	←	2	1	2	A1	2	4	6182.3274	−0.0028	0.0010
3	2	1	A2	1	4	←	2	1	2	A1	1	3	6182.4987	−0.0009	0.0010
7	1	7	A2	2	7	←	6	0	6	A1	2	6	6293.7429	0.0005	0.0020
7	1	7	A2	2	9	←	6	0	6	A1	2	8	6293.8170	0.0022	0.0020
8	4	4	A1	2	8	←	8	3	5	A2	2	8	6683.1789	0.0049	0.0050
8	0	8	A1	2	7	←	7	1	7	A2	2	6	6838.8531	−0.0010	0.0050
8	0	8	A1	2	6	←	7	1	7	A2	2	5	6838.8587	−0.0008	0.0050
8	0	8	A1	2	8	←	7	1	7	A2	2	7	6838.8587	−0.0005	0.0050
8	0	8	A1	0	8	←	7	1	7	A2	0	7	6838.8668	−0.0006	0.0050
8	0	8	A1	1	7	←	7	1	7	A2	1	6	6838.8668	0.0007	0.0050
8	0	8	A1	1	9	←	7	1	7	A2	1	8	6838.8668	0.0035	0.0050
8	0	8	A1	1	8	←	7	1	7	A2	1	7	6838.8668	0.0014	0.0050
8	0	8	A1	2	9	←	7	1	7	A2	2	8	6838.8739	0.0047	0.0050
8	0	8	A1	2	10	←	7	1	7	A2	2	9	6838.8739	0.0022	0.0050
5	4	1	A2			←	5	3	2	A1			7004.3910	−0.0010	0.0100
5	4	1	E			←	5	3	2	E			7004.7260	0.0160	0.0100
7	2	5	A2	1	6	←	6	2	4	A1	1	5	7137.5173	−0.0042	0.0020
7	2	5	A2	2	8	←	6	2	4	A1	2	7	7137.5173	−0.0042	0.0020
7	2	5	A2	2	5	←	6	2	4	A1	2	4	7137.5246	−0.0019	0.0020
7	2	5	A2	2	6	←	6	2	4	A1	2	5	7137.5246	0.0041	0.0020
7	2	5	A2	0	7	←	6	2	4	A1	0	6	7137.5246	−0.0025	0.0020
7	2	5	A2	1	7	←	6	2	4	A1	1	6	7137.5246	−0.0023	0.0020
7	2	5	A2	1	8	←	6	2	4	A1	1	7	7137.5246	0.0032	0.0020
7	2	5	A2	2	9	←	6	2	4	A1	2	8	7137.5246	−0.0027	0.0020
9	0	9	A2	2	8	←	8	1	8	A1	2	7	7700.3406	−0.0003	0.0020
9	0	9	A2	1	10	←	8	1	8	A1	1	9	7700.3487	0.0011	0.0020
9	0	9	A2	2	10	←	8	1	8	A1	2	9	7700.3534	0.0019	0.0020
9	0	9	A2	2	11	←	8	1	8	A1	2	10	7700.3588	0.0023	0.0020
6	2	5	A2	2	8	←	5	1	4	A1	2	7	7736.6670	−0.0041	0.0010
6	2	5	A2	0	6	←	5	1	4	A1	0	5	7736.6757	−0.0038	0.0010
6	2	5	A2	1	6	←	5	1	4	A1	1	5	7736.6867	0.0042	0.0010
6	2	5	A2	2	4	←	5	1	4	A1	2	3	7736.6931	0.0012	0.0010
3	3	0	A1	2	3	←	2	2	1	A2	2	2	7929.0556	−0.0123	0.0020

J'	K_a'	K_c'	S	I'	F'	←	J''	K_a''	K_c''	S	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
10	2	9	A2	2	10	←	9	2	8	A1	2	9	9248.9131	0.0010	0.0020
10	2	9	A2	2	9	←	9	2	8	A1	2	8	9248.9300	0.0007	0.0050
10	2	9	A2	1	11	←	9	2	8	A1	1	10	9248.9300	−0.0009	0.0050
10	2	9	A2	1	10	←	9	2	8	A1	1	9	9248.9456	−0.0007	0.0050
10	2	9	A2	2	8	←	9	2	8	A1	2	7	9248.9456	0.0002	0.0050
