

Nitric Oxide Line Parameters: Review of 1996 HITRAN Update and New Results

A. Goldman†, L. R. Brown‡, M. N. Spencer§, C. Chackerian, Jr.§, L. P. Giver§, C. P. Rinsland¶, L. H. Coudert||, V. Dana||, and J.-Y. Mandin||

†Department of Physics, University of Denver, Denver, CO, 80208,  
‡Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, §NASA AMES Research Center, Moffett Field, CA, 94035, ¶Atmospheric Science Division, NASA Langley Research Center, Hampton, VA 23681-0001, U.S.A., ||Laboratoire de Photophysique Moléculaire, Bâtiment 210, Université Paris-Sud, 91405 Orsay Cedex, ||Laboratoire de Physique Moléculaire et Applications, CNRS, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris Cedex 05, France

**Abstract** - The 1996 HITRAN database incorporated an extensive update of NO line parameters in the 5.3  $\mu\text{m}$  region. Hyperfine lines associated with the O-1 band up to  $J=46.5$  were included and accuracies were greatly improved. Better air- and self-broadened widths were also included for a number of the infrared entries but erroneously omitted for others. These changes, as well as the complete NO database, are critically reviewed. Recent results not yet incorporated into the HITRAN database are described along with ongoing studies and needs for corrections and future improvements.

## I. INTRODUCTION

Nitric oxide (NO) is an important constituent of the Earth's atmosphere. Nitric oxide together with  $\text{NO}_2$  play critical roles in tropospheric chemistry because they act as catalysts in the photochemical production of ozone (Chameides and Walker;<sup>1</sup> WMO Report No. 37,<sup>2</sup> Chapt. 5). Tropospheric NO is produced by a variety of sources, for example, surface-based anthropogenic emissions, lightning (particularly in the tropics), stratospheric injections, aircraft emissions, and in situ photochemical reactions (Singh et al<sup>3</sup>). The primary natural source of NO in the stratosphere is believed to be the reaction of  $\text{O}(^1\text{D})$  with  $\text{N}_2\text{O}$  (Crutzen<sup>4</sup>). The downward transport of NO from the thermosphere and upward transport of NO from lightning are additional, important natural sources of stratospheric NO (WMO Report No. 37,<sup>2</sup> Chapt. 6.2.1.2). Large amounts of thermospheric NO can reach the high latitude stratosphere during winter (Solomon et al<sup>5</sup>). In the stratosphere, reactive nitrogen ( $\text{NO}+\text{NO}_2$ ) is important because it is involved in catalytic cycles which directly destroy  $\text{O}_3$  (WHO Report No. 16,<sup>6</sup> Chapt. 2.1.3).

Nitric oxide is also an important infrared radiator in the thermosphere owing to its fundamental band at  $5.3 \mu\text{m}$  ( $1876 \text{ cm}^{-1}$ ) and its first overtone band at  $2.7 \mu\text{m}$  ( $3727 \text{ cm}^{-1}$ ). Numerous infrared observations of thermospheric NO have been reported in the literature since the mid-seventies. The atmosphere above 80 km is not in local thermodynamic equilibrium. Hence, a detailed model of the steady state NO vibrational distribution and its dependence on local chemical and radiative phenomena is required to model high altitude emission spectra of the NO IR bands (Huppi and Stair;<sup>7</sup> Rawlins et al<sup>8</sup>). Thermospheric NO has been measured in the  $5.3 \mu\text{m}$  by a number of recent satellite experiments, such as HALOE (Luo et al;<sup>9</sup> Russell et al<sup>10</sup>) and ISAMS (Ballard et al;<sup>11</sup> Taylor et al<sup>12</sup>), both on UARS. Successful quantitative modeling of such

observations also requires high quality spectroscopic parameters for the lines of NO up to high  $v$  and high  $J$ .

The infrared spectral parameters of NO have been an important part of the HITRAN trace gases database since its inception, parts of which have been updated a number of times through the 1992 edition. In the 1996 HITRAN update, all the lines of the fundamental band (0-1) and part of the hot-band (1-2) lines of  $^{14}\text{N}^{16}\text{O}$  from the 1992 edition were replaced by new lines which include, for the first time, hyperfine structure (hfs) in vibration-rotation bands, and provide significantly improved line positions and intensities. However, other spectral parameters, such as halfwidths, were incorrectly incorporated for these updated lines, while lineshape parameters for other sub-sets of 1992 lines were improved. Also, some of the  $\Delta v=2$  bands (not updated) show line intensity discrepancies that have been carried over since the 1982 edition. For these reasons, a detailed discussion of the 1996 HITRAN edition is preceded, in Section II, by a review of the development of the NO line parameters into the 1992 edition. Section III will present the more recent studies, with details for those results that were incorporated into the 1996 edition. Section IV will detail more of the recent and new NO studies beyond 1996 HITRAN, and present recommendations for future editions of the database. Additional line parameters in the far IR and UV will also be discussed. Most of the discussion will be organized by spectral region, from long to short wavelength.

## II. NITRIC OXIDE UPDATES IN PRE-1996 HITRAN

The NO pure rotation portion of the HITRAN database was last updated for the 1986 HITRAN edition (Rothman et al<sup>13</sup>). It contains only the (0-0) band of  $^{14}\text{N}^{16}\text{O}$ , taken directly from the JPL catalog (Poynter and Pickett<sup>14</sup>), and includes hyperfine structure. The

extensive update of the NO X<sup>2</sup>11 - X<sup>2</sup>11 infrared line parameters in the 1982 HITRAN database (Rothman et al<sup>15</sup>) was based on the work of Gillis and Goldman<sup>16,17</sup> and contains the vibration-rotation sequences Δv=0,1,2, with v'=0, ...,6, and J<sub>max</sub><40.5 for <sup>14</sup>N<sup>16</sup>O, and v''=0 - v'=1 for <sup>15</sup>N<sup>16</sup>O and <sup>14</sup>N<sup>18</sup>O, with no hyperfine structure. Note, however, that Gillis and Goldman<sup>17</sup> included additional isotopic NO species and bands that were not incorporated into the HITRAN database (available by request from A. Goldman). The halfwidths used for all the bands were taken from the self-broadening results of Abels and Shaw<sup>18</sup> (last column of Table III there) . The NO parameters have been only partially updated since then (Rothman et al;<sup>19</sup> Brown et al;<sup>20</sup> Rothman et al<sup>21</sup>).

Subsequent to 1982 HITRAN, infrared NO measurements and analyses have been completed by Amiot,<sup>22</sup> Falcone et al,<sup>23</sup> Houdeau et al,<sup>24</sup> Pine et al,<sup>25</sup> Phillips and Walker,<sup>26</sup> Hinz et al,<sup>27</sup> and Ballard et al.<sup>28</sup> The 1986 HITRAN version did not report any updates for NO.

In 1992 HITRAN the pure rotation lines (0-0) band remain those from the JPL catalog (Poynter and Pickett<sup>14</sup>). It has been noticed that in the quantum numbers of the hyperfine components for these lines, the .5 has been truncated from each F" value. The air-broadened halfwidths remain the self-broadened halfwidths from 1982, all with temperature dependence of 0.5, and without self-broadened halfwidths.

For the 1992 HITRAN in the infrared, the results of Ballard et al<sup>28</sup> were used to update the intensity of the fundamental and air-broadened individual lines halfwidths for all infrared bands. Thus, the 1992 HITRAN update for the fundamental (0-1) incorporated 128 lines (leading isotope only, main branch P lines having J up to 13.5, and R lines with J up to 19.5) whose line intensities and broadening parameters were taken directly from the work of Ballard

et al.<sup>28</sup> The line intensities were taken from the "talc" values in Table I there, and divided by two to yield the e/f component intensities in the 1992 HITRAN listing. These lines include air-broadened halfwidth and self-broadened width which are J and branch dependent, and also show variations between the  $\Omega=1/2$  and  $3/2$  sub-bands. Ballard et al.<sup>28</sup> measured the  $N_2$ -broadened halfwidth, which was assumed for the air-broadened halfwidth and their average value for the coefficient of temperature dependence (0.71) was assigned to all 128 lines in this subset. For all the remaining  $\Delta v=1$  lines (3 leading isotopes), and all the  $\Delta v=2$  lines (main isotope only), the J-dependent air-broadening parameters were obtained from unpublished values by Ballard (see Rothman et al.<sup>19</sup>). These halfwidths appear to be the result of smoothing and extrapolation to higher J of the data presented in Ballard et al.,<sup>28</sup> and no longer have any dependence on either branch or sub-band. All these lines have been assigned the classical value of 0.5 for the coefficient of temperature-dependent broadening with no self-broadened widths. Pressure shift information is not included for any of the NO lines in 1992 HITRAN.

### III. RECENT WORK AND 1996 HITRAN UPDATE

The more recent works of Spencer et al.,<sup>29,30</sup> Dana et al.,<sup>31</sup> Mandin et al.,<sup>32</sup>, Coudert et al.,<sup>33</sup> and Saupe et al.<sup>34</sup> provide significantly improved line positions, intensities, and halfwidths for several NO bands. Some of these results have been incorporated into the HITRAN 1996 edition (Rothman et al.<sup>21</sup>). The NO data contained in 1996 HITRAN are summarized in Table 1. Table 2 describes the origin of these data, and some of the relevant issues concerning the 1996 update, which are discussed below.

