MARVEL analysis of the measured high-resolution rovibrational spectra of C₂H₂

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Abstract

Rotation-vibration energy levels are determined for the electronic ground state of the acetylene molecule, ¹²C₂H₂, using the Measured Active Rotational-Vibrational Energy Levels (MARVEL) technique. 37,813 measured transitions from 61 publications are considered. The distinct components of the spectroscopic network linking ortho and para states are considered separately. The 20,717 ortho and 17,096 para transitions measured experimentally are used to determine 6013 ortho and 5200 para energy levels. The MARVEL results are compared with alternative compilations based on the use of effective Hamiltonians.

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1. Introduction

Acetylene, HCCH, is a linear tetratomic unsaturated hydrocarbon whose spectrum is important in a large range of environments. The temperatures of these environments range from the hot, oxy-acetylene flames which are widely used for welding and related activities [1], temperate, where monitoring of acetylene in breath gives insights into the nature of exhaled smoke [2], to the cold, where the role of acetylene in the formation of carbon dust in the interstellar medium is a subject of debate [3]. Furthermore, acetylene is observed in star-forming regions [4] and thought to be an important constituent of clouds in the upper atmospheres of brown dwarfs and exoplanets [5]. Acetylene provides a major source of opacity in the atmospheres of cool carbon stars [6, 7]. It is present in various planetary and lunar atmospheres in the solar system, including Jupiter and Titan [8] and has been detected on comets [9]. The first analysis of the atmosphere of a super-Earth, exoplanet 55 Cancri e [10], speculate that acetylene could be present in its atmosphere; however the spectral data currently available does not allow for an accurate verification of its presence in such a high temperature environment.

The spectroscopy of acetylene has long been studied in the laboratory, particularly by the group of Herman in Brussels. A full analysis of these experimental studies is given below. Herman and co-workers have presented a number of reviews of the rovibrational behaviour of acetylene in \( X \, \Sigma^+_v \) ground electronic state [11, 12, 13]. Besides summarizing the status rotation-vibration spectroscopy of the system, these reviews also give insight into the internal dynamics of the system, a topic not considered here.

From a theoretical point of view a number of variational nuclear motion calculations have been performed for the acetylene ground electronic state [14, 15, 16, 17, 18, 19]. New theoretical rovibrational calculations for this molecule are in progress as part of the ExoMol project [20, 21], a database of theoretical line lists for molecules of astrophys-
ical importance, appropriate up to high temperatures of around 300 – 3000K, for use in characterising the atmospheres of cool stars and exoplanets. High accuracy experimental energy levels provide essential input for testing and improving theoretically calculated line positions.

In this work we present the largest compilation of published experimental data on rovibrational transitions for the acetylene molecule, which has been formatted and analysed using the MARVEL (Measured Active Rotational-Vibrational Energy Levels) spectroscopic network software, the results of which are presented and discussed in this paper. The next section gives the underlying theory used for the study. Section 3 presents and discusses the experimental sources used. Results are given in Section 4. Section 5 discusses these results; this section presents comparisons with recent empirical databases due to Amyay et al. [22] (henceforth 16AmFaHe), Lyulin and Campargue [23] (henceforth 17LyCa) and Lyulin and Perevalov, [24] (henceforth 17LyPe), which builds on their earlier work [25], all of which only became available while the present study was being undertaken. Finally section 6 gives our conclusions.

2. Theory

2.1. MARVEL

The MARVEL procedure [26, 27] is based on the theory of spectroscopic networks [28, 29] and is principally based on earlier work by Flaud et al. [30] and Watson [31, 32]. The MARVEL program can be used to critically evaluate and validate experimentally-determined transition wavenumbers and uncertainties collected from the literature. It inverts the wavenumber information to obtain accurate energy levels with an associated uncertainty. MARVEL has been successfully used to evaluate the energy levels for molecules, most recently TiO [33] and others such as $^{14}$NH$_3$ [34, 35], water vapour [36, 37, 38, 39, 40], H$_2$D$^+$ and D$_2$H$^+$ [41], H$_3^+$ [42], and C$_2$ [43]. To be useful for MARVEL, measured transitions
must have an associated uncertainty and each state must be uniquely labelled, typically by a set of quantum numbers. It should be noted that while MARVEL requires uniqueness it does not require these quantum numbers to be strictly correct, or indeed even meaningful, beyond obeying rigorous selection rules; these assignments simply act as labels for each state. Nevertheless, it greatly aids comparisons with other data if they contain physically sensible information. The quantum numbers used in the present study are considered in the following section.

2.2. Quantum number labelling

The 11 quantum numbers that were used for labelling the upper and lower states are detailed in Table 1. This includes the quanta of each vibrational mode in normal mode notation: $v_1, v_2, v_3, v_4, l_4, v_5, l_5, K = |\ell_4 + \ell_5|$ and $J$, where $v_1, \ldots, v_5$ are the vibrational quantum numbers, $\ell_4$ and $\ell_5$ are the vibrational angular momentum quantum numbers associated with $v_4$ and $v_5$, respectively, with $|\ell| = v, v - 2 \ldots 1$ for odd $v$, $|\ell| = v, v - 2 \ldots 0$ for even $v$. $K = |k|$ is the rotational quantum number, with $k$ corresponding to the projection of the rotational angular momentum, $J$, on the $z$ axis. $K$ is also equal to the total vibrational angular momentum quantum number, $|L| = |\ell_4 + \ell_5|$, and therefore $K$ will be also referred to as the total vibrational angular momentum. $J$ is the quantum number associated with rotational angular momentum, $J$. We follow the phase convention of the Belgium group, for $K \equiv |k| = |\ell_4 + \ell_5|$ with $\ell_4 \geq 0$ if $k = 0$. We also use the $e$ or $f$ labelling, along with the nuclear spin state (ortho or para).

The quantum number assignments for this work were taken from the original sources where possible, with any exceptions noted in section 3.1 and 3.2: particular reference should be made to the general comments (1a) and (1b) in 3.2. While MARVEL requires a unique set of quantum numbers for each state, it merely treats these as labels and whether they are strictly correct or not does not effect the validity of results. Nevertheless, the
Table 1: Quantum numbers used to label the upper and lower energy states.

| Label | Description                                                                 |
|-------|-----------------------------------------------------------------------------|
| \(v_1\) | CH symmetric stretch \((\sigma^+_g)\)                                     |
| \(v_2\) | CC symmetric stretch \((\sigma^+_u)\)                                     |
| \(v_3\) | CH antisymmetric stretch \((\sigma^+_u)\)                                  |
| \(v_4\) | Symmetric (trans) bend \((\pi_g)\)                                        |
| \(\ell_4\) | Vibrational angular momentum associated with \(v_4\)                      |
| \(v_5\) | Antisymmetric (cis) bend \((\pi_u)\)                                      |
| \(\ell_5\) | Vibrational angular momentum associated with \(v_5\)                      |
| \(K\) | Total vibrational angular momentum, \(|\ell_4 + \ell_5|\) and Rotational quantum number |
| \(J\) | Rotational angular momentum                                                |
| \(e/f\) | Symmetry relative to the Wang transformation (see text)                   |
| ortho/para | Nuclear spin state (see text)                                               |

attempt to label them with sensible assignments aids comparisons with other datasets.

