Accepted Manuscript

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PII: S0022-2852(18)30320-5
DOI: <https://doi.org/10.1016/j.jms.2018.11.012>
Reference: YJMSP 11101

To appear in: *Journal of Molecular Spectroscopy*

Received Date: 12 October 2018
Revised Date: 26 November 2018
Accepted Date: 26 November 2018

Please cite this article as: L. Morina, R. Alan Aitken, M.H. Palmer, D. Christen, The rotational spectrum and derived structure of 1,2,3- triazine, *Journal of Molecular Spectroscopy* (2018), doi: <https://doi.org/10.1016/j.jms.2018.11.012>

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The rotational spectrum and derived structure of 1,2,3- triazine

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Abstract

The close similarity in patterns of bands in the microwave spectra of the isomeric 1,2,3- and 1,2,4-triazines has enabled assignment for the 1,2,3-isomer. Pure rotational transitions with J up to 65 were identified and fitted to a Watson-type Hamiltonian: $A = 6334.157(14)$., $B = 6271.289(14)$, $C = 3151.230(14)$. A and B thus show near degeneracy. Coupled cluster calculations which include both singles, doubles and selected triple excitations (CCSD(T)), give very close agreement with the spectral data. The theoretical structure which includes estimates of the ^{14}N quadrupole coupling, not determined in the spectrum, is described.

Keyword

1,2,3-triazine; 1,2,4-triazine; Fortrat diagram; rotational constants; stark spectroscopy; structure; ab initio calculations.

1. Introduction

1,2,3-Triazine (Figure 1, I, 123T) is the least studied member of the azines $C_{6-n}H_{6-n}N_n$ ($n = 0$ to 5), where the triazines have $n = 3$. Studies of 123T contrast with those of the 1,2,4-isomer (Figure 1, 2, 124T). Numerous 124T derivatives have excited interest in the pharmaceutical and other industries, and also initiated our previous spectroscopic interest in 124T.[1 – 4] To date no compounds containing the 123T ring system have been found in nature, but the facility with which the molecule loses N_2 has led to considerable interest in its synthetic use as a reverse Diels-Alder reactant in cyclo-addition reactions; the symmetry of the molecule is broken in these processes.[5] Two crystal structures have been reported for 123T [6,7]. Rotational Stark-effect spectra were recorded in Tübingen as early as 2003, but these were not assigned until now. This is the subject of the current paper, where the results will be discussed in the light of theoretical calculations and the x-ray structures.

2. Experimental

2.1. Synthesis of 123T.

The crucial intermediate is N-aminopyrazole (NAP) and we have tried several routes to its synthesis. The procedure from pyrazole and hydroxylamine O-sulfonic acid in aqueous sodium hydroxide solution proved satisfactory. [5,6] The alternative reaction of pyrazole with sodium hydride and anhydrous chloramine [8] in THF also gave a high yield (82%) of NAP. Oxidation

of this using nickel peroxide and acetic acid in methylene chloride[9] gave 1,2,3-triazine (20%) after column chromatography. A more recent procedure, using sodium periodate as oxidising agent,[10] is more convenient and higher yielding.

Our sample of 123T, used in the microwave study, has colourless crystals, mp 67 °C (lit 69.5–71 °C [9,10]). The ^1H NMR spectrum, of AB_2 type, has: δ 9.10 (2H, doublet, J_{AB} 5.7 Hz) and δ 7.42 (1H, triplet, J_{AB} 5.7 Hz).

2.2 Microwave spectroscopy

Spectra of 123T were recorded at room temperature under low pressures. The frequency range was 7 to 35 GHz with a classical square wave modulated Stark effect microwave spectrometer (modulation frequency 50 kHz). Spectra were measured with a computer controlled Gigatronics Model 910 Synthesizer; the step size was 10 kHz. Each point was scanned 10 times, the signals summed, and finally the points were smoothed. The spectral line positions were determined automatically using the ‘peak pick’ facility. Final results of the spectral analysis are shown in Tables I, II and III. The first two bands analysed in detail are shown in Figures 2 and 3. The analysis requires additional description as described below. The lines used in the analysis are summarized in the Appendix.

2.3 Theoretical study

The equilibrium structure of 123T was sought using a variety of basis sets and methods, as shown in Table IV. However, the nearly degenerate A and B rotational constants proved a challenge, which was most closely met by the coupled-cluster with singles and double excitations with selected triples (CCSD(T)) procedure. This is widely regarded as the ‘gold standard’ in computational chemistry for electronic ground state structures.[11 – 14] The Ahlrichs *et al.* default series 2 triple zeta valence with additional p- and d-polarization functions (Def2-TZVPPD) basis set gave the closest rotational constants to the spectroscopic values, and these are shown in Table IV.[15 – 17] The GAUSSIAN-16 suite (G-16),[18] including the Pickett output directive,[19] ensured that all data relate to the inertial axis (IA) system.

3. Spectral analysis of 1,2,3-triazine

Analysis of the original rotational spectrum, were aided by two theoretical calculations by Dr. H.P.S. Müller [20]. More recently, we undertook the coupled cluster and other calculations shown in Tables III and IV.

The objective of this work was to assign the Q-branch rotational transitions in the previously recorded 123T spectrum, and to determine the rotational and centrifugal distortion constants. As shown both by crystallography and NMR spectra, the isolated molecule has C_{2v} symmetry, with symmetrical positions for two nitrogen atoms in the ring (Fig. 1). The dipole moment lies along the C_{2v} axis through the (middle) N_2 atom which must be either the a- or b-axis. However, the nuclear masses dictate that the moments of inertia I_a and I_b are very similar. Using the asymmetry parameter $\kappa = (2B - (A + C)) / (A - C)$, the molecule is nearly an accidental oblate symmetric top, κ close to +1. Analysis of the rotational spectrum below shows the a-axis lies along the symmetry axis. These complexities contrast with 124T where the three nitrogen atoms are unsymmetrically

placed in the ring. 124T is an asymmetric rotor with widely differing moments of inertia I_a and I_b as well as μ_a and μ_b dipole components.