The pure rotation NO lines remain unchanged in the JPL catalog (Pickett et al.<sup>17</sup>) and have not been updated for 1996 HITRAN. The

halfwidths also remained unchanged from 1992. The analysis by Coudert et al<sup>33</sup> provided hyperfine constants, which have been implemented for line positions and intensities of the (0-1), (1-2) main isotopes bands in 1996 HITRAN. Thus, the significant increase in the number of lines in the (0-1) and (1-2) bands from 1992 HITRAN to 1996 HITRAN is due to the hyperfine components. All the (0-1) main isotope lines from 1992 HITRAN (A-doubled) have been replaced in 1996 HITRAN with new line positions and intensities that take into account all the hyperfine components (Coudert et al<sup>33</sup>). Now all the main branch lines include hyperfine structure. In addition, the maximum value of J has been extended to 46.5. The hyperfine component update has been performed for only part of the (1-2) band. The positions and intensities of the (1-2) satellite lines have not been modified. It is noted that the (1-2) band  $J_{\max}=35.5$  in 1992 HITRAN has been reduced to  $J_{\max}=31.5$  for the (1-2) hyperfine lines in 1996 HITRAN while the satellite lines retain their 1992 HITRAN J range.

The comparison of the new (0-1) and (1-2) line positions in 1996 HITRAN with 1992 HITRAN can be done on the basis of Coudert et al<sup>33</sup> A-doubling constants. The newly calculated A-doubling line positions differ (usually less than) from the 1992 values by 0.1 to 2.0 mk, depending on the band and the J-values. Discrepancies up to about 5 mK exist for high J  $^2\Pi_{3/2} - ^2\Pi_{3/2}$  (1-2) lines (Dana et al<sup>31</sup>). The new line intensities are higher than the 1992 values by 2% in the main branches of the (0-1) band, and lower by 8% in the (1-2) main branch transitions. The line intensities are also lower by about 8% for the (0-1) satellite lines. Accuracy indices of 4 were assigned for both frequency ( $\geq 0.0001$  and  $< 0.001$  cm<sup>-1</sup>) and intensity ( $\geq 10\%$  and  $< 20\%$ ) for these (0-1), (1-2) lines. However, based on the convergence of the results from the different laboratories to within a few percent of each other, it is estimated that the HITRAN intensity accuracy index<sup>19</sup> for the strongest lines is 6 ( $\geq 2\%$  and  $< 5\%$ ). Indeed, the (0-1)  $^{14}\text{N}^{16}\text{O}$  band intensity on

1996 HITRAN (see Tables 1,3) is  $4.593 \times 10^{-18} \text{ cm}^{-1} / (\text{molec-cm}^{-2})$ , which is within 1% and 3% of the laboratory values of  $(4.634 \pm 0.14) \times 10^{-18}$  and  $(4.45 \pm 0.04) \times 10^{-18} \text{ cm}^{-1} / (\text{molec-cm}^{-2})$  reported by Spencer et al<sup>29</sup> and Ballard et al,<sup>28</sup> respectively.

The positions and intensities of all the other infrared bands were not changed from 1992 to 1996. A number of deficiencies found in these bands will be discussed below, on the basis of the new work by Goldman.<sup>36</sup>

It should be noted that in a few low J Q-lines hyperfine components are partially resolved in the atmospheric IR spectrum, such as in the  $Q(1/2)_{1/2}$  transitions near 1876.1  $\text{cm}^{-1}$  on the balloon-borne 0.002  $\text{cm}^{-1}$  resolution solar spectra obtained by DU. In such cases, the hyperfine components are important in modeling the observed line shape, as shown in a number of laboratory spectra (Pine et al;<sup>37</sup> Spencer et al<sup>29</sup>).

The weighted transition moments squared (proportional to the transition probabilities) for all the NO lines in the database have been altered slightly in 1996 HITRAN due to an updated version of the partition function (from the TIPS program, Gamache et al<sup>35</sup>). It should be noted that the partition function used had an extraneous nuclear spin factor of  $\prod(2I+1)$ . For  $^{14}\text{N}^{16}\text{O}$ , this amounts to  $(2I(^{14}\text{N})+1) * (2I(^{16}\text{O})+1) = 2I(^{14}\text{N})+1 = 3$  as  $I(^{16}\text{O})=0$  and  $I(^{14}\text{N})=1$  (now to be used as I). This constant factor does not effect the change of line intensity with temperature, in which the ratio of the partition functions is involved. However, in the process of generating the weighted transition moments squared from the listed line intensities (see Gamache and Rothman<sup>37</sup> for the general formulation of this parameter), it was apparently assumed that the lower state degeneracy is always  $(2J+1) * (2I+1)$ . This lead to different errors in the database for transitions sets with different merging of degenerate components. For example, for the

fine structure A components  $^{14}\text{N}^{16}\text{O}$  lines, the listed values of the weighted transition moments squared are too large by the factor of  $2I+1=3$ . In this case,  $(2J+1) * (2I+1)$  is the correct degeneracy but the extra factor of  $2I+1$  in the partition function canceled out the  $2I+1$  term in the degeneracy. For the hyperfine lines and the combined A lines the degeneracy should have been  $(2F+1)$  and  $2*(2J+1)*(2I+1)$ , respectively.

Unfortunately, halfwidth revisions intended for the 1996 version were not uniformly applied, and even some important improvements from 1992 were lost. This occurred because duplicate revisions submitted at different times were merged.

In 1994, one of the authors (L.R. Brown) revised all widths of the infrared NO bands from the 1992 edition using recent results.<sup>28,29,37</sup> The  $\text{N}_2$  widths were either measured or smoothed values of the (0-1) band from Spencer et al.<sup>29</sup> These measurements, involving P and R branch lines up to  $J=26.5$  and Q branch lines up to 11.5, were applied with somewhat different criteria depending on the isotopes, e/f components and sub-bands. The self-broadening widths were based on a smoothing by L.R. Brown of the Ballard et al<sup>25</sup> measurements that first appeared in the 1992 edition for some of the (0-1) lines. Pressure-induced frequency shifts in the (0-1) and (0-2) regions were based on averaged values reported by Spencer et al<sup>29</sup> and Pine et al<sup>37</sup> respectively,  $-0.0017$  and  $-0.004 \text{ cm}^{-1}\text{-atm}^{-1}$  at 296 K. The temperature dependence of  $n=0.71$  from Ballard et al<sup>28</sup> was maintained. It should be reemphasized that the air-broadening coefficients were determined only from  $\text{N}_2$ -broadening measurements.

In 1995, portions of this updated list were overwritten by the hyperfine prediction based on Coudert et al<sup>33</sup> for the (0-1) and some of the (1-2) bands of the main isotope; however, in this second revision, only default constants were applied for the widths and shifts ( $0.05 \text{ cm}^{-1}\text{-atm}^{-1}$  at 296 K for air-, 0.0 for self-, and 0.0 for



shifts) , thus losing the J dependence' given in the 1992 edition, although the temperature dependence coefficient ( $n=0.71$ ) was maintained (see Table 2) . These omissions can be readily corrected (tables are available electronically from L.R. Brown for this).

#### IV. FURTHER DEVELOPMENTS BEYOND 1996 HITRAN

A number of recent studies have been dedicated to validation of the NO line parameters. These are described below, along with the progress in creating a more complete and self consistent data set, applicable over wider spectral regions and atmospheric measurements.

Independent hfs line parameters calculations for the (0-1) and (1-2) bands with Coudert et al" constants (A. Goldman, unpublished, 1997; L.H. Coudert, private communication, 1997) confirm the line positions within 0.0001 MHz. These calculations also confirm the relative intensities of the 1996 HITRAN infrared hfs components. However, the calculations also confirm that the values of the ground state energies ( $E_M$ ) listed in 1996 HITRAN with the transitions, were chosen (for simplicity) as purely rovibrational and do not take into account the hfs. Fortunately, the  $E''$  values are off only in the 4th decimal, and will not cause significant errors in calculating the temperature dependence of the line intensities.

Similar calculations also reproduce well the 1996 HITRAN pure rotation hfs lines. However, it has been concluded from these calculations that the partition function used for these lines is at  $T=300K$ , as in the JPL catalog<sup>14,35</sup> and not at the HITRAN 296K value. Also, the JPL lines do not include the isotopic abundance factor.

The recent heterodyne measurements and analysis of Saupe et

al<sup>34</sup> report improved absolute accuracy for the energy levels and line positions in the fundamental band, and provide new spectroscopic constants (including hfs) for  $v=0,1$ , applicable to  $J$  values up to 38.5. Comparisons with 1996 HITRAN line positions show that the 1996 HITRAN (0-1) lines are consistently higher. The differences increase with  $J$ , and reach  $-0.00008 \text{ cm}^{-1}$  in RR22 (16.5) lines ( $J''=16.5$  is the highest in the  ${}^2\Pi_{3/2} - {}^2\Pi_{3/2}$  transitions tabulated in the paper). The Saupe et al<sup>34</sup> results should be considered for incorporation into the next edition of the HITRAN database.

An extensive use of the recent advances in NO has been described by Goldman,<sup>36</sup> for generating new line parameters with high  $v,J$  for both pure rotation and vibration-rotation transitions in  $X^1\Pi$ . This update is a direct extension of the work on updating the  $X^2\Pi$  lines of OH by Goldman et al.<sup>40</sup> The new set for NO is composed of the  $\Delta v=0, \dots, 5$  dipole allowed transitions between  $v=0, \dots, 14$  and  $J$  up to 125.5, with low intensity cutoffs, applicable to both atmospheric and high temperature research. In all, line parameters for 75 separate bands were calculated; 15 pure rotation bands and 60 vibration-rotation bands. Figs. 1-4 show sample results from this update; Table 3. shows band intensities comparison of 1992 HITRAN, 1996 HITRAN, and 1996 DU, to be discussed below.