Levels with parity \(+(-1)^J\) are called \(e\) levels and those with parity \(-(-1)^J\) are called \(f\) levels. In other words, \(e\) and \(f\) levels transform in the same way as the rotational levels of \(1\Sigma^+\) and \(1\Sigma^-\) states, respectively \[44\]. Table 2 gives the combinations of \(e/f\) and \(J\) with corresponding parity. States of a linear molecular are often also classified based on inversion, with states which are left unchanged called ‘gerade’ and labelled with a subscript \(g\), and those whose phase changes to opposite are called ‘ungerade’ and labelled \(u\). The ortho and para labels are defined based on the the permutation, \(P\), of the identical hydrogen atoms. For the para states the corresponding rovibrational wavefunctions, \(\Psi_{r-v}\), are symmetric, i.e. \(P\Psi_{r-v} = (+1)\Psi_{r-v}\), while for the ortho states they are antisymmetric, \(P\Psi_{r-v} = (-1)\Psi_{r-v}\). The allowed combinations of these labels are shown in Table 3 and explained in more detail below.

Table 2: Parity of states in \(^{12}\text{C}_2\text{H}_2\) based on the symmetry labels used in this work.

| \(e/f\) | \(J\) | Parity |
|--------|--------|--------|
| \(e\)  | Odd    | –      |
| \(e\)  | Even   | +      |
| \(f\)  | Odd    | +      |
| \(f\)  | Even   | –      |
Table 3: Allowed combinations of symmetry labels for rovibrational states (including spin) of $^{12}$C$_2$H$_2$, where $s =$ symmetric, $a =$ antisymmetric, ‘Total’ is how the rovibronic wavefunction, including the nuclear spin, acts under permutation symmetry.

| $u/g$ | $+/−$ | Ro-vib. | Nuclear spin | Total |
|-------|-------|---------|--------------|-------|
| $u$   | +     | $a$     | Ortho        | $a$   |
| $u$   | −     | $s$     | Para         | $a$   |
| $g$   | +     | $s$     | Para         | $a$   |
| $g$   | −     | $a$     | Ortho        | $a$   |

The $e/f$ labelling which has been adopted in this work was originally introduced by Brown et al. [44] in order to eliminate issues relating to Plíva’s $c/d$ labelling [45] and the $s/a$ labelling of Winnewisser and Winnewisser [46]. For more detailed information on the $e/f$ rotational splitting, see the section titled ‘$e/f$ levels’, page 173 of Herman et al. [47].

In summary, an interaction known as $\ell$-doubling occurs in linear molecules, which splits the rotational, $J$, levels in certain vibrational states. The symmetry describing these states is based on the total vibrational angular momentum quantum number, $K$. There are, for example, two distinct states in the $2\nu_4$ band; one with $K = 0$ ($\Sigma^+_g$, (0002000)0) and the other $K = 2$ ($\Delta_g$, (0002200)2). In this case, the interaction with the rotation leads to a splitting of the rovibrational levels in the $K = 2$ ($\Delta_g$) sublevel ($\ell$-doubling). The $\Delta_e$ (corresponding to one of the two bending modes) and $\Sigma_e$ (corresponding to one of the three stretching modes) states repel each other, pushing $\Delta_e$ to a lower energy while $\Delta_f$ is unaffected. For this reason the $e$ state typically lies below the $f$ state, as bending occurs at a lower frequency than stretching [47]. This effect is $J(J + 1)$ dependent and so becomes increasingly important at higher rotational excitations. If a rovibrational state has no rotational splitting (as is the case if both $\ell_4=0$ and $\ell_5 = 0$, but not if $\ell_4 = 1$ and $\ell_5 = −1$), the state is always labelled $e$ and there is no corresponding $f$ state.

Herman and Lievin [48] give an excellent description of the ortho and para states of acetylene which is summarised here. The hydrogen atoms in the main isotopologue of
acetylene are spin-$\frac{1}{2}$ particles and therefore, as Fermions, obey Fermi-Dirac rules. The $^{12}$C carbon atoms, the only isotopologue considered in this work, are spin-0 and so do not need to be considered here. The symmetry operation $P$ describes a permutation of identical particles; when applied to the molecule it implies permutation of the two hydrogen atoms. The total wavefunction must either be symmetric or antisymmetric upon such a transformation. In the case of fermions it must be antisymmetric. The permutation symmetry of the ground electronic state is totally symmetric upon interchange of identical atoms and so the electronic part of the wavefunction can be ignored for this situation. The symmetry of the nuclear spin part of the wavefunction is not usually specified, but can easily be deduced from the remaining symmetry. If the rovibrational part of the wavefunction is antisymmetric under permutation symmetry (resulting from a combination of $g$ and $-$ or $u$ and $+$), then the nuclear spin state must be ortho and if the rovibrational part of the wavefunction is symmetric ($g$, $+$ or $u$, $-$), then the nuclear spin state must be para (see Table 3).

It is important to distinguish the vibrational and rotational symmetries from the symmetry of the rovibrational states of $\Psi_{r-v}$. For a linear molecule such as $^{12}$C$_2$H$_2$ both the rotational $\Psi_r$ and vibrational $\Psi_v$ contributions to $\Psi_{r-v}$ should transform according with the point group $D_{coh}(M)$, spanning an infinite number of irreducible representations such as $\Sigma^+_g$ ($K = 0$), $\Pi^+_g$ ($K = 1$), $\Delta^+_g$ ($K = 2$) etc. However, after combining the rotational and vibrational parts into the rovibrational state $\Psi_{r-v}$, only the $K = 0$ states (i.e. $\Sigma_g^+$, $\Sigma_g^-$, $\Sigma_u^+$, $\Sigma_u^-$) can lead to the total nuclear-rotation-vibrational state obeying the proper nuclear statistics, as described above. These are the irreducible elements of the $D_{2h}(M)$ group \cite{49}, which according to our labeling scheme correspond to the four pairs: $e$ ortho, $e$ para, $f$ ortho and $f$ para. For example the vibrational state $\nu_5$ ($\Pi_u$) can be combined with the $J = 1, K = 1$ ($\Pi_g$) rotational state to produce three rovibrational combinations of $\Sigma_u^+$, $\Sigma_u^-$ and $\Pi_u$ ($D_{coh}$ point group). However only the $\Sigma_u^-$, $\Sigma_u^+$ states are allowed by the nuclear
statistics. Here $\nu_5$, $\Pi_u$, $K$, $\Pi_g$ are not rigorous quantum numbers/labels, while $J = 1$, $e/f$ and ortho/para are. Thus these two rovibrational states are assigned $(0000^1 1^1)^1 J= 1, e$, para and $(0000^0 1^1)^1 J= 1, f$, ortho, respectively. It should be also noted that generally neither $K$ nor $v_1, \ldots, v_5$ are good quantum numbers. However the quantity $(-1)^{v_3+v_5}$ is a good quantum number as it defines the conserved $u/g$ symmetry as follows: a state is ungerade if $(-1)^{v_3+v_5} = -1$ and gerade if $(-1)^{v_3+v_5} = 1$. The $+/-$ labelling is derived from $e/f$ and $J$, as given in Table 2.

Throughout this paper we shall use the notations $(v_1v_2v_3v_4v_5)^K$ to describe vibrational states and $(v_1v_2v_3v_4v_5)^K, J, e/f, \text{ortho/para}$ to describe rovibrational states. The $e$ and $f$ labelling combined with $J$ and nuclear spin state (ortho or para) gives the rigorous designation of each state. Other quantum number labels are approximate but, besides representing the underlying physics, are necessary to uniquely distinguish each state. The symmetry labels of the vibrational states ($\Sigma^{+/-}_{u/g}, \Pi_{u/g}, \Delta_{u/g}, \ldots$) have been added to the end of the output energy files (see Table 8 and supplementary material).