The Q-branches of both 123T and 124T rotational spectra form well defined band heads. Those for 123T are located at 15 GHz, 22 GHz, 28 GHz and 35 GHz. The Fortrat Diagrams shown in Fig.2 enable a comparison of the overall behaviour of the two molecules. Differences in the structure of the rotational spectra between the two compounds rapidly become apparent. The parabolic form of the curves (so prominent in 124T) is not yet reached at the available J-range.

The distance between consecutive band heads for 123T, approximately $(A+B)/2$, is very close to the associated band heads in 124T. The high density of the lines makes it difficult to recognize individual transitions, but with increasing J values the trend to higher intensity, larger spacing, but similar Stark effect gets very obvious. Model calculations based on ab initio and DFT calculations provided a good basis for the analysis of the 123T spectra by using analogy with those for 124T,[1 – 4] as discussed below.

The group of lines near 15.8 GHz was deliberately chosen as the starting point for the analysis of the Q-branches. The diverging Q- branches seen in Fig. 3 go from low J values in the opposite direction with an almost parallel splitting of the lines. It is not easy to find a clear starting transition ($J=K_{+1}$) of the band head (~ 15850 MHz), but the behaviour of the lines seemed to be much simpler than other band heads. Difficulties in assigning transitions to the same branch occurred, so additional criteria to the model calculations were considered. A major criterion was that adjacent members of the same branch should have similar intensities. Similarly, a series must show a continuous increase of distance with increasing J, the Stark effect pattern must also be considered in both magnitude and sign. The transition at 16223.2 MHz (later assigned as $31_{28\ 3-}$

$31_{28\ 4}$) has no obvious Stark effect and therefore, even being strong, is not considered a member of the series. Similarly, the line with the frequency 15508.88 MHz (later assigned as $32_{29\ 3}$ - $32_{29\ 4}$) also shows no prominent Stark effect in contrast to the transitions forming this branch. A first fit was attempted including the first 6 lines of the respective Q branches in the 15 GHz region see Table I and II.

The initial fit results were far-off when compared to the final values of the constants shown in Table IV. However, since Q-branch transitions only depend on $(A-C)/2$ and κ , and these values are almost identical to those of the final analysis, the trial fit assisted the continuing assignment of Q-branch transitions. At higher J values it was necessary to vary some quartic centrifugal distortion constants as well. In order to stabilize these, it was necessary to analyze transitions with a higher K_{+1} value extending to higher values of J.

The 35 GHz range shown in Table III is very different when compared to the 15 GHz region. Particularly, at lower J values the two branches are close together and run in one direction. Again, it was not easy to assign the $J = K_{+1}$ transitions, but predicted lines from the trial-fit could be located. Eventually more and more lines were added to the fit, increasingly improving the predictive power of the model, leading to the assignment of lines from the 28 GHz range, then the 22 GHz and finally the 10 GHz region. The Fortrat diagram clearly shows that the lines in the 10 GHz range do not form a band head, thus becoming the most difficult part of the spectrum to assign. Finally, virtually all predicted transitions were located and measured.

The data were analyzed with the Watson Hamiltonian (S-reduction, III^R - representation), with four quartic centrifugal distortion constants being adjusted. Due to planarity, only 4 quartic constants are linearly independent. Because D_J does not influence the Q-branch transitions, we

kept this value at 0, also when the R-branch transitions were included in the fit. Finally, as transitions with J above 50 were included, 5 sextic centrifugal distortion constants were also added. Unfortunately, the R branch search proved difficult because most of these lines are of a low intensity and mostly located very close to the band heads.

The Stark effect did not produce any resolved splitting patterns, thus it was impossible to determine the size of the permanent electric dipole moment. The weakness of the low-J R-branch transitions and the overlapping of many lines also hindered an analysis of the quadrupole hyperfine structure.

The Appendix contains the Q branches and the subsequently assigned R branch transitions; these are shown in Tables VI onwards.

4. The equilibrium structure of 1,2,3-triazine.

There is a very close identity between the rotational constants in the microwave spectral analysis and the CCSD(T) calculations, leading to adoption of the theoretical structure, shown in Figure 6, as close to reality. The C-C, C-N and N-N bond lengths cover a very small range of 0.057 Å. The C-H bonds, over 1.08 Å, are longer than in many equilibrium structures. The internal ring angles are close to 120° at the N-atoms, but those at C₄ and C₆ are considerably different from C₅. The molecule is accidentally more symmetric than expected, with considerable impact on the microwave spectrum.

The two x-ray structures, [6,7] are considerably different, even after allowing for the alternative axis choices for the crystals. The x-ray structure of Yamaguchi *et al*, [6] after taking the mean of equivalent bonds, gives N-N 1.318 Å, C-C 1.353 Å and C-N 1.371 Å (with a large difference). The corresponding values for Neunhoeffer *et al*, [7] where more detail is given,

are N-N 1.326 Å, C-C 1.385 Å and C-N 1.345 Å; the internal ring angles at each centre have values of 119.7 (N₁,N₃), 121.6 (N₂), 121.8 (C₄,C₆) and 115.4 (C₅). The present results are very similar to those of Neunhoeffer *et al*; b [7] the considerable difference in angles at N₂ and C₅ from the mean angle of 120° is very notable. Although the present spectral study was unable to determine either the ¹⁴N quadrupole coupling or the dipole moment of 123T, the values obtained in the theoretical study, enable subsequent comparison with future measurements. The ¹⁴N quadrupole coupling results reported here are from MP4(SDQ) wave-functions, which have very similar energies to CCSD(T). A comparison between these two methods can be demonstrated for the calculated dipole moments, using CCSD(T) is 5.15 Debye and MP4(SDQ) is 5.012 Debye. The ¹⁴N results in the inertial axis frame are shown in Figure 7. The off-diagonal χ_{ab} -3.8414 MHz at the symmetrically placed N₁/N₃ atoms is numerically larger than the IA diagonal terms, with consequential difficulties in the microwave spectral interpretation. At N₂ χ_{aa} is very large. The out-of-plane χ_{cc} are very similar at all centres.