In this work, the Hamiltonian constants of Coudert et al<sup>33</sup> for A-doubling were used for the rovibrational states of  $v=0,1,2$  and for all the line transitions between these states. The Coudert et al<sup>33</sup> analysis covered  $J$  up to 41.5 for the (0-1) lines and 23.5 for (1-2). For the remaining bands, the Hamiltonian constants of Amiot,<sup>22</sup> which do not include A-doubling, have been used. These include  $v=0, \dots, 22$  and  $J$  in the range of 59.5 (for  $v=0$ ) to 35.5 (for  $v=22$ ). Thus, the new calculations for high  $v,J$  involve significant extrapolation of the available spectroscopic data, beyond the available spectral measurements.

The line *intensity* calculations are based on an improved calculational method for the vibrational-rotational wavefunctions (Goorvitch and Galant;<sup>41,42</sup> Chackerian et al<sup>43</sup>) and a combination of the experimental and theoretical electric dipole moment functions (EDMFs), (Chackerian, private communication, 1996). Figures 1-4 show several results from this work. Figures 1 and 2 show selected  $\Delta v, v'$  line intensities sets. Figure 3 shows the type of EDMFs studied, such as those by Spencer et al,<sup>29</sup> Chackerian et al (unpublished) , and Langhof f et al ."<sup>045</sup> Figure 4 shows high  $v$ , high  $J$  wavefunctions employed in the intensity calculations. The derived intensities are significantly improved compared to those available for use in 1982 HITRAN, as discussed by Gillis and Goldman<sup>16</sup> and are compatible with the intensities assigned to the updated (0-1) and (1-2) lines in 1996 HITRAN.

The intensity comparisons in Table 3 show that the agreement of total DU band intensities with 1996 HITRAN is very close (2% or better) for the bands (0-0), (0-1), (1-2) and (0-2). The rest of the bands show varying degrees of disagreement, as discussed in Goldman,<sup>36</sup> from a comparison of total band intensity ( $S_{sum}$ ) and maximum intensity ( $S_{max}$ ) of the new DU bands. Thus , for the (0-0) band, the  $S_{sum}$  values are nearly equal. The partial sums of the hyperfine components for the given A component in 1992 and 1996 HITRAN show good agreement with  $S_{DU}$ . For the (0-1) and (1-2) bands  $S_{sum}$  are also close;  $S_{DU}$  agrees with the 1992 HITRAN's  $S_{sum}$  and with 1996 HITRAN's  $S_{max}$ . For the (0-2) band, both  $S_{sum}$  and  $S_{max}$  are in good agreement. The (1-3) lines (listed in HITRAN as combined lines, without the label e or f) show  $S_{max}$  in excellent agreement, but  $S_{sum}(DU)$  is twice that of the HITRAN database. It appears that in this case the factor of two is a coincidence, and the HITRAN database retained an inconsistent line intensity normalization, from Gillis and Goldman,<sup>16</sup> of the (1-3) lines with respect to the (2-4), (3-5) and (4-6) lines; the (1-3) line

intensities in HITRAN should be multiplied by 1.488. The (2-4), (3-5) and (4-6) bands also show disagreement in both  $S_{sum}$  and  $S_{max}$  but the adopted 1982 normalization was consistent. Again, the HITRAN database for these 3 bands lists only the combined lines, with  $S_{sum}(hitran)/S_{sum}(DU) \sim 0.8$ , and  $S_{max}(hitran)/S_{max}(DU) \sim 1.6$ . The bands (2-3), (3-4), (4-5) in the HITRAN listings also show combined A-components, except that here the doubled intensities yield  $S_{max}(hitran) \sim 2 * S_{max}(DU)$ , while  $S_{sum}(hitran) \sim 0.9 S_{sum}(DU)$ . The deficiency in the (1-3) band will be corrected in future HITRAN editions. It should be noted that the laboratory intensity measurements of the (0-2) band by Pine et al<sup>25</sup> yielded  $S = 7.57(+0.38, - 0.15) \times 10^{-20} \text{ cm}^{-1}/(\text{molec-cm}^{-2})$  vs. the DU calculated  $S$  of  $8.26 \times 10^{-20} \text{ cm}^{-1}/(\text{molec-cm}^{-2})$ . Laboratory measurements of high Av band intensity are available only for the (0-5) band, as reported by Lee and Ogilvie.<sup>46</sup> Their value of  $S = (2.18 \pm 0.11) \times 10^{-24} \text{ cm}^{-1}/(\text{molec-cm}^{-2})$  is significantly lower than the DU calculated value of  $3.799 \times 10^{-24} \text{ cm}^{-1}/(\text{molec-cm}^{-2})$ .

The recent halfwidths study by Spencer et al<sup>30</sup> has extended the previous works of Falcone et al,<sup>23</sup> Houdeau et al,<sup>24</sup> Phillips and Walker,<sup>26</sup> Ballard et al<sup>28</sup> and Spencer et al,<sup>29</sup> and provided (0-1) band  ${}^2\Pi_{1/2}$ ,  ${}^2\Pi_{3/2}$  NO-N<sub>2</sub> halfwidths with temperature dependence coefficients. The 1996 HITRAN halfwidths have not been fully updated with these values yet. Brown et al<sup>20</sup> used the Spencer et al<sup>29</sup> halfwidths for the ATMOS NO A-doubling lines. In the work of Goldman,<sup>36</sup> the results of Spencer et al<sup>30</sup> have been adopted for  $J$  up to 16.5 for all bands, and single values for higher  $J$ 's have been assumed. The correction to NO-Air halfwidths was determined assuming  $\gamma_{NO-Air}^0 = 0.79\gamma_{NO-N_2}^0 + 0.21\gamma_{NO-O_2}^0$ , with  $\gamma_{NO-O_2}^0(J) \sim 0.05$  based on Houdeau et al.<sup>24</sup> The self-broadening (0-2)  ${}^2\Pi_{1/2}$ ,  ${}^2\Pi_{3/2}$  halfwidths of Pine et al<sup>25</sup> have been adopted, as they may be more consistent with the results of Spencer et al<sup>30</sup> than with Ballard et al.<sup>28</sup> Compiling a set for the "best" halfwidths values still requires an additional study. A new study that has been completed recently

provides  $O_2$ -NO broadening coefficients with  $J$  and  $\Omega$  dependence, as well as  $e/f$  dependence for  $\Omega=1/2$  (Chackerian et al<sup>24</sup>). These will be used to replace the constant value  $0.05 \text{ cm}^{-1}\text{atm}^{-1}$  mentioned above. It should also be noted that the pressure shift coefficients provided by Pine et al<sup>27</sup> and Spencer et al<sup>29</sup> have not been incorporated into the DU database. Accuracy codes for the line positions, intensities, and halfwidths have not been estimated yet. It is clear, however, that lines of  $v'=0,1,2$  and  $J'<50$  have high position accuracy, of  $0.0001$  to  $0.001 \text{ cm}^{-1}$ , and intensity accuracy of 5 to 15%. The 1996 DU line parameters of NO have been incorporated into the 1997 GEISA databank.<sup>44</sup>

More recent infrared studies in progress include work on the spectrum of NO in the first overtone region, using a series of FT laboratory spectra (V. Dana, J.-Y. Mandin and A. Barbe, private communication, 1997). This study is dedicated to line intensities and A-splittings in the (0-2) band for  $J$  values higher than those of Pine et al,<sup>25</sup> to intensities and A splitting in the weak (1-3) hot band, and to  $N_2$ -NO and  $O_2$ -NO broadening coefficients. The results of the first part of this work have been accepted for publication." The newly reported (0-2) line intensities are 5% smaller than those measured by Pine et al.<sup>25</sup>

In the far infrared, it has been noticed that important transitions have not been yet included in the database. The HITRAN database in the far infrared includes only the electric dipole (cd) main branch pure rotation  $X^2\Pi_{1/2}(v=0) - X^2\Pi_{1/2}(v=0)$ ,  $X^2\Pi_{3/2}(v=0) - X^2\Pi_{3/2}(v=0)$  transitions with the hyperfine structure (hfs).

It is known that in addition to the above transitions, weak ed and relatively strong magnetic dipole (red) transitions occur in the satellite branches of  $X^2\Pi_{1/2}(v=0) - X^2\Pi_{3/2}(v=0)$  [Brown et al;<sup>50</sup> Mizushima et al;<sup>51</sup> Saleck et al;<sup>52</sup> Saleck et al<sup>53</sup>]. Saleck et al<sup>52</sup> provide improved analysis of  $^{15}N^{16}O$  and  $^{14}N^{18}O$  pure-rotation (0-0)

main branch lines with hfs, that has not been incorporated yet into the spectroscopic databases. The ed satellite transitions are "forbidden", and originate due to the small mixing of the  ${}^2\Pi_{1/2}$ ,  ${}^2\Pi_{3/2}$  states, similar to those observed and studied in mid infrared  $X^2\Pi_{1/2}(v=0) - X^2\Pi_{3/2}(v=1)$  transitions since the work of James.<sup>5'</sup>

The selection rules for electric dipole and magnetic dipole are opposite in parity. The permanent electric dipole of NO is quite small ( $\mu=0.15872D$ ), and wavefunction mixing is small, so that the md lines (allowed satellite transitions) are '20 times stronger than the corresponding ("forbidden" satellite) ed lines. The md line intensity peaks at the Q-branch near  $124\text{ cm}^{-1}$ , where it approaches the peak intensity of the main branch pure rotation ed lines near  $45\text{ cm}^{-1}$  within a factor of 2. It is thus expected that these md lines will be important in a number of applications.

We have therefore generated HITRAN style hfs line parameters for both types, to supplement the standard HITRAN lines. The energy levels were calculated with the spectroscopic constants and Hamiltonian formalism of Coudert et al.<sup>33</sup> The ed line intensities were calculated in intermediate coupling. The md line intensities were so far calculated only *in* Hund's case (a) (Barrington et al;<sup>55</sup> Brown et al; 50 Saleck et al<sup>53</sup>). Work is in progress with these lines in the far IR atmospheric emission spectrum (I.G. Nolt, private communication, 1997).