2.3. Selection rules

The rigorous selection rules governing rotation-vibration transitions for a symmetric linear molecule (molecular group $D_{coh}(M)$) are given by

1. $\Delta J = \pm 1$ with $e \leftrightarrow e$ or $f \leftrightarrow f$,
2. $\Delta J = \pm 0$ with $e \leftrightarrow f$,
3. $J' + J'' \neq 0$,
4. $u \leftrightarrow g$.

The first two equations here correspond to the standard selection rule $+ \leftrightarrow -$ for the dipole transitions in terms of the parities. The ortho states of $^{12}$C$_2$H$_2$ have the statistical weight $g_{ns} = 3$, while for the para states $g_{ns} = 1.$
3. Experimental sources

A large number of experimentally determined transition frequencies can be found in the literature for the main isotopologue of acetylene, $^{12}$C$_2$H$_2$. As part of this study we attempted to conduct a rigorous and comprehensive search for all useable spectroscopic data. This includes the transition frequency (in cm$^{-1}$) and associated uncertainty, along with quantum number assignments for both the upper and lower energy states. A unique reference label is assigned to each transition, which is required for MARVEL input. This reference indicates the data source, table (or page) and line number that the transition originated from. The data source tag is based on the notation employed by the IUPAC Task Group on water [37, 50] with an adjustment discussed below. The associated uncertainties were taken from the experimental data sources where possible, but it was necessary to increase many of these in order to achieve consistency with the same transition in alternative data sources. As noted by Lyulin and Perevalov [25], these sources often provide overall uncertainties for the strongest lines in a vibrational band which may underestimate the uncertainty associated with some or all of the weaker, and especially of blended, lines.

61 sources of experimental data were considered. Two of the data compilations mentioned in the introduction [22, 23] contain data from multiple other sources, some of which was not directly available to us. Data taken from these compilations is given a tag based on that used in the compilation with the original reference given in Table 5. After processing, 60 sources were used in the final data set. The data from more recent papers is generally provided in digital format, but some of the older papers had to be processed through digitalisation software, or even manually entered in the most extreme cases. After digitalisation the data was converted to MARVEL format; an example of the input file in this format is given in Table 4, the full file can be found in the supplementary data of this paper.
Table 4: Extract from the Marvel input file for the ortho transitions. The full file is supplied as part of the supplementary information to this paper. All energy term values and uncertainties are in units of cm$^{-1}$. The assignments are detailed in Table 1.

| Energy  | Unc   | Upper assignment | Lower assignment | Ref             |
|---------|-------|------------------|------------------|-----------------|
| 1248.2620 | 0.0005 | 0 0 0 1 1 1 -1 0 34 e ortho | 0 0 0 0 0 0 0 0 35 e ortho | 00Vander_table2_l11 |
| 1252.8546 | 0.0005 | 0 0 0 1 1 1 -1 0 32 e ortho | 0 0 0 0 0 0 0 0 33 e ortho | 00Vander_table2_l12 |
| 1257.4230 | 0.0005 | 0 0 0 1 1 1 -1 0 30 e ortho | 0 0 0 0 0 0 0 0 31 e ortho | 00Vander_table2_l14 |
| 1261.9694 | 0.0005 | 0 0 0 1 1 1 -1 0 28 e ortho | 0 0 0 0 0 0 0 0 29 e ortho | 00Vander_table2_l16 |
| 1266.4970 | 0.0005 | 0 0 0 1 1 1 -1 0 26 e ortho | 0 0 0 0 0 0 0 0 27 e ortho | 00Vander_table2_l18 |
| 1271.0098 | 0.0005 | 0 0 0 1 1 1 -1 0 24 e ortho | 0 0 0 0 0 0 0 0 25 e ortho | 00Vander_table2_l10 |
| 1275.5122 | 0.0005 | 0 0 0 1 1 1 -1 0 22 e ortho | 0 0 0 0 0 0 0 0 23 e ortho | 00Vander_table2_l11 |

Table 5 gives a summary of all the data sources used in this work, along with the wavelength range, number of transitions, number of vibrational bands, the approximate temperature of the experiment and comments, which can be found in section 3.1. Table 6 gives those data sources which were considered but not used, with comments on the reasons.

The reference label given in these tables corresponds to the unique labels in the Marvel input files, given in the supplementary data and illustrated in the last column of Table 4. As transitions do not occur between ortho and para states, they form two completely separate components of the experimental spectroscopic network, with no links between them. All input and output files supplied in the supplementary data to this work are split into either ortho or para.

Table 5: Data sources used in this study with wavelength range, numbers of transitions and approximate temperature of the experiment. A/V stands for the number of transitions analysed/verified. ‘RT’ stands for room temperature. See section 3.1 for the notes.

| Tag              | Ref. | Range (cm$^{-1}$) | A/V   | Bands | Temp | Note |
|------------------|------|-------------------|-------|-------|------|------|
| 09YuDrPe         | 51   | 29-55             | 20/20 | 5     | RT   |      |
| 16AmFaHe_kab91   | 52   | 61-1440           | 3233/3233 | 47  | RT   |      |
| 16AmFaHe_amy10   | 53   | 63-7006           | 1232/1232 | 36  | RT   |      |
| 11DrYu           | 54   | 85-92             | 20/20 | 7     | RT   |      |
| 17JaLyPe         | 55   | 429-592           | 627/627 | 9   | RT   |      |
| 81HiKa           | 56   | 628-832           | 684/684 | 5   | RT (3a) |      |
| 93WeBlNa         | 57   | 632-819           | 1610/1609 | 13  | RT (3b) |      |
Table 5: Data sources used in this study with wavelength range, numbers of transitions and approximate temperature of the experiment. A/V stands for the number of transitions analysed/verified. 'RT' stands for room temperature. See section 3.1 for the notes.