5. Discussion

In this work we have assigned more than 350 transitions (mostly Q-branch lines) of the rotational spectrum of the 1,2,3-triazine ground state in the frequency range 8 – 35 GHz. The maximum J value was 65 and K₋₁ equal to 53. Employing the standard Watson Hamiltonian (S-reduction, III^R representation) including 4 quartic and 5 sextic distortion constants led to a standard deviation of 161 kHz, slightly larger than the experimental uncertainty of ~100 kHz, attributable to the lack of an analysis of the quadrupole hyperfine structure caused by the three nitrogen atoms.

Most of the transitions exhibiting hyperfine structure (R-branch transitions at low J values) are either very weak or partly overlapped by much stronger Q branch transitions close to the band heads. The only “hyperfine” corrections made was weighting the components of some obvious doublets to produce a hypothetical frequency of unperturbed transitions.

Acknowledgement:

We are grateful to Dr. Holger S.P. Müller for providing us with his theoretical calculations for the early analysis in Tübingen. MHP wishes to thank the University of Edinburgh, Parallel Computing Centre (EPCC) for the grant of computer time for the current theoretical study.

Declarations of interest: none

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Appendix

Table I. Measured frequencies (MHz) of the diverging Q-branches at 15.8 GHz.

Assignment	Frequency	Assignment	Frequency
$5_{32}-5_{33}$	15732.58	$5_{42}-5_{23}$	15764.39
$6_{42}-6_{43}$	15709.35	$6_{52}-6_{33}$	15775.45
$7_{52}-7_{53}$	15671.34	$7_{62}-7_{43}$	15790.88
$8_{62}-8_{63}$	15615.77	$8_{72}-8_{53}$	15814.55
$9_{72}-9_{73}$	15537.09	$9_{82}-9_{63}$	15848.78
$10_{82}-10_{83}$	15431.32	$10_{92}-10_{73}$	15897.05

Table II. The initial model: Rotational constants (MHz) from an B3LYP calculation with B and C fitted to Q – branch transitions.

Parameter	Value (standard deviation)
A	6334.1478(fixed)
B	6271.288(7)
C	3151.399(8)
(A - C)/2	1575.69
κ	0.960
Microwave RMS	0.442 MHz

Table III. Experimental frequencies (MHz) of 1,2,3-triazine in the 35 GHz range. Low-J assigned transitions.

$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz)	$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz)
$9_{55}-9_{36}$	34659.66	$9_{45}-9_{36}$	34659.66
$10_{65}-10_{46}$	34657.08	$10_{55}-10_{56}$	34657.08
$11_{75}-11_{56}$	34654.20	$11_{65}-11_{66}$	34654.20
$12_{85}-12_{66}$	34649.54	$12_{75}-12_{76}$	34649.54
$13_{95}-13_{76}$	34644.16	$13_{85}-13_{86}$	34644.16
$14_{105}-14_{86}$	34637.69	$14_{95}-14_{96}$	34637.69
$15_{115}-15_{96}$	34629.99	$15_{105}-15_{106}$	34629.99
$16_{125}-16_{106}$	34620.46	$16_{115}-16_{116}$	34620.46
$17_{135}-17_{116}$	34609.55	$17_{125}-17_{126}$	34609.55
$18_{145}-18_{126}$	34596.59	$18_{135}-18_{136}$	
$19_{155}-19_{136}$	34581.44	$19_{145}-19_{146}$	
$20_{165}-20_{146}$	34564.52	$20_{155}-20_{156}$	34562.50
$21_{175}-21_{156}$	34544.07	$21_{165}-21_{166}$	34541.81
$22_{185}-22_{166}$	34521.41	$22_{175}-22_{176}$	34517.44
$23_{195}-23_{176}$	34495.87	$23_{185}-23_{186}$	34489.77
$24_{205}-24_{186}$	34467.31	$24_{195}-24_{196}$	34457.59
$25_{215}-24_{196}$	34435.16	$25_{205}-25_{206}$	34420.93

Table IV. Rotational and centrifugal distortion constants, with standard deviations in parentheses, for 1,2,3-Triazine (MHz). Theoretical values include terms arising from quartic centrifugal distortion constants.

Parameter	Experimental value / MHz	B3LYP + aug-cc-pVT
A	6334.1694(64)	6401.1865
B	6271.3135(64)	6324.6960
C	3151.2485(68)	3181.3531
κ	0.9605	0.9525
D_K	$2.751(80) \times 10^{-3}$	0.00012224
D_{JK}	$-2.7810(32) \times 10^{-3}$	-0.000266870
D_J	0(fixed)	0.00158078
d_1	$0.43890(89) \times 10^{-4}$	-0.0000406914
d_2	$-2.919(23) \times 10^{-3}$	0.192500×10^{-2}
H_J	0.0 (fixed)	
H_{JK}	$-0.0305(35) \times 10^{-6}$	
H_{KJ}	$0.966(108) \times 10^{-6}$	
H_K	0.0 (fixed)	
h_1	$-0.373(90) \times 10^{-9}$	
h_2	$0.338(83) \times 10^{-9}$	
h_3	$-0.084(19) \times 10^{-9}$	
σ	= 0.161	

Table V. Observed and calculated rotational constants

Method	basis set	Rotational constants (GHz)			Asymmetry parameter
		A	B	C	κ
Experiment		6.3341694(64)	6.2712135(64)	3.1512485(68)	0.9605
CCSD(T)	Def2-TZVPPD	6.3285	6.2550	3.1458	0.9539
MP4(SDQ)	Def2-TZVPPD	6.4128	6.3227	3.1837	0.9442
MP2	aug-cc-pVTZ	6.3301	6.2673	3.1493	0.9605
B3LYP	aug-cc-pVTZ	6.4012	6.3247	3.1814	0.9525
M11	Def2-TZVPPD	6.4842	6.3815	3.2162	0.9371
LC-BLYP	Def2-QZVPPD	6.5846	6.4697	3.2633	0.9525

Table VI. ^{14}N quadrupole coupling constants (MHz) calculated from the Def2-TZVPPD basis set