With the expansion of the HITRAN database to the UV, it is important that line parameters for the NO  $\gamma$  band system ( $X^2\Pi - A^2\Sigma'$ ) be added to the compilation. As is widely documented in the literature *since* the mid-sixties, the  $\gamma$  system is prominent in the middle uv spectrum of the earth's airglow, and has been providing high altitude (80-200 km) distribution of NO for many years. The  $\gamma$  system is also used (via fluorescence) for monitoring NO in air pollutants. Some of the recent spectral parameters studies of the

rotational transitions of the  $\gamma$  system have been described by Paul<sup>56</sup> (high  $v$ , high  $J$  calculations of positions and line strengths) , by Vyrodov et al<sup>57</sup> and Di Rosa and Hanson<sup>58</sup> (measurements of collisional broadening and shifts). These spectral parameters can be adapted to the HITRAN database. Other NO electronic band systems, including the shorter  $W \delta$  ( $X^2 11 - C^2 \Sigma'$ ) and  $\epsilon$  ( $X^2 \Pi - D^2 \Sigma'$ ) (some of which are also observable in atmospheric absorption solar spectra) , are important in atmospheric chemistry and physics, and should be considered in the future. For recent discussions, see the review paper by Slanger and Copeland<sup>59</sup> and the proposed ground-based study of NO by Slanger and Kerr.<sup>60</sup>

#### v. CONCLUSIONS

The 1996 HITRAN line parameters update for NO provides a number of improvements, which were, unfortunately, accompanied by some setbacks. Of special significance is the incorporating of the hyperfine line structure with improved intensities for the (0-1) and (1-2) bands, the loss of the individual halfwidths of the (0-1) and some of the (1-2) lines, the intensity discrepancy (carried over from previous editions) in the (1-3) band, and the limited coverage of isotopic line parameters. Extensive recent and new results for the NO spectral parameters from the far infrared to the  $W$  provide significant improvements to be incorporated in future editions of the database.

Acknowledgments - The research at the University of Denver (DU) was supported in part by NSF and in part by Northrop-Grumman Aerospace Corporation. Acknowledgment is made to the National Center for Atmospheric Research, which is sponsored by the National Science Foundation, for computer time used in this project. Part of the work performed at DU was assisted by P.S. Manning and W.G. Schoenfeld. Part of this research was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration.



## REFERENCES

1. Chameides, W. L. and Walker, J. C. G., A photochemical theory of tropospheric ozone. Journal of Geophysical Research, 1973, 78, 8751-8760.
2. World Meteorological Organization, Global Ozone Research and Monitoring Project-Report No. 37, Scientific assessment of ozone depletion: 1994. National Oceanic and Atmospheric Administration, National Aeronautics and Space Administration, United Nations Environment Programme, World Meteorological Organization, 1995.
3. Singh, H. B., Herlth, D., Kolyer, R., Salas, L., Bradshaw, J. D., Sandholm, S. T., Davis, D. D., Crawford, J., Kondo, Y., Koike, M., Talbot, R., Gregory, G. L., Sachse, G. W., Browell, E., Blake, D. R., Rowland, F. S., Newell, R., Merrill, J., Heikes, B., Liu, S. C., Crutzen, P. J. and Kanakidou, M., Reactive nitrogen and ozone over the Western Pacific: distributions, partitioning, and sources. Journal of Geophysical Research, 1996, 101, 1793-1808.
4. Crutzen, P. J., The influence of nitrogen oxides on the atmospheric ozone content. Quarterly Journal of the Royal Meteorological Society, 1970, 96, 320-325.
5. Solomon, S., Crutzen, P. J. and Roble, R. G., Photochemical coupling between the thermosphere and lower atmosphere 1. Odd nitrogen from 50 to 120 km. Journal of Geophysical Research, 1982, 87, 7206-7220.
6. World Meteorological Organization, Global Ozone Research and Monitoring Project-Report No. 16, Atmospheric ozone, 1985-Assessment of our understanding of the processes controlling its present distribution and change. vol. 1, National

Aeronautics and Space Administration, Federal Aviation Administration, National Oceanic and Atmospheric Administration, United Nations Environment Program, World Meteorological Organization, Commission of the European Communities, Bundesministerium fur Forschung und Technologies, 1985.

7. Huppi, R. J. and Stair, Jr. A. T., Aurorally enhanced infrared emissions. Applied Optics, 1979, 18, 3394-3399.
8. Rawlins, W. T., Caledonia, G. E., Gibson, J. J. and Stair, A. T., Jr., Infrared emission from NO ( $\Delta v=1$ ) in an Aurora: Spectral analysis and kinetic interpretation of HIRIS measurements. Journal of Geophysical Research, 1981, 86, 1313-1324.
9. Luo, M., Russell, J. M. III, Cicerone, R. J. and Gordley, L. L., Analysis of selected nitric oxide observations in the lower thermosphere by HALOE on UARS. Geophysical Research Letters, 1993, 20, 1307-1310.
10. Russell, J. M. III, Gordley, L. L., Park, J. H., Drayson, S. R., Hesketh, W. D., Cicerone, R. J., Tuck, A. F., Frederick, J. E., Harries, J. E. and Crutzen, P. J., The halogen occultation experiment. Journal of Geophysical Research, 1993, 90, 10777-10797.
11. Ballard, J., Kerridge, B. J., Morris, P. E. and Taylor, F. W., Observations of  $V=1-0$  emission from thermospheric nitric oxide by ISAMS. Geophysical Research Letters, 1993, 20, 1311-1314.
12. Taylor, F. W., Rodgers, C. D., Whitney, J. G., Werrett, S. T., Barnett, J. J., Peskett, G. D., Venters, P., Ballard, J., Palmer, C. W. P., Knight, R. J., Morris, P., Nightingale, T. and Dudhia, A., Remote sensing of atmospheric structure and

composition by pressure modulator radiometry from space: The ISAMS experiment on UARS. Journal of Geophysical Research, 1993, 90, 10799-10814.

13. Rothman, L. S., Gamache, R. R., Goldman, A., Brown, L. R., Toth, R. A., Pickett, H. M., Poynter, R. L., Flaud, J.-M., Camy-Peyret, C., Barbe, A., Husson, N., Rinsland, C. p. and Smith, M. A. H., The HITRAN database: 1986 Edition. Applied Optics, 1987, 26, 4058-4097.
14. Poynter, R. L. and Pickett, H. M., Submillimeter, Millimeter, and microwave spectral line catalog. Applied Optics, 1985, 24, 2235-2240.
15. Rothman, L. S., Goldman, A., Gillis, J. R., Gamache, R. R., Pickett, H. M., Poynter, R. L., Husson, N. and Chedin, A., AFGL trace gas compilation: 1982 version. Applied Optics, 1983, 22, 1616-1627.
16. Gillis, J. R. and Goldman, A., Nitric oxide IR line parameters for the upper atmosphere. Applied Optics 1982, 21, 1161-1163.
17. Gillis, J. R. and Goldman, A., Infrared line parameters for naturally occurring NO isotopic species. University of Denver, Report, 1982.
18. Abels, L. L. and Shaw, J. H., Widths and strength of vibration-rotation lines in the fundamental band of Nitric Oxide. Journal of Molecular Spectroscopy, 1966, 20, 11-28.
19. Rothman, L. S., Gamache, R. R., Tipping, R. H., Rinsland, C. P., Smith, M. A. H., Chris Benner, D., Malathy Devi, V., Flaud, J.-M., Camy-Peyret, C., Perrin, A., Goldman, A., Massie, S. T., Brown, L. R. and Toth, R. A., The HITRAN molecular database: Editions of 1991 and 1992. Journal of

Quantitative Spectroscopy & Radiative Transfer, 1992, 40, 469-507.

20. Brown, L. R., Gunson, M. R., Toth, R. A., Irion, F. W., Rinsland, C. P. and Goldman, A., 1995 Atmospheric trace molecule spectroscopy (ATMOS) linelist. Applied Optics, 1996, 35, 2828-2848.
21. Rothman, L. S., Rinsland, C. P., Goldman, A., Massie, S. T., Flaud, J.-M., Perrin, A. Dana, V., Mandin, J.-Y., Schroeder, J., McCann, A., Gamache, R. R., Watson, R. B., Yoshino, K., Chance, K., Jucks, K., Brown, L. R., Nemtchinov, V. and Varanasi, P., The HITRAN molecular spectroscopic database and HAWKS (HITRAN Atmospheric Workstation). Journal of Quantitative Spectroscopy & Radiative Transfer, this issue.
22. Amiot, C. The infrared emission spectrum of NO: Analysis of the  $\Delta v=3$  sequence up to  $v=22$ . Journal of Molecular Spectroscopy, 1982, 94, 150-172.
23. Falcone, P. K., Hanson, R. K. and Kruger, C. H., Tunable diode laser measurements of the band strength and collision halfwidths of nitric oxide. Journal of Quantitative Spectroscopy & Radiative Transfer, 1983, 29, 205-221.
24. Houdeau, J. P., Boulet, C., Bonamy, J., Khayar, A. and Guelachvili, G., Air broadened NO linewidths in a temperature range of atmospheric interest. Journal of Chemical Physics, 1983, 79, 1634-1640.
25. Pine, A. S., Maki, A. G. and Chou, N.-Y., Pressure Broadening, Lineshapes, and Intensity Measurements in the  $2 \leftarrow 0$  Band of NO. Journal of Molecular Spectroscopy, 1985, 114, 132-147.
26. Phillips, W. J. and Walker, H. C., Nitrogen-broadened

linewidths and strengths of nitric oxide utilizing tunable diode laser spectroscopy. Journal of Chemical Physics, 1986, 05, 3211-3216.