| Tag            | Ref. | Range (cm$^{-1}$) | A/V | Bands | Temp | Note               |
|----------------|------|-------------------|-----|-------|------|--------------------|
| 00MaDaCl       | 58   | 644-820           | 77/77 | 1     | RT   |                    |
| 01JaClMa       | 59   | 656-800           | 355/355 | 4    | RT   |                    |
| 50BeNi         | 60   | 671-1460          | 500/0 | 13    | RT   | (3c)               |
| 16AmFaHe_gom10 | 61   | 1153-1420         | 27/27 | 3     | RT   |                    |
| 16AmFaHe_gom09 | 62   | 1247-1451         | 66/66 | 8     | RT   |                    |
| 00Vander       | 63   | 1248-1415         | 64/64 | 2     | RT   |                    |
| 16AmFaHe_amy09 | 64   | 1253-3422         | 3791/3777 | 57   | Up to 1455K | (3d) |
| 03JaMaDa       | 65   | 1810-2235         | 486/486 | 14   | RT   |                    |
| 03JaMaDab      | 66   | 3207-3358         | 109/109 | 2    | RT   |                    |
| 16AmFaHe_jac02 | 67   | 1860-2255         | 150/150 | 3    | RT   |                    |
| 72Pliva        | 68   | 1865-2598         | 1016/1015 | 15   | RT   |                    |
| 16AmFaHe_ber98 | 69   | 1957-1960         | 19/19  | 1     | RT   | (3e)               |
| 16AmFaHe_jac07 | 70   | 2515-2752         | 148/148 | 3    | RT   |                    |
| 16AmFaHe_pal72 | 71   | 2557-5313         | 42/42  | 3    | RT   |                    |
| 16AmFaHe_vda93 | 72   | 2584-3364         | 499/499 | 5    | RT   |                    |
| 93DeSaJo       | 73   | 2589-2760         | 372/372 | 3    | RT   |                    |
| 82RiBaRa       | 74   | 3140-3399         | 1789/1788 | 21   | RT and 433K |       |
| 16AmFaHe_sarb95| 75   | 3171-3541         | 401/401 | 8    | RT   |                    |
| 06LyPeMa       | 76   | 3182-3327         | 167/167 | 13   | RT   |                    |
| 16AmFaHe_man05 | 77   | 3185-3355         | 288/288 | 5    | RT   |                    |
| 16AmFaHe_sara95| 78   | 3230-3952         | 424/424 | 5    | RT   |                    |
| 16AmFaHe_ber99 | 79   | 3358-3361         | 21/21  | 1    | RT   | (3e)               |
| 16AmFaHe_lyub07| 80   | 3768-4208         | 668/668 | 8    | RT   |                    |
| 16AmFaHe_gr06  | 81   | 3931-4009         | 91/91  | 10   | RT   |                    |
| 16AmFaHe_dcu91 | 82   | 3999-4143         | 251/251 | 6    | RT   |                    |
| 72BaGhNa       | 83   | 4423-4791         | 472/408 | 8    | RT   | (3f)               |
| 16AmFaHe_lyua07| 84   | 4423-4786         | 440/440 | 8    | RT   |                    |
| 16AmFaHe_lyu08 | 85   | 5051-5562         | 320/320 | 5    | RT   |                    |
| 16AmFaHe_kep96 | 86   | 5705-6802         | 1957/1957 | 30   | RT   |                    |
| 17LyCa         | 87   | 5852-8563         | 4941/4941 | 108  | RT   | (3g)               |
| 16AmFaHe_rob08 | 88   | 5885-6992         | 568/568 | 20   | RT   |                    |
| 07TrMaDa       | 89   | 6299-6854         | 546/546 | 13   | RT   | (3h)               |
| 16AmFaHe_lyu09 | 90   | 6300-6666         | 89/89  | 5    | RT   |                    |
| 16KaNaVa       | 91   | 6386-6541         | 19/19  | 2    | RT   | (3i)               |
| 16AmFaHe_kou94 | 92   | 6439-6629         | 73/73  | 1    | RT   |                    |
| 15TwCiSe       | 93   | 6448-6564         | 135/135 | 2    | RT   |                    |
| 02HaVa         | 94   | 6448-6685         | 271/271 | 4    | RT   |                    |
| 77BaGhNa       | 95   | 6460-6680         | 860/859 | 15   | RT   | (3j)               |
| 05EdBaMa       | 96   | 6472-6579         | 41/41  | 1    | RT   |                    |
Table 5: Data sources used in this study with wavelength range, numbers of transitions and approximate temperature of the experiment. A/V stands for the number of transitions analysed/verified. 'RT' stands for room temperature. See section 3.1 for the notes.

| Tag            | Ref. | Range (cm\(^{-1}\)) | A/V | Bands | Temp | Note     |
|----------------|------|----------------------|-----|-------|------|----------|
| 13ZoGiBa       | [94] | 6490-6609            | 37/37 | 1     | RT   |          |
| 00MoDuJa       | [95] | 6502-6596            | 36/36 | 1     | RT   |          |
| 96NaLaAw       | [96] | 6502-6596            | 36/36 | 1     | RT   |          |
| 16AmFaHe_amy11 | [97] | 6667-7868            | 2259/2256 | 79 | RT   | (3k)     |
| 15LyVaCa       | [98] | 7001-7499            | 2471/2471 | 29 | RT   | (3l)     |
| 09JaLaMa       | [99] | 7043-7471            | 233/233 | 4  | RT   |          |
| 02VaElBr       | [100]| 7062-9877            | 626/626 | 11 | RT   | (3m)     |
| 16LyVaCa       | [101]| 8283-8684            | 627/627 | 14 | RT   | (3n)     |
| 17BeLyHu       | [102]| 8994-9414            | 432/432 | 11 | RT   |          |
| 89HeHuVe       | [103]| 9362-10413           | 657/657 | 14 | RT   | (3o)     |
| 93SaKa         | [104]| 12428-12538          | 91/73 | 1   | RT   | (3p)     |
| 03HeKeHu       | [105]| 12582-12722          | 60/60 | 1   | RT   |          |
| 92SaKa         | [106]| 12904-13082          | 216/212 | 3  | RT   | (3q)     |
| 94SaSeKa       | [107]| 13629-13755          | 53/53 | 1   | <RT (223K) | (3r) |
| **Total**      |      |                      |      | 29-13755 | 37813/37206 |        |

Table 6: Data sources considered but not used in this work.

| Tag            | Ref. | Comments                                           |
|----------------|------|---------------------------------------------------|
| 16AmFaHe_abb96 | [108]| 0 transitions in 16AmFaHe; data not available in original paper. |
| 16AmFaHe_eli98 | [109]| 0 transitions in 16AmFaHe; data not available in original paper. |
| 72Plivaa       | [110]| Energy levels only                                |
| 02MeYaVa       | [111]| No suitable data                                  |
| 01MeYaVa       | [112]| No suitable data                                  |
| 99SaPeHa       | [113]| No suitable data                                  |
| 97JuHa         | [114]| No suitable data                                  |
| 93ZhHa         | [115]| No suitable data                                  |
| 93ZhVaHa       | [116]| No suitable data                                  |
| 91ZhVaKa       | [117]| No suitable data                                  |
| 13SiMeVa       | [118]| No suitable data                                  |
| 83ScLeKl       | [119]| No assignments given                             |

3.1. Comments on the experimental sources in Table 5

(3a) 81HiKa [56] has an apparent misprint in column 2 of their Table 6: the R(19) line should be 780.2601 cm\(^{-1}\) not 790.2601 cm\(^{-1}\), as confirmed by 01JaClMa [59], and in col-
umn 5 of their Table 4: the Q(3) line should be 728.9148 cm$^{-1}$ not 729.9148 cm$^{-1}$, also confirmed by 01JaClMa [59].

(3b) 93WeBlNa_page14_l38 from 93WeBlNa [57] is not consistent with other data sources. It was marked in the original dataset as a transition that the authors did not include in their analysis and so has been removed from our dataset.

(3c) 50BeNi [60] was deemed too unreliable to use in the final dataset: data are directly contradicted by other sources.

(3d) Many of the transitions included from 16AmFaHe_amy09 [64] are not duplicated in any other source. While this means they represent a valuable source of data, and have thus been kept in the MARVEL dataset, the fact that there is no other experimental data to back them up means they should be treated with some degree of caution. As stated in the original paper, modelling such a high temperature region is a challenge. There are a small number of transitions - 14 out of 3791 - that do not match those from other data sources and have been removed from our dataset.

(3e) 16AmFaHe_ber98 [68] and 16AmFaHe_ber99 [77] are Raman spectra and so the transitions do not follow the selection rules detailed in section 2.3 of this paper.

(3f) 72BaGhNa [81] has a band labelled (0013$^{1}0^{0}$)$^{1}$ - (0001$^{1}0^{0}$)$^{1}$ which is not consistent with other data sources. It was found that the band labelled (0104$^{0}1^{1}$)$^{1}$ - (0001$^{1}0^{0}$)$^{1}$ gave energies consistent with those labelled (0013$^{1}0^{0}$)$^{1}$ - (0001$^{1}0^{0}$)$^{1}$ in other data sources (16AmFaHe_lyua07, 16AmFaHe_lyu08). Bands including (0104$^{0}1^{1}$)$^{1}$ are not present in other data sources. We have swapped the labelling of these bands accordingly. All other bands from this dataset were included, with the exception of the single transition labelled 72BaGhNa_table2_c2_l32, which was not consistent with other datasets.