10	2	9	A2	2	12	←	9	2	8	A1	2	11	9248.9456	−0.0017	0.0050
10	2	9	A2	0	10	←	9	2	8	A1	0	9	9248.9456	−0.0010	0.0050
9	2	8	A1	2	9	←	8	1	7	A2	2	8	9399.8607	−0.0009	0.0050
9	2	8	A1	1	8	←	8	1	7	A2	2	7	9399.8689	0.0040	0.0020
5	3	2	A1	2	3	←	4	2	3	A2	2	2	9948.6875	0.0023	0.0020
5	3	2	A1	0	5	←	4	2	3	A2	0	4	9948.7029	−0.0115	0.0020
5	3	2	A1	2	5	←	4	2	3	A2	2	4	9948.9115	0.0038	0.0020
12	0	12	A1	2	12	←	11	1	11	A2	2	11	10 204.5764	−0.0028	0.0020
6	2	4	E	2	4	←	5	1	5	E	2	3	10 654.4786	0.0009	0.0010
6	2	4	A1	2	4	←	5	1	5	A2	2	3	10 654.4884	0.0022	0.0010
6	2	4	E			←	5	1	5	E			10 654.7650	0.0080	0.0020
6	2	4	E	2	6	←	5	1	5	E	2	5	10 655.1633	0.0009	0.0010
6	2	4	A1	2	6	←	5	1	5	A2	2	5	10 655.1736	0.0026	0.0010
11	4	8	A1	2	11	←	10	4	7	A2	2	10	10 723.8987	−0.0071	0.0020
11	4	8	A1	1	12	←	10	4	7	A2	1	11	10 723.9133	−0.0082	0.0050
11	4	8	A1	2	10	←	10	4	7	A2	2	9	10 723.9133	−0.0086	0.0050
11	4	8	A1	2	12	←	10	4	7	A2	2	11	10 723.9187	−0.0002	0.0020
11	4	8	A1	1	10	←	10	4	7	A2	1	9	10 723.9192	−0.0002	0.0020
11	4	8	A1	2	13	←	10	4	7	A2	2	12	10 723.9289	−0.0057	0.0050
11	4	8	A1	0	11	←	10	4	7	A2	0	10	10 723.9289	−0.0061	0.0050
11	4	8	A1	1	11	←	10	4	7	A2	1	10	10 723.9289	−0.0062	0.0050
11	4	8	A1	2	9	←	10	4	7	A2	2	8	10 723.9289	−0.0066	0.0050
4	4	1	A2	2	6	←	3	3	0	A1	2	5	10 897.1957	0.0010	0.0020
4	4	0	A1	2	6	←	3	3	1	A2	2	5	10 898.1865	0.0014	0.0050
4	4	0	A1	1	3	←	3	3	1	A2	1	2	10 898.2149	0.0002	0.0050
4	4	0	A1	2	2	←	3	3	1	A2	2	1	10 898.2149	0.0000	0.0050
4	4	0	A1	2	5	←	3	3	1	A2	2	4	10 898.2149	−0.0031	0.0050
4	4	0	A1	2	4	←	3	3	1	A2	2	3	10 898.2673	0.0006	0.0050
13	0	13	A2	2	13	←	12	1	12	A1	2	12	11 027.7449	0.0007	0.0050
13	0	13	A2	2	12	←	12	1	12	A1	2	11	11 027.7449	−0.0020	0.0050
13	0	13	A2	1	12	←	12	1	12	A1	1	11	11 027.7532	0.0039	0.0050
13	0	13	A2	2	14	←	12	1	12	A1	2	13	11 027.7532	0.0023	0.0050
13	0	13	A2	2	11	←	12	1	12	A1	2	10	11 027.7532	0.0015	0.0050
13	0	13	A2	1	14	←	12	1	12	A1	1	13	11 027.7532	0.0033	0.0050

J'	K_a'	K_c'	S	I'	F'	$\leftarrow$	J''	K_a''	K_c''	S	I''	F''	$\nu_{\mathrm{obs.}}$	$\nu_{\mathrm{obs.}} - \nu_{\mathrm{calc.}}$	exp. error
13	0	13	A2	0	13	←	12	1	12	A1	0	12	11 027.7568	0.0024	0.0050