Centre	Method	1.5 χ_{aa}	0.25 ($\chi_{bb} - \chi_{cc}$)
N2	MP4(SDQ)	-9.259	-0.258
N1/N3	MP4(SDQ)	-1.593	-1.544
N2	M11	-10.456	-0.3814
N1/N3	M11	-1.9618	-1.7918

Table VII. Calculated and experimental frequencies (MHz) of 1,2,3- Triazine belonging to the 10 GHz band head (disregarding quadrupole hyperfine structure)

$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated	$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated
4 ₄₁ -4 ₂₂	9784.35	9784.47	4 ₃₁ -4 ₃₂	9141.92	9141.79486
5 ₅₁ -5 ₃₂	9962.27	9962.22	5 ₄₁ -5 ₄₂		8986.68
6 ₆₁ -6 ₄₂	10186.29	10186.41	6 ₅₁ -6 ₅₂	8801.55	8801.55
7 ₇₁ -7 ₅₂	10462.50	10462.74	7 ₆₁ -7 ₆₂	8587.11	8587.04
8 ₈₁ -8 ₆₂	10797.53	10797.47	8 ₇₁ -8 ₆₂	8343.95	8343.96
9 ₉₁ -9 ₇₂	11197.27	11197.30	9 ₈₁ -9 ₈₂	8073.38	8073.33
10 ₁₀₁ -10 ₈₂	11669.07	11669.00	10 ₉₁ -10 ₉₂	7776.58	7776.41
11 ₁₁₁ -11 ₉₂	12218.85	12219.11			
12 ₁₂₁ -12 ₁₀₂	12853.30	12853.59			
13 ₁₃₁ -13 ₁₁₂	13577.63	13577.54			
14 ₁₄₁ -14 ₁₂₂	14394.74	14394.90			
15 ₁₅₁ -15 ₁₃₂	15308.56	15308.38			
16 ₁₆₁ -16 ₁₄₂	16319.33	16319.41			
17 ₁₇₁ -17 ₁₅₂	17427.79	17428.19			

18 ₁₈₁ -18 ₁₆₂		18633.79			
19 ₁₉₁ -19 ₁₇₂	19934.16	19934.33			
20 ₂₀₁ -20 ₁₈₂	21327.00	21327.03			
21 ₂₁₁ -21 ₁₉₂	22808.56	22808.45			
22 ₂₂₁ -22 ₂₀₂	24373.94	24374.35			
23 ₂₃₁ -23 ₂₁₂	26020.14	26019.99			
24 ₂₄₁ -24 ₂₂₂	27739.91	27740.04			
25 ₂₅₁ -25 ₂₃₂	29528.80	29528.61			
26 ₂₆₁ -26 ₂₄₂	31379.22	31379.30			
27 ₂₇₁ -27 ₂₅₂	33285.16	33285.22			

Table VIII. Calculated and experimental frequencies (MHz) of 1,2,3-Triazine belonging to the 15 GHz band head (disregarding quadrupole hyperfine structure)

$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated	$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated
3 ₁₂ - 3 ₁₃		15753.36	3 ₂₂ - 3 ₀₃		15758.07
4 ₂₂ - 4 ₂₃	15746.67	15746.43	4 ₃₂ - 4 ₁₃		15760.60
5 ₃₂ - 5 ₃₃	15732.58	15732.78	5 ₄₂ - 5 ₂₃		15765.88
6 ₄₂ - 6 ₄₃	15709.35	15709.09	6 ₅₂ - 6 ₃₃	15775.45	15775.37
7 ₅₂ - 7 ₅₃	15671.34	15671.51	7 ₆₂ - 7 ₄₃	15790.88	15790.87

$8_{62} - 8_{63}$	15615.77	15615.72	$8_{72} - 8_{53}$	15814.55	15814.56
$9_{72} - 9_{73}$	15537.09	15537.15	$9_{82} - 9_{63}$	15848.78	15848.98
$10_{82} - 10_{83}$	15431.32	15431.18	$10_{92} - 10_{73}$	15897.05	15897.14
$11_{92} - 11_{93}$	15293.46	15293.46	$11_{102} - 11_{83}$	15962.52	15962.49
$12_{102} - 12_{103}$	15120.32	15120.13	$12_{112} - 12_{93}$	16048.97	16048.97
$13_{112} - 13_{113}$	14908.13	14908.11	$13_{122} - 13_{103}$	16161.04	16161.08
$14_{122} - 14_{123}$	14655.43	14655.27	$14_{132} - 14_{113}$	16303.84	16303.82
$15_{132} - 15_{133}$	14360.57	14360.52	$15_{142} - 15_{123}$	16482.86	16482.80
$16_{142} - 16_{143}$	14024.10	14023.79	$16_{152} - 16_{133}$	16704.12	16704.14
$17_{152} - 17_{153}$	13645.85	13645.92	$17_{162} - 17_{143}$	16974.56	16974.47
$18_{162} - 18_{163}$	13228.62	13228.57	$18_{172} - 18_{153}$	17300.88	17300.81
$19_{172} - 19_{173}$	12774.20	12774.04	$19_{182} - 19_{163}$	17690.53	17690.50
$20_{182} - 20_{183}$	12285.33	12285.14	$20_{192} - 20_{173}$	18150.10	18150.95
$21_{192} - 21_{193}$	11765.07	11765.06	$21_{202} - 21_{183}$		18689.45
$22_{202} - 22_{203}$	11217.54	11217.35	$22_{212} - 22_{193}$	19312.76	19312.85
$23_{212} - 23_{213}$	10645.89	10645.81	$23_{222} - 23_{203}$	20027.36	20027.41
$24_{222} - 24_{223}$	10054.81	10054.52	$24_{232} - 24_{213}$	20838.31	20838.37
$25_{232} - 25_{233}$	9447.98	9447.83	$25_{242} - 25_{223}$	21749.80	21749.87
$26_{242} - 26_{243}$	8830.42	8830.36	$26_{252} - 26_{233}$	22764.63	22764.72
$27_{252} - 27_{253}$	8206.95	8206.99	$27_{262} - 27_{243}$	23884.39	23884.40
$28_{262} - 28_{263}$	7583.02	7582.83	$28_{272} - 28_{253}$	25109.17	25109.03
$29_{262} - 29_{273}$			$29_{282} - 29_{263}$	26437.44	26437.46