(3g) 17LyCa [23] provides a collection of data recorded in Grenoble using cavity ring down spectroscopy (CRDS) from several papers. 15LyVaCa (FTS15 in the notation of 17LyCa) [98], 16LyVaCa (FTS16) [101] and 17BeLyHu (FTS17) [102] were all already
included as separate files in our dataset and so were removed from the 17LyCa [23] dataset. The remaining data, CRDS13 [120], CRDS14 [121] and CRDS16 [122] are all included in the final dataset with the tag ‘17LyCa’. See also comment (3i).

(3h) 07TrMaDa [86] contains a band labelled $2\nu_2 + (\nu_4 + 3\nu_5)^0$. $\ell_4$ and $\ell_5$ were assigned as 1 and -1 respectively, to be consistent with the labelling of 16AmFaHe_kee96.

(3i) Full data for 16KaNaVa [88] was provided in digital format from the corresponding author (private communication, Juho Karhu).

(3j) 77BaGhNa_table3_1205 of 77BaGhNa [92] does not fit with the same transition in two other sources.

(3k) 16AmFaHe_amy11 [97] includes a band $((1000^60^6) - (0000^00^0)^0)$ which has transitions from $J = 0$ to $J = 10, 11, 12$. These are not physical and so have been removed from the dataset. There is one other transition which we have removed which we have found to be inconsistent with the other datasets.

(3l) There has been some changes in the authors approach to labelling levels between 15LyVaCa [98] and 17LyCa [23], see comment (3g) (Alain Campargue, private communication). This was partly to allow all bands to have unique labelling, as duplicate labels were provided in 15LyVaCa as indicated by ** or * superscripts. We have relabelled these bands to fit with other data sources, for example 16AmFaHe_amy11 [97]. We have been informed by the authors of 17LyCa that they are currently making amendments to their published dataset (Alain Campargue, private communication). Table 7 summarises the changes in labelling between 15LyVaCa, the current version of 17LyCa_FTS15 (see supplementary data of [23]) and this work.

(3m) 02VaElBr [100] is missing one band labelling in the footnote to their Table 3. The missing label for the penultimate level is $I = (v_1 v_2 v_3 v_4^{i} v_5^{j}) K = (0020^011^1)$. Full data for this source was provided in digital format by the corresponding author (Jean Vander Auwera, private communication).
(3n) 16LyVaCa [101] has duplicate lines in the (1110000) band. Those which are inconsistent with other sources were removed and thus not included in the final data set for the MARVEL analysis. It is possible that they should be re-assigned.

(3o) The assignments given for the band labelled (0122020) - (0000000) in 89HeHuVe [103] require the upper state to have the parity of an f-level, which is unphysical if both $\ell_4=0$ and $\ell_5=0$. There can be no e/f splitting in this case. We assumed this upper state should be labelled (012222-2)0. We have amended and included these reassigned transitions in our dataset.

(3p) Table 1 of 93SaKa [104] has duplicates for the $e\leftrightarrow e$ transitions in the (202110) - (000011) vibrational band. Those which are inconsistent with other sources were removed and thus not included in the final data set.

(3q) 92SaKa [106] contains some duplicate lines which have been assigned identical quantum numbers. Those which are inconsistent with other sources were removed and thus not included in the final data set.

(3r) 94SaSeKa [107] gives two tables of data but only one is assigned with vibrational quantum numbers, so data from the other table were not considered in this study.

Table 7: Changes in labelling between 15LyVaCa [98], 17LyVa_FTS15 [23] and this work, in the form ($e_1e_2e_3e_4s_{e_3}l_{s}^3$). See comment (3l) in the text.

| 15LyVaCa       | 17LyVa_FTS15       | This work       |
|----------------|--------------------|----------------|
| (020411−1)1**  | (011300)1          | (020410)1      |
| (011300)1      | (020411)1          | (011300)1      |
| (1102101)1     | (1102101)1         | (1102100)1     |
| (110211−1)1**  | (020231−1)1        | (1102011)1     |
| (110211−1)1**  | (110231−1)1        | (110211−1)1    |
3.2. General comments

A number of general issues had to be dealt with before consistent networks could be obtained.

(1a) 16AmFaHe [22] released a collation and analysis of experimental data in the middle of our collation and analysis stage. The entire database was formatted into Marvel format so it could subsequently be run through the software and combined with the other experimental sources referenced in this paper. Some of the experimental sources featured in the 16AmFaHe database paper had already been collated and formatted to Marvel format prior to its publication. These are 03JaMaDa [65], 91KaHeDi [52], 06LyPeMa [74], 07LyPeGu [82], 82RiBaRa [6], 02VaElBr [100] and 00MoDuJa [95]. We used a Marvel format version of 16AmFaHe’s compilation to compare to our data, as a further check to validate data had been digitised and formatted correctly; the versions included in the present study come from the original datasets for these papers. A few of the sources that were cited in 16AmFaHe were not included in our final dataset. There were 0 transitions in 16AmFaHe from [108] (abb96), [109] (eli98) or [54] (drou11). The data for [54] was taken from the original paper (see 11DrYu in Table 5), but there was no data obviously available in the original papers for the other two sources. We have tried to keep the quantum number labelling consistent with that of 16AmFaHe as much as possible (see comment (1b) for an exception). Some other sources were labelled in order to make them consistent, in particular those cases were \( \ell_4 \) and \( \ell_5 \) were not defined in the original source.

(1b) Many of the \( \ell_4 \) and \( \ell_5 \) assignments were inconsistent between different sources, were not given in the original data (often only the total \( K = |\ell_4 + \ell_5| \) is given) or were inconsistent between data in the same dataset. Examples include the bands with upper energies labelled \((v_1v_2v_3\ell_4^4\ell_5^4)^K = (0002^+1^*)^1\), \((1102^+1^*)^1\) or \((0102^+1^*)^1\) in 16AmFaHe. Using simple combination differences, with the known lower value and given transition wavenumber, there was found to be more than one value for the upper energy. We assume this duplication of
quantum numbers for different states is down to the different method of analysis used in 16AmFaHe, which does not require a completely unique set. For example, for the upper level \((1102^2 1^{-1})^1\), \(J=2\), \(e\), there are two transitions which give as upper energy level of 7212.93 cm\(^{-1}\) (from 16AmFaHe_kee96) and three that give 7235.29 cm\(^{-1}\) (from 16AmFaHe_vda02 and 16AmFaHe_rob08). These same two energies can be found in multiple other sources (07TrMaDa, 15LyVaCa, 77BaGhNa, 02VaElBr), but the \(\ell_4\) and \(\ell_5\) assignment was inconsistent for states of the same upper energy. The decision was made to batch them together and assign the first energy level (7212.94 cm\(^{-1}\) in this example) as \((1102^2 1^{-1})^1\) and the second (7235.29 cm\(^{-1}\) in this example) as \((1102^0 1^1)^1\). The same logic was applied to other bands with \(K = |\ell_4 + \ell_5| = 1\).

(1c) The \(e/f\) notation (see section 2.2) was mostly specified in experimental papers, but some required additional investigation in order to assign them in such a way as to be consistent with other papers. The \(c/d\) notation in \([45]\), for example, is analogous to the \(e/f\) notation used in this work.

(1d) All transitions which were considered but not processed in the final dataset are labelled with _ct at the end of the reference and have a minus sign in front of the transition frequency, at the start of the file. Marvel software ignores any line with a negative wavenumber.