27. Hinz, A., Wells, J. S. and Maki, A. G., Heterodyne frequency measurements on the nitric oxide fundamental band. Journal of Molecular Spectroscopy, 1986, 119, 120-125.
28. Ballard, J., Johnston, W. B., Kerridge, B. J. and Remidios, J. J., Experimental spectral line parameters in the 1-0 band of nitric oxide. Journal of Molecular Spectroscopy, 1988, 127, 70-82.
29. Spencer, M. N., Chackerian, Jr., C., Giver, L. P. and Brown, L. R., The nitric oxide fundamental band: frequency and shape parameters for rovibrational lines. Journal of Molecular Spectroscopy, 1994, 165, 506-524.
30. Spencer, M. N., Chackerian, Jr., C., Giver, L. P. and Brown, L. R., Temperature dependence of nitrogen broadening of the NO fundamental vibrational band. Journal of Molecular Spectroscopy, 1997, 181, 307-315.
31. Dana, V., Mandin, J.-Y., Coudert, L. H., Badaoui, M., Le Roy, F., Guelachvili, G. and Rothman, L. S., A-splitting and line intensities in the 2 ← 1 hot band of nitric oxide. Journal of Molecular Spectroscopy, 1994, 165, 525-540.
32. Mandin, J.-Y., Dana, V., Coudert, L. H., Badaoui, M., Le Roy, F., Morillon-Chapey, R. Farrenq, and G. Guelachvili, Line positions and intensities in the fundamental 1 ← 0 forbidden  ${}^1\Pi_{3/2}$  -  ${}^2\Pi_{3/2}$  and  ${}^2\Pi_{3/2}$  -  ${}^2\Pi_{1/2}$  subbands of nitric oxide. Journal of Molecular Spectroscopy, 1994, 167, 262-271.

33. Coudert, L. H., Dana, V., Mandin, J.-Y., Morillon-Chapey, M., Farrenq, R. and Guelachvili, G., The spectrum of nitric oxide between 1700 and 2100  $\text{cm}^{-1}$ . Journal of Molecular Spectroscopy, 1995, 172, 435-448.
34. Saupe, S., Meyer, B., Wappelhorst, M. H., Urban, W. and Maki, A. G., Sub-doppler heterodyne frequency measurements and calibration tables for the nitric oxide fundamental band. Journal of Molecular Spectroscopy, 1996, 179, 13-21.
35. Pickett, H. M., Poynter, R. L., Cohen, E. A., Delitsky, M. Lo, Pearson, J. C. and Müller, H. S. P., Submillimeter, millimeter, and microwave spectral line catalogue. JPL Publication 80-23, Rev.4, 1996.
36. Goldman, A., Updated line parameters for NO  $X^2\text{II} - X^2\text{II}(v'',v')$  transitions. Progress Report, University of Denver, Dec. 1996.
37. Pine, A. S., Johns, J. W. C. and Robiette, A. G., A-Doubling in the  $v=2+0$  overtone band in the infrared spectrum of NO. Journal of Molecular Spectroscopy, 1979, 74, 52-69.
38. Gamache, R. R., Hawkins, R. L. and Rothman, L. S., Total internal partition sums in the temperature range 70-3000K: atmospheric linear molecules. Journal of Molecular Spectroscopy & Radiative Transfer, 1990, 142, 205-219.
39. Gamache, R.R. and Rothman, L.R., Extension of the HITRAN database to non-LTE applications. Journal of Quantitative Spectroscopy & Radiative Transfer, 1992, 48, 519-525.
40. Goldman, A., Schoenfeld, W. G., Goorvitch, D., Chackerian, Jr., C., Dothe, H., Mélen, F., Abrams, M. C. and Selby, J. E. A.\* Updated line parameters for OH  $X^2\text{II} - X^2\text{II}(v'',v')$

transitions. Journal of Quantitative Spectroscopy & Radiative Transfer, 1997, in press.

41. Goorvitch, D. and Galant, D. C., Schrodinger's radial equation: solution by extrapolation. Journal of Quantitative Spectroscopy & Radiative Transfer, 1992, 47, 393-399.
42. Goorvitch, D. and Galant, D. C., The solution of coupled Schrödinger equations using an extrapolation method. Journal of Quantitative Spectroscopy & Radiative Transfer, 1992, 47, 505-513.
43. Chackerian, C., Jr., Goorvitch, D., Benidar, A., Farreng, R., Guelachvili, G., Martin, P. M., Abrams, M. C. and Davis, S. P., Rovibrational intensities and electric dipole moment function of the X<sup>2</sup>11 hydroxyl radical. Journal of Quantitative Spectroscopy & Radiative Transfer, 1992, 40, 667-673.
44. Langhoff, S. R., Bauschlicher, C. W., Jr. and Patridge, H., Theoretical study of the NO  $\gamma$  system. Journal of Chemical Physics, 1988, 89, 4909-4917.
45. Langhoff, S. R., Bauschlicher, C. W., Jr. and Patridge, H., Theoretical dipole moment for the X<sup>2</sup>11 state of NO. Chemical Physics Letters, 1994, 223, 416-422.
46. Lee, Y. P. and Ogilvie, J. F., Strengths of absorption lines in the vibration-rotational band  $v=5+v=0$  of NO X<sup>2</sup>11. Infrared Physics, 1988, 28, 321-324.
47. Chackerian, C., Jr., Freedman, R. S., Giver, L. P. and Brown, L. R., The NO vibrational fundamental band: O<sub>2</sub>-broadening coefficients. to be submitted to Journal of Molecular Spectroscopy, 1997.

48. Jaquinet-Husson, N., Arie, E., Barbe, A., Brown, L. R., Bonnet, B., Camy-Peyret, C., Champion, J. p., Chedin, A., Chursin, A., Clerbaux, C., Duxbury, G., Flaud, J.-M., Fourrie, N., Fayt, A., Graner, G., Gamache, R. R., Goldman, A., Guelachvilli, G., Hartmann, J. M., Hillico, J. C., Lefevre, G., Nikitin, A., Perrin, A., Reuter, D., Rosenmann, L., Rothman, L. S., Scott, N.A., Selby, J. E., Sirota, J. O. M., Smith, A., Smith, K., Tipping, R. H., Urban, S., Varanasi, P. and Weber, M., The 1997 spectroscopic GEISA databank. Journal of Quantitative Spectroscopy & Radiative Transfer, 1997, to be submitted.
49. Mandin, J.-Y., Dana, V., Régalia, L., Barbe, A. and Thomas, X., A-splitting and line intensities in the first overtone of nitric oxide. Journal of Molecular Spectroscopy, 1997, in press.
50. Brown, J. M., Cole, A. R. H. and Honey, F. R., Magnetic dipole transitions in the far infra-red spectrum of nitric oxide. Molecular Physics, 1972, 23, 287-295.
51. Mizushima, M., Evenson, K. M. and Wells, J. S., Laser magnetic resonance of the NO molecule using 78-, 79-, and 119- $\mu\text{m}$   $\text{H}_2\text{O}$  laser lines. Physical Review A, 1972, 5, 2276-2287.
52. Saleck, A. H., Yamada, K. M. T. and Winnewisser, G., Isotopic nitric oxide spectra and breakdown of the Born-Oppenheimer approximate ion. Molecular Physics, 1991, 72, 1135-1148.
53. Saleck, A. H., Winnewisser, G. and Yamada, K. M. T., High resolution spectrum of  $^{14}\text{N}^{16}\text{O}$  in the far infrared region:  $^2\Pi_{3/2} - ^2\Pi_{1/2}$  transitions. Molecular Physics, 1992, 76, 1443-1455.
54. James, T. C., Intensity of the forbidden  $X^2\Pi_{3/2} - X^2\Pi_{1/2}$



- satellite bands in the infrared spectrum of nitric oxide. Journal of Chemical Physics, 1964, 40, 762-771.
55. Barrington, A., Levy, D. H. and Miller, T. A., Electron resonance of gaseous diatomic molecules. Advances in Chemical Physics, 1970, 18, 149-248.
56. Paul, P. H., Calculation of transition frequencies and rotational line strengths in the  $\gamma$ -bands of nitric oxide. Journal of Quantitative Spectroscopy & Radiative Transfer, 1997, 57, 581-589.
57. Vyrodov, A. O., Heinze, J. and Meier, U. E., Collisional broadening of spectral lines in the A - X(0-0) system of NO by N<sub>2</sub>, Ar, and He at elevated pressures measured by laser-induced fluorescence. Journal of Quantitative Spectroscopy & Radiative Transfer, 1995, 53, 277-287.
58. Di Rosa, M. D. and Hanson, R. K., Collision broadening and shift of NO  $\gamma(0,0)$  absorption lines by O<sub>2</sub> and H<sub>2</sub>O at high temperatures. Journal of Quantitative Spectroscopy & Radiative Transfer, 1994, 52, 515-529.
59. Slanger T. G. and Copeland, R. A., Energy transfer, spectroscopy, and atmospheric significance of excited O<sub>2</sub>, NO, and OH, Chap. 13 in Progress and Problems in Atmospheric Chemistry, J. R. Barker cd., World Scientific, Singapore, 1995.
60. Slanger, T. G. and Kerr, R. B., Ground-based detection of NO in the lower thermosphere. 8th Scientific Assembly of IAGA with ICMA and STP symposia, Uppsala, Sweden, August 4-15, 1997, Abstract Book, p. 163.