$30_{272} - 30_{283}$			$30_{292} - 30_{273}$	27867.40	27867.41
			$31_{302} - 31_{283}$	29395.72	29395.55
			$32_{312} - 32_{293}$	31017.63	31017.65
			$33_{322} - 33_{303}$	32728.82	32728.83
			$34_{332} - 34_{313}$	34523.19	34523.30

Table IX. Calculated and experimental frequencies (MHz) of 1,2,3-Triazine belonging to the 22 GHz band head (disregarding quadrupole hyperfine structure)

$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated	$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated
$4_{13} - 4_{14}$	22058.75	22058.76	$4_{23} - 4_{04}$	22058.75	22058.83
$5_{33} - 5_{14}$	22057.56	22057.58	$5_{23} - 5_{24}$	22057.56	22057.34
$6_{43} - 6_{34}$	22055.30	22055.63	$6_{33} - 6_{34}$	22054.97	22054.89
$7_{53} - 7_{34}$	22052.81	22052.78	$7_{43} - 7_{44}$	22050.94	22050.92
$8_{63} - 8_{44}$	22048.86	22048.89	$8_{53} - 8_{54}$	22044.38	22044.80
$9_{73} - 9_{54}$	22043.91	22043.90	$9_{63} - 9_{64}$	22035.93	22035.71
$10_{83} - 10_{64}$	22037.74	22037.82	$10_{73} - 10_{74}$	22022.81	22022.60
$11_{93} - 11_{74}$	22030.69	22030.81	$11_{83} - 11_{84}$	22004.08	22004.16
$12_{103} - 12_{84}$	22023.07	22023.18	$12_{93} - 12_{94}$	21978.83	21978.78
$13_{113} - 13_{94}$	22015.43	22015.45	$13_{103} - 13_{104}$	21944.60	21944.49
$14_{123} - 14_{104}$	22008.45	22008.41	$14_{113} - 14_{114}$	21899.34	21898.95
$15_{133} - 15_{114}$	22003.36	22003.09	$15_{123} - 15_{124}$	21839.20	21839.37

16 ₁₄₃ - 16 ₁₂₄	22000.90	22000.86	16 ₁₃₃ -16 ₁₃₄	21762.48	21762.57
17 ₁₅₃ - 17 ₁₃₄	22003.36	22003.44	17 ₁₄₃ -17 ₁₄₄	21664.93	21664.97
18 ₁₆₃ - 18 ₁₄₄	22012.98	22012.96	18 ₁₅₃ -18 ₁₅₄	21542.41	21542.61
19 ₁₇₃ -19 ₁₅₄	22031.98	22031.93	19 ₁₆₃ -19 ₁₆₄	21391.31	21391.29
20 ₁₈₃ -20 ₁₆₄	22063.44	22063.37	20 ₁₇₃ -20 ₁₇₄	21206.56	21206.71
21 ₁₉₃ -21 ₁₇₄	22110.82	22110.74	21 ₁₈₃ -21 ₁₈₄	20984.47	20984.64
22 ₂₀₃ -22 ₁₈₄	22178.09	22178.04	22 ₁₉₃ -22 ₁₉₄	20721.20	20721.16
23 ₂₁₃ -23 ₁₉₄	22269.86	22269.80	23 ₂₀₃ -23 ₂₀₄	20412.79	20412.86
24 ₂₂₃ -24 ₂₀₄	22391.14	22391.10	24 ₂₁₃ -24 ₂₁₄	20057.20	20057.12
25 ₂₃₃ -25 ₂₁₄	22547.61	22547.56	25 ₂₂₃ -25 ₂₂₄	19652.38	19652.23
26 ₂₄₃ -26 ₂₂₄	22745.40	22745.35	26 ₂₃₃ -26 ₂₃₄	19197.67	19197.50
27 ₂₅₃ -27 ₂₃₄	22991.20	22991.16	27 ₂₄₃ -27 ₂₄₄		18693.34
28 ₂₆₃ -28 ₂₄₄	23292.14	23292.08	28 ₂₅₃ -28 ₂₅₄	18140.72	18141.09
29 ₂₇₃ -29 ₂₅₄	23655.58	23655.58	29 ₂₆₃ -29 ₂₆₄	17543.20	17543.12
30 ₂₈₃ -30 ₂₆₄	24089.25	24089.30	30 ₂₇₃ -30 ₂₇₄	16902.36	16902.51
31 ₂₉₃ -31 ₂₇₄	24600.90	24600.92	31 ₂₈₃ -31 ₂₈₄	16223.20	16223.00
32 ₃₀₃ -32 ₂₈₄	25197.88	25197.86	32 ₂₉₃ -32 ₂₉₄	15508.88	15508.85
33 ₃₁₃ -33 ₂₉₄	25887.17	25887.14	33 ₃₀₃ -33 ₃₀₄	14764.55	14764.74
34 ₃₂₃ -34 ₃₀₄	26675.03	26675.00	34 ₃₁₃ -34 ₃₁₄	13995.79	13995.66
35 ₃₃₃ -35 ₃₁₄	27566.83	27566.72	35 ₃₂₃ -35 ₃₂₄	13206.90	13206.90
36 ₃₄₃ -36 ₃₂₄	28566.47	28566.42	36 ₃₃₃ -36 ₃₃₄	12403.87	12403.92
37 ₃₅₃ -37 ₃₃₄	29676.98	29676.84	37 ₃₄₃ -37 ₃₄₄	11592.67	11592.51

38 ₃₆₃ -38 ₃₄₄	30899.39	30899.33	38 ₃₅₃ -38 ₃₅₄	10778.59	10778.57
39 ₃₇₃ -39 ₃₅₄	32233.84	32233.81	39 ₃₆₃ -39 ₃₆₄	9968.18	9968.18
40 ₃₈₃ -40 ₃₆₄	33678.85	33678.85	40 ₃₇₃ -40 ₃₇₄	9167.50	9167.50
			41 ₃₈₃ -41 ₃₈₄	8382.35	8382.69
			42 ₃₉₃ -42 ₃₉₄	7619.68	7619.79