### 3.3. Other comments

The following are sources of the acetylene data in the HITRAN database ([66, 123, 124, 125]): 16AmFaHe_gom09 [62], 16AmFaHe_gom10 [61], 96NaLaAw [96], 05Ed-BaMa [93], 16AmFaHe_lyua07 [82], 16AmFaHe_jac07 [69], 16AmFaHe_jac09 [99], 00Vander [63], 02HaVa [91], 03JaMaDab [66], 16AmFaHe_kab91 [52], 72Pliva [45], 03JaMaDa [65], 82RiBaRa [6], 16AmFaHe_vda93 [71].

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4. Results

The MARVEL website (http://kkrk.chem.elte.hu/marvelonline/marvel_full.php) has a version of MARVEL which can be run online. The variable NQN (number of quantum numbers) is 11 in the case of acetylene, given in Table 1. These are required for both the lower and upper levels, as illustrated in Table 4.

All energies are measured from the zero point energy (ZPE). This is the energy of the ground rovibrational state, which is given a relative energy of 0 and is included in the para set of energy levels. The ortho set of energies therefore needs a ‘magic number’ to be added to all the MARVEL ortho-symmetry energies. Here the magic number was taken as the ground vibrational \((0000^00)^0, J = 1\) state of 16AmFaHe [22] who determined the value 2.3532864 cm\(^{-1}\), see Table 10 below. The output for the ortho energies in the supplementary data, and the extract of the output file in Table 8, all have this magic number added. The para component of the spectroscopic network does not require a magic number as it contains the ground rovibrational level, \((0000^00)^0, J = 0\). There are a small number (284 for ortho and 119 for para) of energy levels which are not joined to the two principal components (PCs) of the network. If more experimental transitions became available in the future it would be possible to link these to the PCs.

A total of 37,813 transitions were collated and considered (20,717 ortho and 17,096 para) from the data sources detailed in section 3. Of those 607 were found to be inconsistent with others (353 ortho and 254 para) and thus removed from the final data set, leaving a total of 37,206 transitions used as input into MARVEL (20,364 ortho and 16,842 para). A plot of energy as a function of rotational quantum number, \(J\), was made for each vibrational band as a check that quantum numbers had been assigned consistently. Figure 1 and 2 show this for each vibrational band, for the ortho and para states respectively. Figures 3 and 4 illustrate the ortho and para spectroscopic networks, respectively. The nodes are
Table 8: Extract from the Marvel output file for the ortho transitions. The full file is supplied as part of the supplementary information to this paper. All energies and uncertainties are in units of cm$^{-1}$. The assignments are detailed in Table 1.

| Assignment | Energy   | Unc | NumTrans | u/g | Symmetry     |
|------------|----------|-----|----------|-----|--------------|
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 e ortho | 2.35329 | 0.00003 | 204 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3 e ortho | 14.11952 | 0.00002 | 289 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5 e ortho | 35.29793 | 0.00002 | 306 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7 e ortho | 65.88710 | 0.00002 | 298 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9 e ortho | 105.88501 | 0.00002 | 306 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11 e ortho | 155.28899 | 0.00002 | 306 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13 e ortho | 214.09576 | 0.00002 | 306 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15 e ortho | 282.30144 | 0.00002 | 310 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17 e ortho | 359.90150 | 0.00002 | 294 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19 e ortho | 446.89078 | 0.00003 | 282 | g | sigma_g_plus |
| 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21 e ortho | 543.26353 | 0.00002 | 274 | g | sigma_g_plus |
| 0 0 0 1 1 0 0 0 1 1 e ortho | 614.04436 | 0.00018 | 98 | g | pi_g |
| 0 0 0 1 1 0 0 0 1 2 f ortho | 618.77696 | 0.00013 | 133 | g | pi_g |

Energy levels and the edges the transitions between them. Each consists of a large main network with a series of smaller networks currently unattached. Different algorithms can be used to present these networks in a variety of ways; figure 5, for example, gives alternative representations of the structure. They highlight the intricate relationships between different energy levels and illustrate how the variety of sources collated in this work link together. We note that the inclusion of transitions intensities as weights in the spectroscopic network can aid in the determination of transitions which should preferentially be investigated in new experiments [28].
Figure 1: MARVEL energy levels (cm$^{-1}$) as a function of rotational quantum number, $J$, for all the vibrational energy bands in the ortho network analysed in this paper.
Figure 2: MARVEL energy levels (cm$^{-1}$) as a function of rotational quantum number, $J$, for all the vibrational energy bands in the para network analysed in this paper.
Figure 3: The ortho component of the spectroscopic network produced using MARVEL input data.
Figure 4: The *para* component of the spectroscopic network produced using *MARVEL* input data.
Table 9 gives the vibrational ($J=0$) energies resulting from the Marvel analysis, with associated uncertainty, vibrational assignment and the number of transitions (NumTrans) which were linked to the particular energy level. The higher the number of transitions the more certainty can be given to the energy value. See comment (3o) of section 3.1 relating to the band (0122$^22^{-2}$)$^0$ which may not have the correct assignment.