## Legend for Tables

Table 1. Summary of all NO bands (part 1) and sub-bands (part 2) for each isotope on 1996 HITRAN. The bands updated in 1996 are followed by the previous, 1992, values, designated by parenthesis.

Table 2. The origin of NO line parameters in the 1996 HITRAN database and related issues.

Table 3. Comparison of  $^{14}\text{N}^{16}\text{O}$   $X^2\Pi(v'',v')$  total band intensities and maximum intensities in 1992 HITRAN, 1996 HITRAN, and 1996 DU.

## Legend for Figures

Figure 1. Line intensities vs wavenumber from the 1996 DU set<sup>36</sup> at T=296 K for  $^{14}\text{N}^{16}\text{O X}^2\Pi$  pure rotation and vibration-rotation transitions for  $\Delta v=0, \dots, 5$ , with  $v'=0, \dots, 14$ , with J Up to 125.5. Satellite transitions are included. Plotted with  $10^{-8}$  intensity cutoff .

Figure 2. Line intensity vs wavenumber at T=296 K for  $^{14}\text{N}^{16}\text{O X}^2\Pi$  vibration-rotation transitions for  $\Delta v=1$  with  $v'=3, \dots, 14$ , Amiot<sup>22</sup> constants with J up to 125.5. Satellite transitions are included. Plotted with  $10^{-62}$  intensity cutoff (from the 1996 DU line parameters set<sup>36</sup>).

Figure 3. Comparison of electric dipole moment functions (EDMF) used in the 1996 DU study.<sup>36</sup> The Spencer et al<sup>29</sup> EDMF (solid line) and the Chackerian et al (unpublished) EDMF (dotted curve), and the Langhoff et al<sup>44,45</sup> EDMF (dashed curve) .

Figure 4. Wavefunction overlap plots showing the upper level, lower level, and their product wavefunctions for the  $v=11-13$  PP11  $J''=124.5$  transition (The  $\Omega=1/2$  component), as used in the 1996 DU study.<sup>36</sup>

Table 1. Summary of **NO** bands on 1996 HITRAN

la. Isotope $^{14}\text{N}^{16}\text{O}$ (46), total band summary								
$\nu_0$	$v'-v''$	$\nu_{\min}$	$\nu_{\max}$	#lines	$\Sigma S$	$S_{\min}$	$S_{\max}$	$J_{\max}$
0.00000	0-0	0.00002	98.43997	599	3.441E-20	1.280E-35	2.950E-22	29.5
1763.89421	5-4	1463.17330	2019.87770	416	7.675E-33	8.464E-43	2.040E-34	35.5
1791.85814	4-3	1488.86950	2050.21700	416	3.792E-29	3.800E-39	1.010E-30	35.5
1819.85684	3-2	1514.60570	2080.57280	416	2.016E-25	1.840E-35	5.400E-27	35.5
1847.89817	2-1	1540.30870	2111.05110	2722	1.003E-21	7.887E-34	5.038E-24	35.5
(1875.8983)	2-1	1540.30870	2111.05110	831	1.081E-21	4.380E-32	1.450E-23	35.5
1675.98911	1-0	1487.36591	2188.44755	<b>6888</b>	4.593E-18	1.114E-39	2.322E-20	4G.5
(1875.9893)	1-0	1566.15200	2141.45503	833	4.532E-18	4.300E-29	6.040E-20	35.5
3499.84723	6-4	3177.86990	3732.23210	416	3.303E-34	9.809E-45	8.680E-36	35.5
3555.75234	5-3	3231.55890	3790.57850	416	1.291E-30	3.320E-41	3.420E-32	35.5
3611.71498	4-2	3285.30650	3848.95850	416	5.435E-27	1.280E-37	1.440E-28	35.5
3667.75515	3-1	3339.13240	3907.39480	416	1.391E-23	3.020E-34	3.720E-25	35.5
3723.88758	2-0	3392.97240	3966.00070	832	8.079E-20	7.690E-31	1.090E-21	35.5

The total number of lines of the isotope  $^{14}\text{N}^{16}\text{O}$  is **13,953**

lb. Isotope $^{14}\text{N}^{16}\text{O}$ (46), sub-band summary								
sub-band	$\nu_{\min}$	$\nu_{\max}$	#lines	$\Sigma S$	$S_{\min}$	$S_{\max}$	$J_{\max}$	
0 $X_{3/2}$ - 0 $X_{3/2}$	0.00002	97.22389	3 0 1	1.218E-20	1.280E-35	1.650E-22	2 8 . 5	
0 $X_{1/2}$ - 0 $X_{1/2}$	0.00687	98.43997	2 9 s	2.222E-20	1.530E-31	2.950E-22	29.5	
5 $X_{3/2}$ - 4 $X_{3/2}$	1626.11170	1855.89030	1 0 3	2.685E-33	7.360E-41	1.090E-34	35.5	
5 $X_{1/2}$ - 4 $x_{3/*}$	1463.17330	1691.40890	1 0 3	7.974E-37	8.4 64E-43	3.340E-38	35.5	
5 $X_{3/2}$ - 4 $X_{1/2}$	1792.30260	2019. s7770	1 0 4	1.739E-36	2. 840E-42	7.180E-38	3 5 . 5	
5 $X_{1/2}$ - 4 $X_{1/2}$	1629.36420	1S54.77110	1 0 G	4.9 88E-33	3. 680E-41	2.040E-34	3 5 . 5	

4 $X_{3/2}$ - 3 $X_{3/2}$	1652. s5690	1865.19030	1 0 3	1.324E-29	3.280E-37	5.420E-31	3 5 . 5
4 $X_{1/2}$ - 3 $X_{3/2}$	1488.86950	1719.609S0	1 0 3	4.003E-33	3.800E-39	1. 690E-34	3 5 . 5
4 $X_{3/2}$ - 3 $X_{1/2}$	1820.12240	2050.21 700	1 0 4	8.734E-33	1.280E-38	3.620E-34	3 5 . 5
4 $X_{1/2}$ - 3 $X_{1/2}$	1656.13490	1SS4.02610	106	2.466E-29	1.650E-37	1. 010E30	35.5
3 $X_{3/2}$ - 2 $X_{3/2}$	1679.63240	1914.51470	1 0 3	7.034E-26	1.570E-33	2.900E-27	3 5 . 5
3 $X_{1/2}$ - 2 $X_{3/2}$	1514.60570	1747.84590	1 0 3	2.164E-29	1. 840E-35	9.200E-31	3 5 . 5
3 $X_{3/2}$ - 2 $X_{1/2}$	1847.96460	2080.57280	1 0 4	4.720E-29	6.240E-35	1.970E-30	3 5 . 5
3 $X_{1/2}$ - 2 $X_{1/2}$	1682.93790	1913.30740	1 0 6	1.312E-25	8.020E-34	5.400E-27	3 5 . 5
2 $X_{3/2}$ - 1 $X_{3/2}$	1724.36683	1935.55054	1140	3.496E-22	7.887E-34	2. 688E-24	31.5
(2 $X_{3/2}$ - 1 $X_{3/2}$ )	1706.43400	1943. s8590	205	3.767E-22	3.780E-30	7.800E-24	35.5
2 $X_{1/2}$ - 1 $X_{3/2}$	1540.30s70	1776.19330	206	1.175E-25	4.380E32	2.520E-27	35.5
(2 $X_{1/2}$ - 1 $X_{3/2}$ )	1540.30s70	1776.19330	206	1.175E-25	4.380E-32	2.520E-27	35.5
2 $X_{3/2}$ - 1 $X_{1/2}$	1875.77760	2111.05110	208	2.562S25	1.490E-31	5.390E-27	35.5
(2 $X_{3/2}$ - 1 $X_{1/2}$ )	1875.77760	2111.05110	208	2.562E-25	1.490E-31	5.390E-27	35.5
2 $X_{1/2}$ - 1 $X_{1/2}$	1727.43703	1934.28638	1168	6.528E-22	1.725E-33	5.038E-24	31.5
(2 $X_{1/2}$ - 1 $X_{1/2}$ )	1709.77750	1942.62150	212	7.034E22	1.950E-30	1.450E-23	35.5
1 $X_{3/2}$ - 0 $X_{3/2}$	1681.19055	1993.20160	1710	1.600S18	5. 632E-35	1.238E-20	46.5
(1 $X_{3/2}$ - 0 $X_{3/2}$ )	1733.30330	1973.2s430	205	1.5 85E-18	1. 600E-26	3.40E20	35.5
1 $X_{1/2}$ - 0 $X_{3/2}$	14s7.36591	1804.53175	1720	5.145E-22	1.114E-39	4.038E-24	46.5
(1 $X_{1/2}$ - 0 $X_{3/2}$ )	15 66.15200	1804.53270	206	5.530E-22	1.870E-28	1.190E-23	35.5
1 $X_{3/2}$ - 0 $X_{1/2}$	1S79.02261	21S8,44755	1720	1.098E-21	4.447s39	8.613E-24	46.5
(1 $X_{3/2}$ - 0 $X_{1/2}$ )	1903.69740	2141.45500	210	1.2 05E-21	4.300S29	2.550E-23	35.5
1 $X_{1/2}$ - 0 $X_{1/2}$	16 S5.19629	1992.06796	1738	2.991E-18	1.478E-34	2.322E-20	46.5
(1 $X_{1/2}$ - 0 $X_{1/2}$ )	173 G. 7140	1971.9890	212	2.945E-18	8.200E-27	6.040E-20	35.5
G $X_{3/2}$ - 4 $X_{3/2}$	3339.74S50	356 S.24400	1 0 3	1.155E-34	3.180E-42	4. 680E-36	3 5 . 5
6 $X_{1/2}$ - 4 $X_{3/2}$	3177.86990	3415.18670	103	3.555E-38	9. 809E-45	1.460E-39	35.5