Table X. Calculated and experimental frequencies (MHz) of 1,2,3-Triazine belonging to the 28 GHz band head (disregarding quadrupole hyperfine structure)

$J_{Ka',Kc'} \leftarrow J_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated	$J_{Ka',Kc'} \leftarrow J_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated
5 ₂₄ -5 ₀₅	28361.53	28362.76	5 ₁₄ -5 ₁₅	28361.53	28362.75
6 ₃₄ -6 ₁₅	28360.74	28360.62	6 ₂₄ -6 ₂₅	28360.74	28360.61
7 ₄₄ -7 ₂₅	28359.28	28358.93	7 ₃₄ -7 ₃₅	28359.28	28359.92
8 ₅₄ -8 ₃₅	28356.32	28356.54	8 ₄₄ -8 ₄₅	28356.32	28356.51
9 ₆₄ -9 ₄₅	28353.37	28353.27	9 ₅₄ -9 ₅₅	28363.37	28353.18
10 ₇₄ -10 ₅₅	28348.82	28348.90	10 ₆₄ -10 ₆₅	28348.82	28348.71
11 ₈₄ -11 ₆₅	28343.10	28343.27	11 ₇₄ -11 ₇₅		28342.82
12 ₉₄ -12 ₇₅	28336.15	28336.11	12 ₈₄ -12 ₈₅		28335.21
13 ₁₀₄ -13 ₈₅	28327.33	28327.22	13 ₉₄ -13 ₉₅	28325.70	28325.54
14 ₁₁₄ -14 ₉₅	28316.46	28316.38	14 ₁₀₄ -14 ₁₀₅	28313.29	28313.37
15 ₁₂₄ -15 ₁₀₅	28303.45	28303.40	15 ₁₁₄ -15 ₁₁₅	28298.27	28298.20

16 ₁₃₄ -16 ₁₁₅	28288.09	28288.11	16 ₁₂₄ -16 ₁₂₅	28279.45	28279.44
17 ₁₄₄ -17 ₁₂₅	28270.44	28270.40	17 ₁₃₄ -17 ₁₃₅	28256.48	28256.40
18 ₁₅₄ -18 ₁₃₅	28250.33	28250.20	18 ₁₄₄ -18 ₁₄₅	28228.30	28228.24
19 ₁₆₄ -19 ₁₄₅	28227.63	28277.54	19 ₁₅₄ -19 ₁₅₅	28194.12	28193.94
20 ₁₇₄ -20 ₁₅₅	28202.17	28203.56	20 ₁₆₄ -20 ₁₆₅	28152.36	28152.30
21 ₁₈₄ -21 ₁₆₅	28175.64	28175.54	21 ₁₇₄ -21 ₁₇₅	28102.15	28101.88
22 ₁₉₄ -22 ₁₇₅	28146.93	28146.92	22 ₁₈₄ -22 ₁₈₅		28040.98
23 ₂₀₄ -23 ₁₈₅	28117.41	28117.31	23 ₁₉₄ -23 ₁₉₅	27967.10	27967.57
24 ₂₁₄ -24 ₁₉₅	28087.64	28087.59	24 ₂₀₄ -24 ₂₀₅	27878.97	27879.30
25 ₂₂₄ -25 ₂₀₅	28058.87	28058.88	25 ₂₁₄ -25 ₂₁₅	27772.98	27773.44
26 ₂₃₄ -26 ₂₁₅	28032.56	28032.58	26 ₂₂₄ -26 ₂₂₅	27646.56	27646.90
27 ₂₄₄ -27 ₂₂₅	28010.53	28010.45	27 ₂₃₄ -27 ₂₃₅		27496.20
28 ₂₅₄ -28 ₂₃₅	27994.58	27994.61	28 ₂₄₄ -28 ₂₄₅	27317.28	27317.49
29 ₂₆₄ -29 ₂₄₅	27987.53	27987.57	29 ₂₅₄ -29 ₂₄₅	27106.54	27106.69
30 ₂₇₄ -30 ₂₅₅	27867.40	27867.28	30 ₂₆₄ -30 ₂₆₅	26859.24	26859.50
31 ₂₈₄ -31 ₂₆₅	28012.13	28012.15	31 ₂₇₄ -31 ₂₇₅	26571.32	26571.62
32 ₂₉₄ -32 ₂₇₅	28050.87	28051.10	32 ₂₈₄ -32 ₂₈₅	26238.71	26238.85
33 ₃₀₄ -33 ₂₈₅	28113.62	28113.53	33 ₂₉₄ -33 ₂₉₅	25857.17	25857.40
34 ₃₁₄ -34 ₂₉₅	28204.38	28204.48	34 ₃₀₄ -34 ₃₀₅	25424.02	25424.03
35 ₃₂₄ -35 ₃₀₅	28329.39	28329.39	35 ₃₁₄ -35 ₃₁₅	24936.35	24936.28
36 ₃₃₄ -36 ₃₁₅	28494.17	28494.34	36 ₃₂₄ -36 ₃₂₅	24392.75	24392.66
37 ₃₄₄ -37 ₃₂₅	28705.87	28705.89	37 ₃₃₄ -37 ₃₃₅	23792.72	23792.74