13	0	13	A2	1	13	←	12	1	12	A1	1	12	11 027.7568	0.0029	0.0050
13	0	13	A2	2	15	←	12	1	12	A1	2	14	11 027.7568	0.0006	0.0050
7	3	5	A2	2	5	←	6	2	4	A1	2	4	11 212.2672	0.0037	0.0020
13	1	12	A1	2	13	←	12	2	11	A2	2	12	11 669.4783	−0.0041	0.0020
13	1	12	A1	1	12	←	12	2	11	A2	1	11	11 669.4847	−0.0039	0.0050
13	1	12	A1	2	14	←	12	2	11	A2	2	13	11 669.4847	−0.0048	0.0050
13	1	12	A1	2	12	←	12	2	11	A2	2	11	11 669.4847	−0.0029	0.0050
13	1	12	A1	1	14	←	12	2	11	A2	1	13	11 669.4847	−0.0047	0.0050
13	1	12	A1	2	11	←	12	2	11	A2	2	10	11 669.4928	−0.0008	0.0050
13	1	12	A1	0	13	←	12	2	11	A2	0	12	11 669.4928	−0.0024	0.0020
13	1	12	A1	1	13	←	12	2	11	A2	1	12	11 669.4928	−0.0020	0.0020
13	1	12	A1	2	15	←	12	2	11	A2	2	14	11 669.4928	−0.0034	0.0020
12	5	8	A1	2	12	←	11	5	7	A2	2	11	11 696.2420	0.0076	0.0050
12	5	8	A1	2	13	←	11	5	7	A2	2	12	11 696.2420	−0.0066	0.0050
12	5	8	A1	1	11	←	11	5	7	A2	1	10	11 696.2420	−0.0073	0.0050
12	5	8	A1	1	13	←	11	5	7	A2	1	12	11 696.2571	0.0053	0.0050
12	5	8	A1	2	11	←	11	5	7	A2	2	10	11 696.2571	0.0044	0.0050
12	5	8	A1	2	14	←	11	5	7	A2	2	13	11 696.2713	0.0053	0.0050
12	5	8	A1	0	12	←	11	5	7	A2	0	11	11 696.2713	0.0046	0.0050
12	5	8	A1	1	12	←	11	5	7	A2	1	11	11 696.2713	0.0044	0.0050
12	5	8	A1	2	10	←	11	5	7	A2	2	9	11 696.2713	0.0037	0.0050
8	3	6	A1	2	8	←	7	2	5	A2	2	7	11 819.3374	−0.0056	0.0050
14	0	14	A1	2	14	←	13	1	13	A2	2	13	11 848.8375	0.0008	0.0030
14	0	14	A1	2	13	←	13	1	13	A2	2	12	11 848.8375	−0.0018	0.0030
14	0	14	A1	1	15	←	13	1	13	A2	1	14	11 848.8434	0.0016	0.0030
14	0	14	A1	1	13	←	13	1	13	A2	1	12	11 848.8434	0.0022	0.0030
14	0	14	A1	2	15	←	13	1	13	A2	2	14	11 848.8434	0.0008	0.0030
14	0	14	A1	2	12	←	13	1	13	A2	2	11	11 848.8434	−0.0001	0.0030
14	0	14	A1	0	14	←	13	1	13	A2	0	13	11 848.8471	0.0013	0.0030
14	0	14	A1	1	14	←	13	1	13	A2	1	13	11 848.8471	0.0018	0.0030
14	0	14	A1	2	16	←	13	1	13	A2	2	15	11 848.8480	0.0006	0.0030
13	2	12	A1	2	13	←	12	1	11	A2	2	12	11 982.1592	0.0066	0.0100
13	2	12	A1	1	14	←	12	1	11	A2	1	13	11 982.1764	−0.0039	0.0050
13	2	12	A1	2	12	←	12	1	11	A2	2	11	11 982.1764	−0.0039	0.0050
13	2	12	A1	2	14	←	12	1	11	A2	2	13	11 982.1764	0.0014	0.0050
13	2	12	A1	1	12	←	12	1	11	A2	1	11	11 982.1764	0.0010	0.0050