6 X<sub>3/2</sub> - 4 X<sub>1/2</sub> 3505.93940 3732.23210 104 7.217E-38 3.503E-44 3.020E-39 35.5  
6 X<sub>1/2</sub> - 4 X<sub>1/2</sub> 3344.06080 3566.22050 106 2.147E-34 1.581E-42 8.680E-36 35.5

5 X<sub>3/2</sub> - 3 X<sub>3/2</sub> 3394.49740 3625.55190 103 4.511E-31 1.120E-38 1.840E-32 35.5  
5 X<sub>1/2</sub> - 3 X<sub>3/2</sub> 3231.55890 3471.25530 103 1.411E-34 3.320E-41 5.820E-36 35.5  
5 X<sub>3/2</sub> - 3 X<sub>1/2</sub> 3561.76280 3790.57850 104 2.868E-34 1.260E-40 1.210E-35 35.5  
5 X<sub>1/2</sub> - 3 X<sub>1/2</sub> 3398.82440 3625.47190 106 8.394E-31 5.620E-39 3.420E-32 35.5

4 X<sub>3/2</sub> - 2 X<sub>3/2</sub> 3449.29400 3682.90040 103 1.896E-27 4.220E-35 7.760E-29 35.5  
4 X<sub>1/2</sub> - 2 X<sub>3/2</sub> 3285.30650 3527.45500 103 6.036E-31 1.280E-37 2.500E-32 35.5  
4 X<sub>3/2</sub> - 2 X<sub>1/2</sub> 3617.62620 3848.95850 104 1.228E-30 4.900E-37 5.200E-32 35.5  
4 X<sub>1/2</sub> - 2 X<sub>1/2</sub> 3453.63570 3682.76760 106 3.537E-27 2.160E-35 1.440E-28 35.5

3 X<sub>3/2</sub> - 1 X<sub>3/2</sub> 3504.15910 3740.31210 103 4.848E-24 9.740E-32 1.990E-25 35.5  
3 X<sub>1/2</sub> - 1 X<sub>3/2</sub> 3339.13240 3583.70660 103 1.570E-27 3.020E-34 6.540E-29 35.5  
3 X<sub>3/2</sub> - 1 X<sub>1/2</sub> 3673.55130 3907.39480 104 3.194E-27 1.160E-33 1.360E-28 35.5  
3 X<sub>1/2</sub> - 1 X<sub>1/2</sub> 3508.52460 3740.12930 106 9.054E-24 5.020E-32 3.720E-25 35.5

2 X<sub>3/2</sub> - 0 X<sub>3/2</sub> 3559.09560 3797.81770 206 2.814E-20 2.550E-28 5.820E-22 35.5  
2 X<sub>1/2</sub> - 0 X<sub>3/2</sub> 3392.97240 3640.13470 206 9.235E-24 7.690E-31 1.940E-25 35.5  
2 X<sub>3/2</sub> - 0 X<sub>1/2</sub> 3729.49350 3966.00070 208 1.879E-23 2.980E-30 4.030E-25 35.5  
2 X<sub>1/2</sub> - 0 X<sub>1/2</sub> 3563.49340 3797.37020 212 5.262E-20 1.330E-28 1.090E-21 35.5

The total number of lines of the isotope <sup>14</sup>N<sup>16</sup>O is 13,953

2a. Isotope <sup>15</sup>N<sup>16</sup>O (56), total band summary

$\nu_0$	V'-v''	$\nu_{min}$	$\nu_{max}$	#lines	$\Sigma$	S	$S_{min}$	$S_{max}$	$J_{max}$
1842.91770	1-0	1609.38540	2060.46250	699	1.917E-20	4.430E-28	2.550E-22	35.5	

---

2b. Isotope  $^{15}\text{N}^{16}\text{O}$  (56), sub-band summary

---

sub-band	$\nu_{\min}$	$\nu_{\max}$	#lines	$\Sigma S$	$S_{\min}$	$S_{\max}$	$J_{\max}$
1 $X_{3/2} - 0 X_{3/2}$	1705.67090	1937.21230	199	6.683E-21	5.000E-28	1.370E-22	3 5 . 5
1 $X_{1/2} - 0 X_{3/2}$	1609.58540	1768.04290	142	1.972E-24	4.430E-28	4.1 80E-26	26.5
1 $X_{3/2} - 0 X_{1/2}$	1892.71620	2060.46250	156	4.307E-24	4.750E-28	8.950E-26	28.5
1 $X_{1/2} - 0 X_{1/2}$	1708.85690	1935.97950	202	1.248E-20	6.380E-28	2.550E-22	3 5 . 5

The total number of lines of the isotope  $^{15}\text{N}^{16}\text{O}$  is 699

---

3a. Isotope  $^{14}\text{N}^{18}\text{O}$  (48), sub-band summary

---

$\nu_0$	$v'-v''$	$\nu_{\min}$	$\nu_{\max}$	#lines	$\Sigma S$	$S_{\min}$	$S_{\max}$	$J_{\max}$
1S27.28440	1-0	1601.90940	2038.84610	679	1.054E-20	4.190E-28	1.390E-22	3 5 . 5

The total number of lines of the isotope  $^{14}\text{N}^{18}\text{O}$  is 679

---

3b. Isotope  $^{14}\text{N}^{18}\text{O}$ , sub-band summary

---

sub-band	$\nu_{\min}$	$\nu_{\max}$	#lines	$\Sigma S$	$S_{\min}$	$S_{\max}$	$J_{\max}$
1 $X_{3/2} - 0 X_{3/2}$	1692.55850	1920.16370	197	3.674E-21	5.4 60E-28	7.440E-23	35.5
1 $X_{1/2} - 0 X_{3/2}$	1601.90940	1750.35060	132	1.045E-24	4.490E-28	2.200E-26	24.5
1 $X_{3/2} - 0 X_{1/2}$	1880.24190	2038.84610	150	2.289E-24	4.190E-28	4.720E-26	27.5
1 $X_{1/2} - 0 X_{1/2}$	1695.65800	1918.95830	200	6.861E-21	6.310E-28	1.390E-22	35.5

The total number of lines of the isotope  $^{14}\text{N}^{18}\text{O}$  is 679

---

$\nu$  values are in units of  $\text{cm}^{-1}$

S values are in units of  $\text{cm}^{-1}/(\text{molec}\cdot\text{cm}^{-2})$  at 296K

Sub-bands notation  $v X_{\Omega'} - v'' X_{\Omega''}$  is short for  $v X^2\Pi_{\Omega'} - v'' X^2\Pi_{\Omega''}$

Band centers ( $\nu_0$ ) for  $^{14}\text{N}^{16}\text{O}$  (0-1), (1-2) are from Coudert et al.<sup>33</sup>

All other  $^{14}\text{N}^{16}\text{O}$   $\nu_0$  are from Amiot.<sup>22</sup> For  $^{15}\text{N}^{16}\text{O}$ ,  $^{14}\text{N}^{18}\text{O}$   $\nu_0$  see Gillis & Goldman.<sup>17</sup>

Table 2. Origin of NO parameters in the 1996 HITRAN Database

Bands	Isotope	Data References						
		Positions	HFS	Intensities	Halfwidths		T-dep	P-shft
Av=0	<sup>14</sup> N <sup>16</sup> O				Air	Self		
0-0		P&P	Y	P&P <sup>a</sup>	A&S <sup>b</sup>	N	0.5	N
Δv=1	<sup>14</sup> N <sup>16</sup> O							
0-f	main, satl	C. et al	Y	C. et al	0.05 <sup>d</sup>	N	0.71 <sup>e</sup>	N
1-2 <sup>c</sup>	main	C. et al	Y	C. et al	0.05 <sup>d</sup>	N	0.71 <sup>e</sup>	N
1-2	satl	G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
2-3 <sup>i</sup>		G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
3-4 <sup>i</sup>		G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
4-5 <sup>i</sup>		G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
0-1	<sup>15</sup> N <sup>16</sup> O	G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
0-1	<sup>14</sup> N <sup>18</sup> O	G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>w</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
Δv=2	<sup>14</sup> N <sup>16</sup> O							
0-2		G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
1-3 <sup>ij</sup>		G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
2-4 <sup>i</sup>		G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
3-5 <sup>i</sup>		G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>
4-6 <sup>ij</sup>		G&G	N	G&G	S. et al <sup>f</sup>	L. Brown <sup>g</sup>	0.71 <sup>e</sup>	Y <sup>h</sup>

<sup>a</sup> Poynter & Pickett<sup>14</sup>, used Q(300K), no isotopic abundance factor  
<sup>b</sup> Self broadening, Abels & Shaw<sup>18</sup>  
<sup>c</sup> Update of all (0-1) lines, main branch (1-2) lines  
<sup>d</sup> Inadvertently, assumed 0.05 cm<sup>-1</sup>atm<sup>-1</sup> (296K) for all lines  
<sup>e</sup> Ballard et al<sup>28</sup>

<sup>f</sup> N<sub>2</sub> broadening  
<sup>g</sup> Estimated from S. et al<sup>29f</sup> by L.R. Brown, 1996

<sup>h</sup> -0.0017 cm<sup>-1</sup>atm<sup>-1</sup> for unupdated Av=1 (S. et al<sup>29</sup>)  
 -0.004 cm<sup>-1</sup>atm<sup>-1</sup> for Δv=2 (Poynter et al<sup>3,17</sup>)  
<sup>i</sup> two A components combined  
<sup>j</sup> Error in intensity normalization (see text)

A&S=Abels & Shaw<sup>18</sup>  
 C. et al=Coudert et al<sup>33</sup>  
 G&G=Gillis & Goldman<sup>16</sup>