38 ₃₅₄ -38 ₃₃₅	28971.10	28971.09	38344-38 ₃₄₅	23137.23	23137.19
39 ₃₆₄ -39 ₃₄₅	29297.43	29297.40	39 ₃₅₄ -39 ₃₅₅	22427.88	22427.80
40 ₃₇₄ -40 ₃₅₅	29692.60	29692.55	40 ₃₆₄ -40 ₃₆₅	21667.11	21667.35
41 ₃₈₄ -41 ₃₆₅	30164.46	30164.44	41 ₃₇₄ -41 ₃₇₅	20859.60	20859.51
42 ₃₉₄ -42 ₃₇₅	30721.09	30720.90	42 ₃₈₄ -42 ₃₈₅	20008.75	20008.70
43 ₄₀₄ -43 ₃₈₅	31369.48	31369.54	43 ₃₉₄ -43 ₃₉₅	19119.94	19191.97
44 ₄₁₄ -44 ₃₉₅	32117.40	32117.43	44 ₄₀₄ -44 ₄₀₅	18198.56	18198.83
45 ₄₂₄ -45 ₄₀₅	32970.98	32970.89	45 ₄₁₄ -45 ₄₁₅	17251.42	17251.19
46 ₄₃₄ -46 ₄₁₅	33935.24	33935.23	46 ₄₂₄ -46 ₄₂₅	16283.51	16283.28
			47 ₄₃₄ -47 ₄₃₅	15301.60	15301.56
			48 ₄₄₄ -48 ₄₄₅	14312.85	14312.67
			49 ₄₅₄ -49 ₄₅₅	13323.33	13323.43
			50 ₄₆₄ -50 ₄₆₅	12340.99	12340.75
			51 ₄₇₄ -51 ₄₇₅	11371.62	11371.54
			52 ₄₈₄ -52 ₄₈₅	10422.48	10422.68
			53 ₄₉₄ -53 ₄₉₅	9500.73	9500.84

Table XI. Calculated and experimental frequencies (MHz) of 1,2,3-Triazine belonging to the 35 GHz band head (disregarding quadrupole hyperfine structure)

$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated	$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated
6 ₂₅ .6 ₀₆		34664.75	6 ₁₅ .6 ₁₆		34664.75

7 ₃₅ -7 ₁₆		34663.62	7 ₂₅ -7 ₂₂₆		34663.62
8 ₄₅ -8 ₂₆		34662.08	8 ₃₅ -8 ₃₆		34662.08
9 ₅₅ -9 ₃₆	34659.66	34660.08	9 ₄₅ -9 ₃₆	34659.66	34660.08
10 ₆₅ -10 ₄₆	34657.08	34657.43	10 ₅₅ -10 ₅₆	34657.08	34657.42
11 ₇₅ -11 ₅₆	34654.20	34654.03	11 ₆₅ -11 ₆₆	34654.20	34654.03
12 ₈₅ -12 ₆₆	34649.54	34649.75	12 ₇₅ -12 ₇₆	34649.54	34649.76
13 ₉₅ -13 ₇₆	34644.16	34644.47	13 ₈₅ -13 ₈₆	34644.16	34644.45
14 ₁₀₅ -14 ₈₆	34637.69	34638.00	14 ₉₅ -14 ₉₆	34637.69	34637.95
15 ₁₁₅ -15 ₉₆	34629.99	34630.17	15 ₁₀₅ -15 ₁₀₆	34629.99	34630.08
16 ₁₂₅ -16 ₁₀₆	34620.46	34620.82	16 ₁₁₅ -16 ₁₁₆	34620.46	34620.65
17 ₁₃₅ -17 ₁₁₆	34609.55	34609.40	17 ₁₂₅ -17 ₁₂₆	34609.55	34609.43
18 ₁₄₅ -18 ₁₂₆	34596.59	34596.75	18 ₁₃₅ -18 ₁₃₆		34596.19
19 ₁₅₅ -19 ₁₃₆	34581.44	34581.60	19 ₁₄₅ -19 ₁₄₆		34581.44
20 ₁₆₅ -20 ₁₄₆	34564.52	34564.17	20 ₁₅₅ -20 ₁₅₆	34562.50	34562.59
21 ₁₇₅ -21 ₁₅₆	34544.07	34544.18	21 ₁₆₅ -21 ₁₆₆	34541.81	34541.62
22 ₁₈₅ -22 ₁₆₆	34521.41	34521.45	22 ₁₇₅ -22 ₁₇₆	34517.44	34521.39
23 ₁₉₅ -23 ₁₇₆	34495.87	34495.79	23 ₁₈₅ -23 ₁₈₆	34489.77	34489.48
24 ₂₀₅ -24 ₁₈₆	34467.31	34467.03	24 ₁₉₅ -24 ₁₉₆	34457.59	34457.42
25 ₂₁₅ -24 ₁₉₆	34435.16	34435.02	25 ₂₀₅ -25 ₂₀₆	34420.93	34420.66
26 ₂₂₅ -26 ₂₀₆	34399.74	34399.67	26 ₂₁₅ -26 ₂₁₆	34378.85	34378.54
27 ₂₃₅ -27 ₂₁₆	34361.07	34360.93	27 ₂₂₅ -27 ₂₂₆	34330.45	34330.30
28 ₂₄₅ -28 ₂₂₆	34318.97	34318.80	28 ₂₃₅ -28 ₂₃₆	34275.0	34275.07