13	2	12	A1	2	15	←	12	1	11	A2	2	14	11 982.2055	0.0029	0.0050
13	2	12	A1	0	13	←	12	1	11	A2	0	12	11 982.2055	0.0027	0.0050

J'	K_a'	K_c'	S	I'	F'	←	J''	K_a''	K_c''	S	I''	F''	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error
13	2	12	A1	1	13	←	12	1	11	A2	1	12	11 982.2055	0.0026	0.0050
13	2	12	A1	2	11	←	12	1	11	A2	2	10	11 982.2055	0.0026	0.0050
7	2	5	E	2	9	←	6	1	6	E	2	8	12 552.7668	0.0027	0.0020
7	2	5	A2	2	9	←	6	1	6	A1	2	8	12 552.7794	0.0034	0.0010
7	2	5	E			←	6	1	6	E			12 552.9310	−0.0040	0.0020
7	2	5	E	2	7	←	6	1	6	E	2	6	12 553.3552	0.0002	0.0010
7	2	5	A2	2	7	←	6	1	6	A1	2	6	12 553.3680	0.0011	0.0010
15	0	15	A2	2	15	←	14	1	14	A1	2	14	12 668.8022	0.0090	0.0050
15	0	15	A2	1	14	←	14	1	14	A1	1	13	12 668.8022	0.0051	0.0050
15	0	15	A2	2	16	←	14	1	14	A1	2	15	12 668.8022	0.0038	0.0050
15	0	15	A2	2	14	←	14	1	14	A1	2	13	12 668.8022	0.0066	0.0050
15	0	15	A2	2	13	←	14	1	14	A1	2	12	12 668.8022	0.0030	0.0050
15	0	15	A2	0	15	←	14	1	14	A1	0	14	12 668.8022	0.0009	0.0050
15	0	15	A2	1	16	←	14	1	14	A1	1	15	12 668.8022	0.0044	0.0050
15	0	15	A2	1	15	←	14	1	14	A1	1	14	12 668.8022	0.0013	0.0050
15	0	15	A2	2	17	←	14	1	14	A1	2	16	12 668.8022	−0.0006	0.0050
14	2	13	A2	2	14	←	13	1	12	A1	2	13	12 734.6503	−0.0025	0.0050
14	2	13	A2	2	13	←	13	1	12	A1	2	12	12 734.6706	−0.0029	0.0050
14	2	13	A2	2	15	←	13	1	12	A1	2	14	12 734.6706	0.0003	0.0050
14	2	13	A2	1	13	←	13	1	12	A1	1	12	12 734.6706	0.0004	0.0050
14	2	13	A2	1	15	←	13	1	12	A1	1	14	12 734.6706	−0.0034	0.0050
14	2	13	A2	0	14	←	13	1	12	A1	0	13	12 734.6952	0.0040	0.0050
14	2	13	A2	2	12	←	13	1	12	A1	2	11	12 734.6952	0.0044	0.0050
14	2	13	A2	2	16	←	13	1	12	A1	2	15	12 734.6952	0.0039	0.0050
14	2	13	A2	1	14	←	13	1	12	A1	1	13	12 734.6952	0.0041	0.0050
15	1	14	A1	2	15	←	14	2	13	A2	2	14	13 403.0512	−0.0037	0.0020
15	1	14	A1	1	14	←	14	2	13	A2	1	13	13 403.0609	−0.0021	0.0020
15	1	14	A1	2	14	←	14	2	13	A2	2	13	13 403.0609	−0.0026	0.0020
15	1	14	A1	1	16	←	14	2	13	A2	1	15	13 403.0609	−0.0037	0.0020
15	1	14	A1	2	16	←	14	2	13	A2	2	15	13 403.0609	−0.0027	0.0020
15	1	14	A1	2	13	←	14	2	13	A2	2	12	13 403.0716	0.0002	0.0020
15	1	14	A1	0	15	←	14	2	13	A2	0	14	13 403.0716	−0.0009	0.0020