Table 9: Vibrational energy levels (cm$^{-1}$) from Marvel analysis

| $(v_1v_2v_3^4v_4^3)^K$ | e/f | State | MARVEL Energy (cm$^{-1}$) | Uncertainty (cm$^{-1}$) | NumTrans |
|-------------------------|-----|-------|---------------------------|-------------------------|----------|
| (000$^00^00^0$)$^0$     | e   | para  | 0.000000                  | 0.000000                | 85       |
| (0002$^00^00^0$)$^0$    | e   | para  | 1230.390303               | 0.000559                | 10       |
| (0001$^11^{-1}$)$^0$    | e   | ortho | 1328.073466               | 0.000319                | 19       |
| (0001$^11^{-1}$)$^0$    | f   | para  | 1340.550679               | 0.001551                | 9        |
| (0000$^02^0^0$)$^0$     | e   | para  | 1449.112363               | 0.001189                | 10       |
| (0100$^00^0^0$)$^0$     | e   | para  | 1974.316617               | 0.006000                | 1        |
| (0003$^11^{-1}$)$^0$    | e   | ortho | 2560.594937               | 0.002000                | 3        |
| (0002$^22^{-2}$)$^0$    | e   | para  | 2648.014468               | 0.004000                | 1        |
| (0001$^13^{-1}$)$^0$    | e   | ortho | 2757.797907               | 0.001897                | 3        |
| (0000$^04^0^0$)$^0$     | e   | para  | 2880.220077               | 0.004000                | 1        |
| (0101$^11^{-1}$)$^0$    | e   | ortho | 3281.899025               | 0.001744                | 5        |
| (0010$^00^0^0$)$^0$     | e   | ortho | 3294.839579               | 0.001903                | 4        |
| (0101$^11^{-1}$)$^0$    | f   | para  | 3300.635590               | 0.007682                | 2        |
|      |      |       |       |       |
|------|------|-------|-------|-------|
| (1000^00^0)^0 | e   | para | 3372.838987 | 0.016000 | 1     |
| (0103^1-1)^0  | e   | ortho| 4488.838166 | 0.001200 | 2     |
| (0012^00^0)^0 | e   | ortho| 4508.012219 | 0.002666 | 4     |
| (0102^2-2)^0  | f   | ortho| 4599.774669 | 0.003905 | 2     |
| (0011^1-1)^0  | e   | para | 4609.341046 | 0.005902 | 3     |
| (0011^1-1)^0  | f   | ortho| 4617.925870 | 0.005083 | 4     |
| (1001^1)^0    | e   | ortho| 4673.631058 | 0.001789 | 3     |
| (1001^1)^0    | f   | para | 4688.846488 | 0.011400 | 1     |
| (0101^2-1)^0  | e   | ortho| 4710.739822 | 0.018000 | 1     |
| (0010^2)^0    | e   | ortho| 4727.069907 | 0.001193 | 3     |
| (1000^2)^0    | e   | para | 4800.137287 | 0.006000 | 1     |
| (0201^1-1)^0  | e   | ortho| 5230.229286 | 0.010000 | 1     |
| (0110^2)^0    | e   | ortho| 5260.021842 | 0.003328 | 2     |
| (0103^2-1)^0  | e   | ortho| 5893.260496 | 0.010000 | 1     |
| (1001^3-1)^0  | e   | ortho| 6079.693064 | 0.003714 | 2     |
| (0010^4)^0    | e   | ortho| 6141.127536 | 0.010000 | 1     |
| (0112^0)^0    | e   | ortho| 6449.106486 | 0.006000 | 1     |
| (1102^0)^0    | e   | para | 6513.991447 | 0.008000 | 1     |
| (1010^0)^0    | e   | ortho| 6556.464783 | 0.001000 | 4     |
| (1101^1)^0    | e   | ortho| 6623.139603 | 0.011915 | 2     |
| (0110^2)^0    | e   | ortho| 6690.577636 | 0.012000 | 1     |
| (2000^0)^0    | e   | para | 6709.021187 | 0.003714 | 2     |
| (1100^2)^0    | e   | para | 6759.239077 | 0.010000 | 1     |
| (0114^0)^0    | e   | ortho| 7665.441780 | 0.010000 | 1     |
| (0022^0)^0    | e   | para | 7686.078947 | 0.002000 | 1     |
| (0204^2-2)^0  | e   | para | 7707.277687 | 0.004000 | 1     |
| (1012^0)^0    | e   | ortho| 7732.793472 | 0.005291 | 4     |
| (0203^3-3)^0  | e   | ortho| 7787.324394 | 0.010000 | 1     |
| (0021^1-1)^0  | e   | ortho| 7805.004672 | 0.001876 | 3     |
| (1103^1)^0    | e   | ortho| 7816.006736 | 0.010000 | 1     |
| (1011^1)^0    | f   | ortho| 7853.277713 | 0.012000 | 1     |
| (1010^2)^0    | e   | ortho| 7961.820133 | 0.007660 | 3     |
| (2001^1)^0    | e   | ortho| 7994.394918 | 0.002578 | 2     |
| (2001^1)^0    | f   | para | 8001.204086 | 0.009877 | 2     |
| (2000^2)^0    | e   | para | 8114.362883 | 0.003705 | 3     |
| (1100^4)^0    | e   | para | 8164.554028 | 0.008000 | 1     |
| (1110^0)^0    | e   | ortho| 8512.056241 | 0.000429 | 3     |
| (1201^1)^0    | e   | ortho| 8556.589655 | 0.010000 | 1     |
| (1201^1-1)^0  | f   | para | 8570.322888 | 0.010000 | 1     |
| (2100^0)^0    | e   | para | 8661.149087 | 0.010000 | 1     |
| (0300^4)^0    | e   | para | 8739.814487 | 0.010000 | 1     |
| (0310^0)^0    | e   | ortho| 9151.727686 | 0.010000 | 1     |
| (0030^0)^0    | e   | ortho| 9639.863579 | 0.015435 | 2     |
| (1112^0)^0    | e   | ortho| 9668.161468 | 0.015435 | 2     |
| (0122^2-2)^0  | f   | ortho| 9741.622286 | 0.030000 | 1     |
| (0121^1-1)^0  | e   | ortho| 9744.541486 | 0.030000 | 1     |
5. Comparison to other derived energy levels

Table 10 compares our rotational energy levels for the vibrational ground state, which are determined up to $J = 69$, with those obtained by 16AmFaHe [22] from an effective Hamiltonian fit to the observed data. In general the agreement is excellent. However for the highest few levels with $J \geq 55$ we find differences which are significantly larger than our uncertainties; our levels are systematically below those of 16AmFaHe. This suggests that the effective Hamiltonian treatment used by 16AmFaHe becomes unreliable for these high $J$ levels. It should be noted that data relating to these highly excited levels originated from 16AmFaHe_amy9, a high temperature experiment which has not been reproduced; see comment (3d), section 3.1. It is interesting to note that a further comparison with rotational energies extrapolated as part of 17LyPe’s ASD-1000 spectroscopic databank [24], also given in table 10, yields differences of approximately the same magnitude but, in contrast, consistently lower than our work.

### Table 10: Comparison of pure rotational levels with those of 16AmFaHe [22].

| $J$ | This work | Uncertainty | 16AmFaHe | Difference | 17LyPe | Difference | State |
|-----|------------|-------------|----------|------------|--------|------------|-------|
| 1   | 2.35329    | 0.00003     | 2.353286417 | 0         | 2.3533  | 0.00001    | ortho |
| 2   | 7.05982    | 0.00003     | 7.05982021 | 0         | 7.0598  | -0.00002   | para  |
| 3   | 14.11952   | 0.00002     | 14.119523294 | 0.00001  | 14.1195 | -0.00002   | ortho |
| 4   | 23.53228   | 0.00003     | 23.532278547 | 0         | 23.5322 | -0.00008   | para  |
| 5   | 35.29793   | 0.00002     | 35.297929811 | 0         | 35.2978 | -0.00013   | ortho |
| 6   | 49.41629   | 0.00003     | 49.416281896 | -0.00001 | 49.4161 | -0.00019   | para  |
| 7   | 65.88710   | 0.00002     | 65.887100587 | 0         | 65.8869 | -0.00002   | ortho |
| 8   | 84.71012   | 0.00002     | 84.710112648 | -0.00001 | 84.7098 | -0.00032   | para  |
| 9   | 105.88501  | 0.00002     | 105.88505832 | 0         | 105.8846 | -0.00041   | ortho |
| 10  | 129.41144  | 0.00003     | 129.411428888 | -0.00001 | 129.411 | -0.00044   | para  |
| 11  | 155.28899  | 0.00002     | 155.28899157 | 0.00001  | 155.2885 | -0.00049   | ortho |
| 12  | 183.51727  | 0.00003     | 183.517264652 | -0.00001 | 183.5167 | -0.00057   | para  |
The supplementary data from 17LyCa [23] contains lower energy levels, frequency and assignments, from which upper energy levels can be calculated. Figure 6 gives the differences between the energies given in 17LyCa and this work as a function of \( J \). The vast majority are within 0.005 cm\(^{-1}\). Note that the difference in labelling of some bands has been taken into account when comparisons are made (see comment (3l) in section 3.1 and comment (1b) in section 3.2).