29 ₂₅₅ -29 ₂₃₆	34273.50	34273.41	29 ₂₄₅ -29 ₂₄₆	34212.18	34211.77
30 ₂₆₅ -30 ₂₄₆	34225.08	34224.95	30 ₂₅₅ -30 ₂₅₆		34139.20
31 ₂₇₅ -31 ₂₅₆	34174.13	34173.77	31 ₂₆₅ -31 ₂₆₆		34055.89
32 ₂₈₅ -32 ₂₆₆	34120.66	34120.37	32 ₂₇₅ -32 ₂₇₆	33960.14	33959.38
33 ₂₉₅ -33 ₂₇₆	34065.51	34065.42	33 ₂₈₅ -33 ₂₈₆	33849.00	33851.74
34 ₃₀₅ -34 ₂₈₆	34010.01	34009.80	34 ₂₉₅ -34 ₂₉₆	33722.56	33722.95
35 ₃₁₅ -35 ₂₉₆	33954.68	33954.67	35 ₃₀₅ -35 ₃₀₆	33576.33	33576.59
36 ₃₂₅ -36 ₃₀₆	33901.53	33901.40	36 ₃₁₅ -36 ₃₁₆	33407.81	33407.82
37 ₃₃₅ -37 ₃₁₆	33851.70	33851.73	37 ₃₂₅ -37 ₃₂₆	33213.08	33213.25
38 ₃₄₅ -38 ₃₄₆	33807.65	33807.70	38 ₃₃₅ -38 ₃₃₆	32989.02	32989.15
39 ₃₅₅ -39 ₃₃₆	33771.62	33771.74	39 ₃₄₅ -39 ₃₄₆	32731.40	32731.49
40 ₃₆₅ -40 ₃₄₆	33746.75	33746.70	40 ₃₅₅ -40 ₃₅₆	32435.78	32435.96
41 ₃₇₅ -41 ₃₅₆	33735.89	33735.86	41 ₃₆₅ -41 ₃₆₆	32098.01	32098.16
42 ₃₈₅ -42 ₃₆₆	33743.04	33742.96	42 ₃₇₅ -42 ₃₇₆	31713.69	31713.68
43 ₃₉₅ -43 ₃₇₆	33772.03	33772.28	43 ₃₈₅ -43 ₃₈₆	31278.21	31278.30
44 ₄₀₅ -44 ₃₈₆	33828.64	33288.56	44 ₃₉₅ -44 ₃₉₆	30788.08	30788.20
45 ₄₁₅ -45 ₃₉₆	33917.21	33917.14	45 ₄₀₅ -45 ₄₀₆	30240.19	30240.20
46 ₄₂₅ -46 ₄₀₆	34043.62	34043.85	46 ₄₁₅ -46 ₄₁₆	29631.88	29631.89
47 ₄₃₅ -47 ₄₁₆	34215.01	34215.07	47 ₄₂₅ -47 ₄₂₆	28961.71	28961.87
48 ₄₄₅ -48 ₄₂₆	34437.77	34437.69	48 ₄₃₅ -48 ₄₃₆	28229.81	28229.85
49 ₄₅₅ -49 ₄₃₆	34719.18	34719.04	49 ₄₄₅ -49 ₄₄₆	27436.48	27436.71
			50 ₄₅₅ -50 ₄₅₆	26584.56	26584.46

			51 ₄₆₅ -51 ₄₆₆	25676.42	25676.24
			52 ₄₇₅ -52 ₄₇₆	24716.29	24716.15
			53 ₄₈₅ -53 ₄₈₆	23709.25	23709.12
			54 ₄₉₅ -54 ₄₉₆	22660.94	22660.80
			55 ₅₀₅ -55 ₅₀₆	21577.68	21577.41
			56 ₅₁₅ -56 ₅₁₆	20465.65	20465.60
			57 ₅₂₅ -57 ₅₂₆	19332.46	19332.36
			58 ₅₃₅ -58 ₅₃₆	18185.13	18184.96
			60 ₅₅₅ -60 ₅₅₆	15877.34	15877.58

Table XII. Calculated and experimental frequencies (MHz) of 1,2,3-triazine belonging to the 42 GHz band head (disregarding quadrupole hyperfine structure)

$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental.	ν (MHz) calculated	$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated
56 ₅₀₆ -56 ₅₀₇	34919.67	34919.41	56 ₅₀₆ -56 ₅₀₇	34919.67	34919.41
57 ₅₁₆ -57 ₅₁₇	34201.29	34201.24	57 ₅₁₆ -57 ₅₁₇	34201.29	34201.24
58 ₅₂₆ -58 ₅₂₇	33416.02	33416.16	58 ₅₂₆ -58 ₅₂₇	33416.02	33416.16
59 ₅₃₆ -59 ₅₃₇	32564.12	32563.92	59 ₅₃₆ -59 ₅₃₇	32564.12	32563.92
60 ₅₄₆ -60 ₅₄₇	31645.52	31645.49	60 ₅₄₆ -60 ₅₄₇	31645.52	31645.49
61 ₅₅₆ -61 ₅₅₇	30662.83	30663.04	61 ₅₅₆ -61 ₅₅₇	30662.83	30663.04
62 ₅₆₆ -62 ₅₆₇	29619.70	29619.92	62 ₅₆₆ -62 ₅₆₇	29619.70	29619.92
63 ₅₇₆ -63 ₅₇₇	28520.54	28520.54	63 ₅₇₆ -63 ₅₇₇	28520.54	28520.54

$65_{596}-65_{597}$	26175.00	26175.08	$65_{596}-65_{597}$	26175.00	26175.08
$56_{506}-56_{507}$	34919.67	34919.41	$56_{506}-56_{507}$	34919.67	34919.41

Table XIII. Calculated and experimental frequencies (MHz) of 1,2,3-Triazine for the R-branch transitions (disregarding quadrupole hyperfine structure)

$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated	$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν (MHz) experimental	ν (MHz) calculated
$2_{12}-1_{11}$	15724.71	15725.02	$2_{02}-1_{01}$		15786.95
$3_{13}-2_{12}$		22058.41	$3_{03}-2_{02}$		22059.34
$2_{11}-1_{10}$	21965.38	21965.13			
$4_{14}-3_{13}$	28361.53	28361.44	$4_{04}-3_{03}$	28361.53	28361.44
$3_{22}-2_{21}$	28267.66	28267.69	$3_{12}-2_{11}$		28451.59
$2_{20}-1_{01}$	28394.81	28394.77			
$5_{15}-4_{14}$	34664.08	34664.13	$5_{05}-4_{04}$	34664.08	34664.13
$3_{21}-2_{20}$		34475.99			
$4_{23}-3_{22}$		34662.21	$4_{13}-3_{12}$		34666.85

Figure 1. Structures of 1,2,3 -triazine and 1,2,4 -triazines

Figure 2. Fortrat diagrams of 1,2,4-triazine and 1,2,3-triazine.

Figure 3. The band head near 15.8 GHz with $K_{+1} = 2-3$ (room temperature, pressure = 20 mtorr; time constant = 300 ms; delay = 125 ms; electric field = 400 V/cm; frequency step = 10 kHz.

Figure 4. The band head at 35 GHz (room temperature, pressure = 20 mtorr; time constant = 300 ms; delay = 125 ms; electric field = 400 V/cm; frequency step = 10 kHz)

Figure 5. The CCSD(T) equilibrium structure of 1,2,3-triazine.

Figure 6. The ^{14}N quadrupole coupling constants (MHz) in the inertial axis frame.

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Highlights

1,2,3-triazine

1,2,4-triazine

Fortrat diagram

rotational constants

stark spectroscopy

structure

ab initio calculations

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Graphical abstract