15	1	14	A1	1	15	←	14	2	13	A2	1	14	13 403.0716	−0.0007	0.0020
16	0	16	A1	2	14	←	15	1	15	A2	2	13	13 488.1457	0.0008	0.0050
16	0	16	A1	1	15	←	15	1	15	A2	1	14	13 488.1457	0.0028	0.0050
16	0	16	A1	2	15	←	15	1	15	A2	2	14	13 488.1457	0.0041	0.0050
16	0	16	A1	0	16	←	15	1	15	A2	0	15	13 488.1457	−0.0010	0.0050
16	0	16	A1	1	16	←	15	1	15	A2	1	15	13 488.1457	−0.0007	0.0050
16	0	16	A1	2	16	←	15	1	15	A2	2	15	13 488.1457	0.0062	0.0050

J'	K_a'	K_c'	S	I'	F'	←	J''	K_a''	K_c''	S	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
16	1	16	A1	2	14	←	15	1	15	A2	2	13	13 488.6970	0.0005	0.0050
16	1	16	A1	1	15	←	15	1	15	A2	1	14	13 488.6970	0.0025	0.0050
16	1	16	A1	2	15	←	15	1	15	A2	2	14	13 488.6970	0.0038	0.0050
16	1	16	A1	0	16	←	15	1	15	A2	0	15	13 488.6970	−0.0013	0.0050
16	1	16	A1	1	16	←	15	1	15	A2	1	15	13 488.6970	−0.0010	0.0050
16	1	16	A1	2	16	←	15	1	15	A2	2	15	13 488.6970	0.0060	0.0050
16	1	16	A1	2	14	←	15	0	15	A2	2	13	13 489.7573	0.0008	0.0050
16	1	16	A1	1	15	←	15	0	15	A2	1	14	13 489.7573	0.0029	0.0050
16	1	16	A1	2	15	←	15	0	15	A2	2	14	13 489.7573	0.0041	0.0050
16	1	16	A1	0	16	←	15	0	15	A2	0	15	13 489.7573	−0.0011	0.0050
16	1	16	A1	1	16	←	15	0	15	A2	1	15	13 489.7573	−0.0007	0.0050
16	1	16	A1	2	16	←	15	0	15	A2	2	15	13 489.7573	0.0064	0.0050
15	2	14	A1	2	15	←	14	1	13	A2	2	14	13 511.9023	−0.0015	0.0050
15	2	14	A1	2	14	←	14	1	13	A2	2	13	13 511.9194	−0.0004	0.0050
15	2	14	A1	1	16	←	14	1	13	A2	1	15	13 511.9194	−0.0011	0.0050
15	2	14	A1	1	14	←	14	1	13	A2	1	13	13 511.9194	0.0019	0.0050
15	2	14	A1	2	16	←	14	1	13	A2	2	15	13 511.9194	0.0016	0.0050
15	2	14	A1	2	13	←	14	1	13	A2	2	12	13 511.9378	0.0044	0.0050
15	2	14	A1	0	15	←	14	1	13	A2	0	14	13 511.9378	0.0038	0.0050
15	2	14	A1	1	15	←	14	1	13	A2	1	14	13 511.9378	0.0039	0.0050
15	2	14	A1	2	17	←	14	1	13	A2	2	16	13 511.9378	0.0035	0.0050
7	4	3	A2	2	9	←	6	3	4	A1	2	8	13 809.1542	0.0015	0.0020
7	4	3	A2			←	6	3	4	A1			13 809.1790	−0.0010	0.0050
7	4	3	E			←	6	3	4	E			13 809.2200	0.0110	0.0050
7	4	3	E	2	7	←	6	3	4	E	2	6	13 809.2780	0.0010	0.0020
16	1	15	A2	2	16	←	15	2	14	A1	2	15	14 242.9662	−0.0032	0.0020