The energy levels given as supplementary data in annex 5 of 16AmFaHe [22] are separated into polyads which are characterised by a small number of quantum numbers; \( N_{rmv} = 5v_1 + 3v_2 + 5v_3 + v_4 + v_5, \) \( J, e/f \) symmetry and \( u/g \) symmetry. As there are more than one state defined by these quantum numbers, the only comparison that was possible to make was to match these and find the closest energy value within these bounds. As such, we cannot be certain that bands have been matched correctly. 17LyCa compared what they could against 16AmFaHe’s data but also could not find a reliable way to determine unambiguously which energy of each polyad block corresponds to their energy levels. Figure 7 gives the difference between the energies in this work and those matched with 16AmFaHe as a function of rotational angular momentum quantum number, \( J \). 6160 out of the 11,154 energies differ by less than 0.01 cm\(^{-1}\). However, this leaves 4994 energies with a difference of higher than 0.01 cm\(^{-1}\). 2176 of these energies also appear in 17LyCa, so a comparison could be made between the three. Only 7 of the energies in the 17LyCa dataset are closer to 16AmFaHe than this work, and of those all are within 0.02 cm\(^{-1}\) with this

| Energy Levels | Difference | Assignment |
|---------------|------------|------------|
| 4284.80143    | 0.00181    | para       |
| 4426.87720    | 0.00154    | ortho      |
| 4571.24409    | 0.00142    | para       |
| 4717.87442    | 0.00142    | para       |
| 4866.79028    | 0.00232    | para       |
| 5017.97095    | 0.00168    | ortho      |
| 5171.43923    | 0.00366    | para       |
| 5327.14526    | 0.00195    | para       |
| 5645.38676    | 0.00300    | ortho      |
Figure 6: Differences between the energy term values given in 17LyCa²³ and this work as a function of rotational angular momentum quantum number, $J$. 
work.

It should be noted, however, that the differences between this work and 16AmFaHe are largest for those energy levels with a low value of NumTrans (the number of transitions that link the energy state to other energies within the dataset); see figure 8. The vast majority of energy levels which only have one transition are not in the 17LyCa dataset. Many of these transitions came from the data source 16AmFaHe_amy09; see comment (3d) in section 3.1. It would be of use to have more experimental data on transitions to these levels in order to confirm their validity. The entire band \((012^2 2 \rightarrow 2^0)\) has differences of over 900 cm\(^{-1}\) in comparison to the matched values in 16AmFaHe. This indicates that this band has been misassigned (see comment (3o in section 3.1)). We are uncertain currently as what it should be reassigned to. We have excluded this band from figures 7 and 8.

It should be made clear, as mentioned above, that those energy levels present in the input data which are only linked to the main components of the spectroscopic network by one transition should be treated with caution; this number is given as a parameter in the third to last column of the output files included in the supplementary data. It can be used, along with the uncertainties, as an indication of the reliability of each energy level. Note, finally, that Marvel only processes data given as input; it does not extrapolate to higher excitations.
Figure 7: Deviations in cm$^{-1}$ between this work and 16AmFaHe [22] as a function of rotational angular momentum quantum number, $J$. Different colours represent different designations of e/f and u/g.
Figure 8: Deviations in cm$^{-1}$ between this work and 16AmFaHe [22] as a function of the number of transitions that link to the energy level in our dataset.

6. Conclusions

A total of 37,813 measured experimental transitions from 61 publications have been considered in this work. From this 6013 ortho and 5200 para energy levels have been determined using the Measured Active Rotational-Vibrational Energy Levels (MARVEL) technique. These results have been compared with alternative compilations based on the use of effective Hamiltonians. An \textit{ab initio} high temperature linelist for acetylene is in preparation as part of the ExoMol project [126], for which this data will be used in the process of validation of theoretical calculations.

A significant part of this work was performed by pupils from Highams Park School in
London, as part of a project known as ORBYTS (Original Research By Young Twinkle Scientists). The Marvel study of TiO \(^{33}\) was also performed as part of the ORBYTS project and further studies on other key molecules will be published in due course. A paper discussing our experiences of performing original research in collaboration with school children will be published elsewhere \(^{127}\).

7. Supplementary Data

Supplementary material associated with this article can be found, in the online version, at 10.1016/j.jqsrt.2017.08.018. There are four files provided, as listed in Table 11. The column definitions are given in Table 12 for files 1 and 2 (Marvel input files) and Table 13 for files 3 and 4 (Marvel output files).

| File   | Name                                      |
|--------|-------------------------------------------|
| 1      | MARVEL_ortho_transitions_input.txt        |
| 2      | MARVEL_para_transitions_input.txt         |
| 3      | MARVELenergylevels_ortho_output.txt       |
| 4      | MARVELenergylevels_para_output.txt        |
Table 12: Definition of columns in files 1 and 2.

| Column | Label | Description |
|--------|-------|-------------|
| 1      | Energy (cm\(^{-1}\)) | Transition wavenumber |
| 2      | Uncertainty (cm\(^{-1}\)) | Associated uncertainty |
| 3      | \(v_1\) | CH symmetric stretch (\(\sigma_g^+\)) |
| 4      | \(v_2\) | CC symmetric stretch (\(\sigma_g^+\)) |
| 5      | \(v_3\) | CH antisymmetric stretch (\(\sigma_u^+\)) |
| 6      | \(v_4\) | Symmetric (trans) bend (\(\pi_g\)) |
| 7      | \(\ell_4\) | Vibrational angular momentum associated with \(v_4\) |
| 8      | \(v_5\) | Antisymmetric (cis) bend (\(\pi_u\)) |
| 9      | \(\ell_5\) | Vibrational angular momentum associated with \(v_5\) |
| 10     | \(J\) | Total vibrational angular momentum |
| 11     | \(e/f\) | Symmetry relative to the Wang transformation (see section 2.2) |
| 12     | ortho/para | Nuclear spin state (see section 2.2) |
| 13     | \(v_1\) | CH symmetric stretch (\(\sigma_g^+\)) |
| 14     | \(v_2\) | CC symmetric stretch (\(\sigma_g^+\)) |
| 15     | \(v_3\) | CH antisymmetric stretch (\(\sigma_u^+\)) |
| 16     | \(v_4\) | Symmetric (trans) bend (\(\pi_g\)) |
| 17     | \(\ell_4\) | Vibrational angular momentum associated with \(v_4\) |
| 18     | \(\ell_5\) | Vibrational angular momentum associated with \(v_5\) |
| 19     | \(K\) | Total vibrational angular momentum |
| 20     | \(J\) | Rotational angular momentum |
| 21     | \(e/f\) | Symmetry relative to the Wang transformation (see section 2.2) |
| 22     | ortho/para | Nuclear spin state (see section 2.2) |
| 23     | Ref | Unique reference label (see section 2.2) |
### Table 13: Definition of columns in files 3 and 4.

| Column | Label | Description |
|--------|-------|-------------|
| 1      | \(v_1\) | CH symmetric stretch \((\sigma^+_{\delta})\) |
| 2      | \(v_2\) | CC symmetric stretch \((\sigma^+_{\delta})\) |
| 3      | \(v_3\) | CH antisymmetric stretch \((\sigma^-_{u})\) |
| 4      | \(v_4\) | Symmetric (trans) bend \((\pi_g)\) |
| 5      | \(\ell_4\) | Vibrational angular momentum associated with \(v_4\) |
| 6      | \(v_5\) | Antisymmetric (cis) bend \((\pi_u)\) |
| 7      | \(\ell_5\) | Vibrational angular momentum associated with \(v_5\) |
| 8      | \(K\) | \(|\ell_4 + \ell_5|\), total vibrational angular momentum |
| 9      | \(J\) | Rotational angular momentum |
| 10     | \(e/f\) | Symmetry relative to the Wang transformation (see section 2.2) |
| 11     | ortho/para | Nuclear spin state (see section 2.2) |
| 12     | Energy (cm\(^{-1}\)) | MARVEL energy assignment |
| 13     | Uncertainty (cm\(^{-1}\)) | MARVEL uncertainty |
| 14     | NumTrans | The number of transitions in the dataset which link to this state |
| 15     | \(u/g\) symmetry | See section 2.2 |
| 16     | Symmetry label | See section 2.2 |

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