16	1	15	A2	1	15	←	15	2	14	A1	1	14	14 242.9756	−0.0018	0.0020
16	1	15	A2	2	15	←	15	2	14	A1	2	14	14 242.9756	−0.0025	0.0020
16	1	15	A2	2	14	←	15	2	14	A1	2	13	14 242.9864	0.0004	0.0020
16	1	15	A2	0	16	←	15	2	14	A1	0	15	14 242.9864	−0.0005	0.0020
16	1	15	A2	1	16	←	15	2	14	A1	1	15	14 242.9864	−0.0004	0.0020
16	2	15	A2	2	16	←	15	2	14	A1	2	15	14 265.5461	−0.0016	0.0050
16	2	15	A2	2	15	←	15	2	14	A1	2	14	14 265.5556	−0.0023	0.0050
16	2	15	A2	1	17	←	15	2	14	A1	1	16	14 265.5566	−0.0022	0.0050
16	2	15	A2	1	15	←	15	2	14	A1	1	14	14 265.5566	−0.0002	0.0050
16	2	15	A2	2	17	←	15	2	14	A1	2	16	14 265.5566	−0.0007	0.0050
16	2	15	A2	2	14	←	15	2	14	A1	2	13	14 265.5680	0.0011	0.0050
16	2	15	A2	0	16	←	15	2	14	A1	0	15	14 265.5680	0.0003	0.0050
16	2	15	A2	1	16	←	15	2	14	A1	1	15	14 265.5680	0.0004	0.0050

J'	K'_a	K'_c	S	I'	F'	$\leftarrow$	J''	K''_a	K''_c	S	I''	F''	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error
16	2	15	A2	2	18	←	15	2	14	A1	2	17	14 265.5680	−0.0003	0.0050
16	2	15	A2	2	16	←	15	1	14	A1	2	15	14 305.3471	−0.0022	0.0050
16	2	15	A2	2	15	←	15	1	14	A1	2	14	14 305.3613	−0.0008	0.0050
16	2	15	A2	1	17	←	15	1	14	A1	1	16	14 305.3613	−0.0016	0.0050
16	2	15	A2	1	15	←	15	1	14	A1	1	14	14 305.3613	0.0009	0.0050
16	2	15	A2	2	17	←	15	1	14	A1	2	16	14 305.3613	0.0005	0.0050
16	2	15	A2	2	14	←	15	1	14	A1	2	13	14 305.3764	0.0033	0.0050
16	2	15	A2	0	16	←	15	1	14	A1	0	15	14 305.3764	0.0026	0.0050
16	2	15	A2	1	16	←	15	1	14	A1	1	15	14 305.3764	0.0027	0.0050
16	2	15	A2	2	18	←	15	1	14	A1	2	17	14 305.3764	0.0021	0.0050
17	0	17	A2	2	15	←	16	1	16	A1	2	14	14 307.1694	0.0003	0.0020
17	0	17	A2	1	16	←	16	1	16	A1	1	15	14 307.1694	0.0021	0.0020
17	0	17	A2	2	16	←	16	1	16	A1	2	15	14 307.1694	0.0031	0.0020
17	1	17	A2	2	15	←	16	1	16	A1	2	14	14 307.4537	−0.0006	0.0020
17	1	17	A2	1	16	←	16	1	16	A1	1	15	14 307.4537	0.0012	0.0020
17	1	17	A2	2	16	←	16	1	16	A1	2	15	14 307.4537	0.0022	0.0020
17	1	17	A2	2	15	←	16	0	16	A1	2	14	14 308.0061	0.0001	0.0020
17	1	17	A2	1	16	←	16	0	16	A1	1	15	14 308.0061	0.0020	0.0020
17	1	17	A2	2	16	←	16	0	16	A1	2	15	14 308.0061	0.0030	0.0020
8	4	5	E	2	6	←	7	3	4	E	2	5	14 602.0532	−0.0024	0.0020
8	2	6	E			←	7	1	7	E			14 651.1200	−0.0060	0.0020
8	2	6	E	2	8	←	7	1	7	E	2	7	14 651.5548	−0.0007	0.0010
8	2	6	A1	2	8	←	7	1	7	A2	2	7	14 651.5694	−0.0017	0.0010
8	4	4	A1	2	6	←	7	3	5	A2	2	5	14 809.2848	−0.0036	0.0010
8	4	4	A1	1	8	←	7	3	5	A2	1	7	14 809.2953	−0.0004	0.0010
8	4	4	A1	2	7	←	7	3	5	A2	2	6	14 809.3342	0.0011	0.0010
6	5	2	A1	2	4	←	5	4	1	A2	2	3	14 836.0507	0.0037	0.0020
6	5	1	A2	2	6	←	5	4	2	A1	2	5	14 836.6131	0.0006	0.0020
17	1	16	A1	1	16	←	16	2	15	A2	1	15	15 073.7179	−0.0013	0.0020
17	1	16	A1	2	16	←	16	2	15	A2	2	15	15 073.7179	−0.0021	0.0020
17	1	16	A1	2	15	←	16	2	15	A2	2	14	15 073.7281	0.0006	0.0020
17	2	16	A1	2	17	←	16	1	15	A2	2	16	15 108.9249	−0.0010	0.0020
17	2	16	A1	2	16	←	16	1	15	A2	2	15	15 108.9364	−0.0001	0.0050
17	2	16	A1	1	16	←	16	1	15	A2	1	15	15 108.9364	0.0012	0.0050
17	2	16	A1	1	18	←	16	1	15	A2	1	17	15 108.9364	−0.0009	0.0050
17	2	16	A1	2	18	←	16	1	15	A2	2	17	15 108.9364	0.0008	0.0050
17	2	16	A1	2	15	←	16	1	15	A2	2	14	15 108.9487	0.0030	0.0050
17	2	16	A1	0	17	←	16	1	15	A2	0	16	15 108.9487	0.0023	0.0050
17	2	16	A1	1	17	←	16	1	15	A2	1	16	15 108.9487	0.0024	0.0050

J'	K_a'	K_c'	S	I'	F'	←	J''	K_a''	K_c''	S	I''	F''	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error
17	2	16	A1	2	19	←	16	1	15	A2	2	18	15 108.9487	0.0018	0.0050
18	0	18	A1	2	16	←	17	1	17	A2	2	15	15 126.0276	0.0000	0.0020
18	1	18	A1	2	16	←	17	0	17	A2	2	15	15 126.4594	−0.0001	0.0020
9	4	6	A1	2	9	←	8	3	5	A2	2	8	15 408.3349	−0.0284	0.0100
9	4	6	A1	2	8	←	8	3	5	A2	2	7	15 408.3392	−0.0317	0.0100
9	4	6	A1	1	9	←	8	3	5	A2	1	8	15 408.3931	0.0159	0.0020
7	5	3	E			←	6	4	2	E			15 794.9400	−0.0090	0.0050
7	5	3	E	2	7	←	6	4	2	E	2	6	15 794.9957	−0.0090	0.0020
7	5	3	A2	2	5	←	6	4	2	A1	2	4	15 795.5768	0.0001	0.0020
7	5	3	A2	1	7	←	6	4	2	A1	1	6	15 795.5795	−0.0016	0.0020
7	5	3	A2	0	7	←	6	4	2	A1	0	6	15 795.5885	0.0064	0.0020
7	5	3	A2	2	9	←	6	4	2	A1	2	8	15 795.5887	0.0027	0.0020
7	5	3	A2	2	6	←	6	4	2	A1	2	5	15 795.6036	−0.0112	0.0020
7	5	3	A2	1	8	←	6	4	2	A1	1	7	15 795.6134	−0.0070	0.0020
7	5	3	A2	1	6	←	6	4	2	A1	1	5	15 795.6377	0.0097	0.0020
7	5	3	A2	2	8	←	6	4	2	A1	2	7	15 795.6428	0.0111	0.0020
7	5	3	A2	2	7	←	6	4	2	A1	2	6	15 795.6666	0.0009	0.0020
7	5	2	A1	2	5	←	6	4	3	A2	2	4	15 797.9939	0.0000	0.0020
7	5	2	A1	2	9	←	6	4	3	A2	2	8	15 798.0030	−0.0004	0.0020
7	5	2	A1	2	8	←	6	4	3	A2	2	7	15 798.0536	0.0036	0.0020
7	5	2	A1	2	7	←	6	4	3	A2	2	6	15 798.0854	0.0009	0.0020
7	5	2	E			←	6	4	3	E			15 798.6750	−0.0070	0.0050
7	5	2	E	2	7	←	6	4	3	E	2	6	15 798.7297	−0.0090	0.0020
18	1	17	A2	1	17	←	17	2	16	A1	1	16	15 899.0273	−0.0016	0.0020
18	1	17	A2	2	17	←	17	2	16	A1	2	16	15 899.0273	−0.0024	0.0020
18	1	17	A2	1	19	←	17	2	16	A1	1	18	15 899.0273	−0.0033	0.0020
18	1	17	A2	2	19	←	17	2	16	A1	2	18	15 899.0273	−0.0021	0.0020
18	1	17	A2	2	16	←	17	2	16	A1	2	15	15 899.0369	0.0002	0.0020
18	1	17	A2	0	18	←	17	2	16	A1	0	17	15 899.0369	−0.0006	0.0020
18	1	17	A2	1	18	←	17	2	16	A1	1	17	15 899.0369	−0.0004	0.0020
18	1	17	A2	2	20	←	17	2	16	A1	2	19	15 899.0369	−0.0011	0.0020
18	2	17	A2	2	18	←	17	1	16	A1	2	17	15 918.6468	−0.0013	0.0050
18	2	17	A2	2	17	←	17	1	16	A1	2	16	15 918.6568	−0.0003	0.0050
18	2	17	A2	1	17	←	17	1	16	A1	1	16	15 918.6568	0.0008	0.0050
18	2	17	A2	1	19	←	17	1	16	A1	1	18	15 918.6568	−0.0011	0.0050
18	2	17	A2	2	19	←	17	1	16	A1	2	18	15 918.6568	0.0003	0.0050
18	2	17	A2	2	16	←	17	1	16	A1	2	15	15 918.6687	0.0037	0.0050
18	2	17	A2	0	18	←	17	1	16	A1	0	17	15 918.6687	0.0030	0.0050
18	2	17	A2	1	18	←	17	1	16	A1	1	17	15 918.6687	0.0031	0.0050

J'	K'_a	K'_c	S	I'	F'	←	J''	K''_a	K''_c	S	I''	F''	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$	exp. error
18	2	17	A2	2	20	←	17	1	16	A1	2	19	15 918.6687	0.0025	0.0050
19	2	18	A1	2	19	←	18	1	17	A2	2	18	16 732.0200	−0.0003	0.1000
19	2	18	A1	2	18	←	18	1	17	A2	2	17	16 732.0288	0.0006	0.0050
19	2	18	A1	1	18	←	18	1	17	A2	1	17	16 732.0288	0.0016	0.0050
19	2	18	A1	1	20	←	18	1	17	A2	1	19	16 732.0288	−0.0001	0.0050
19	2	18	A1	2	20	←	18	1	17	A2	2	19	16 732.0288	0.0011	0.0050
19	2	18	A1	2	17	←	18	1	17	A2	2	16	16 732.0375	0.0025	0.0020
19	2	18	A1	0	19	←	18	1	17	A2	0	18	16 732.0375	0.0017	0.0020
19	2	18	A1	1	19	←	18	1	17	A2	1	18	16 732.0375	0.0019	0.0020
19	2	18	A1	2	21	←	18	1	17	A2	2	20	16 732.0375	0.0012	0.0020
8	5	4	E			←	7	4	3	E			16 748.9000	0.0350	0.0100
8	5	4	A1			←	7	4	3	A2			16 749.2690	0.0020	0.0050