P&P=Poynter & Pickett<sup>14</sup>  
 S. et al=Spencer et al<sup>29</sup>



Table 3.  $^{14}\text{N}^{16}\text{O}$   $X^2\Pi(v'', v')$ : Band intensities and maximum intensities

Band	Hitran 92		Hitran 96		DU 96	
	$S_{sum}$	$S_{max}$	$S_{sum}$	$S_{max}$	$S_{sum}$	$S_{max}$
		$S_{max\Lambda}$		$S_{max\Lambda}$		
O-O	.344e-19	.295e-21	.344e-19	.295e-21	.336e-19	.805e-21
0-0		.826e-21		.826e-21		.805e-21
O-1	.453e-17	.604e-19	.459e-17	.232e-19	.45e-17	.621e-19
0-1				.619e-19		.621e-19
1-2	.108e-20	.145e-22	.100e-20	.504e-23	.986e-21	.133e-22
1-2				.134e-22		.133e-22
2-3	.202e-24	.540e-26	.202e-24	.540e-26	.183e-24	.245e-26
3-4	.379e-28	.101e-29	.379e-28	.101e-29	.344e-28	.458e-30
4-5	.786e-32	.204e-33	.768e-32	.204e-33	.695e-32	.921e-34
O-2	.808e-19	.109e-20	.808e-19	.109e-20	.826e-19	.114e-20
1-3	.139e-22	.372e-24	.139e-22	.372e-24	.271e-22	.371e-24
2-4	.543e-26	.144e-27	.543e-26	.144e-27	.678e-26	.922e-28
3-5	.129e-29	.342e-31	.129e-29	.342e-31	.162e-29	.219e-31
4-6	.330e-33	.868e-35	.330e-33	.868e-35	.400e-33	.537e-35

ALL BRANCHES T= 296.0 AFTER CUT

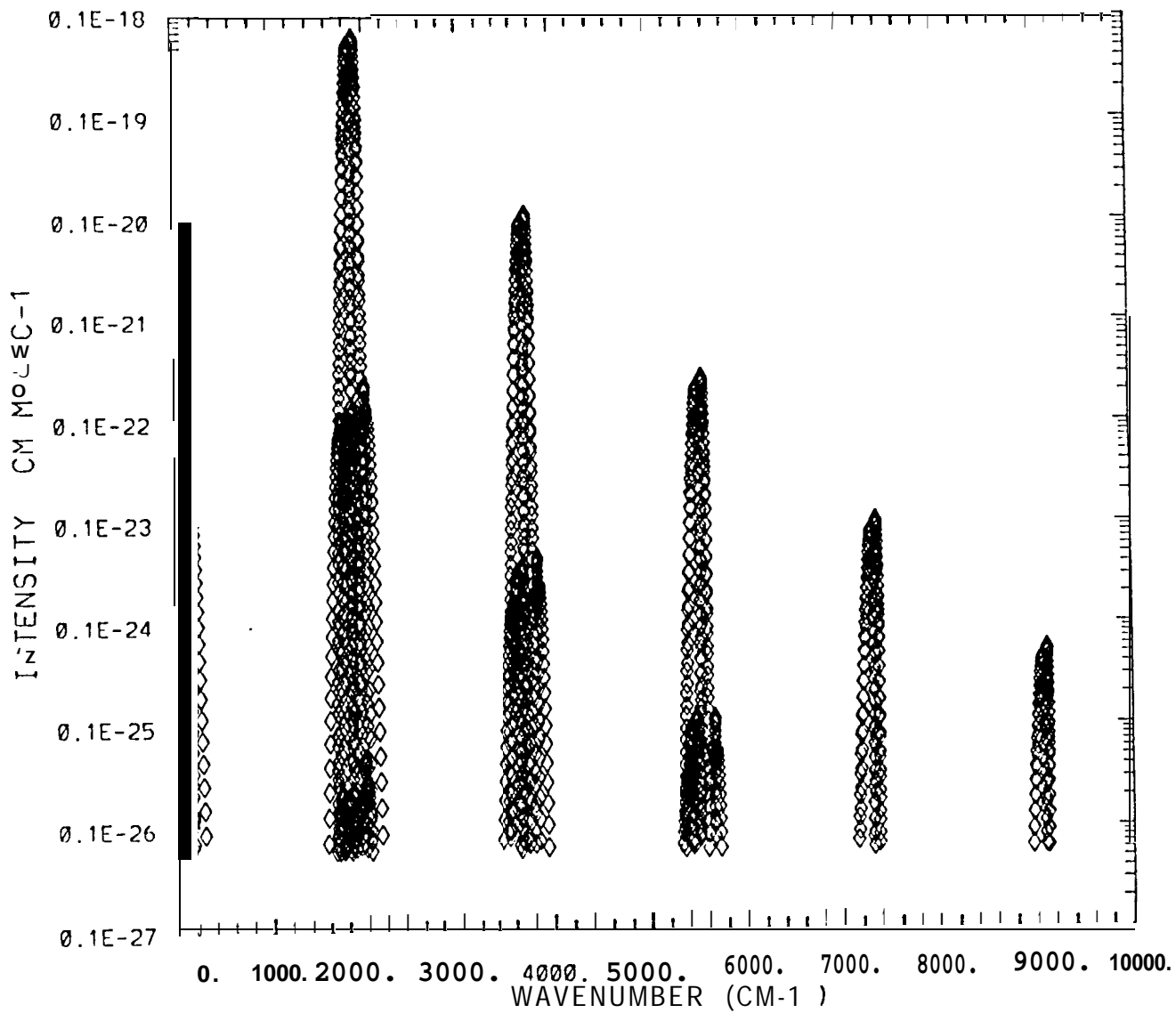


Fig. 1.

NO ALL BRANCHES T= 296.0 FIRST CUT

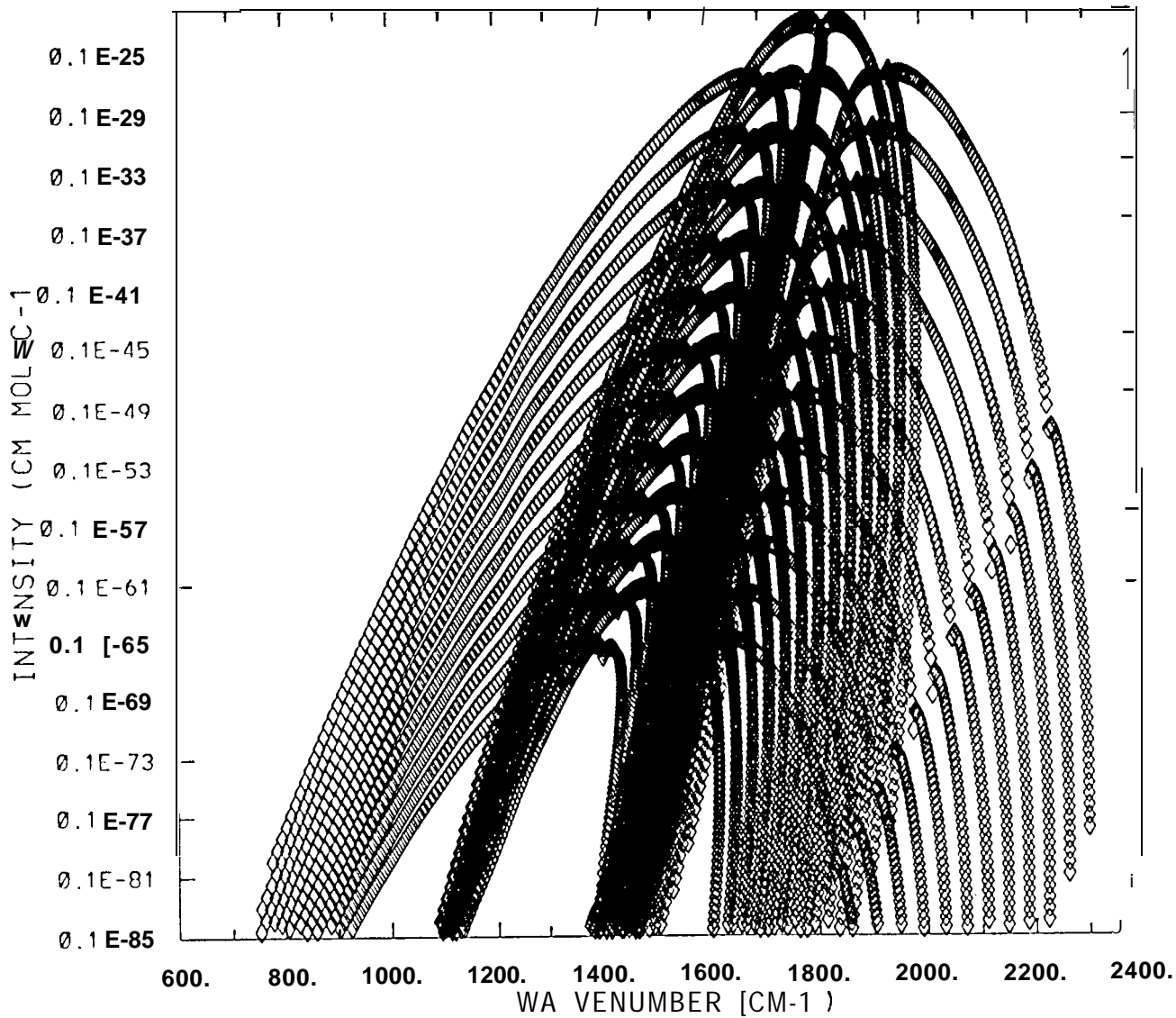


Fig. 2.

35

Spencer(sol id) Chackerian(dot) Langhoff(dash)

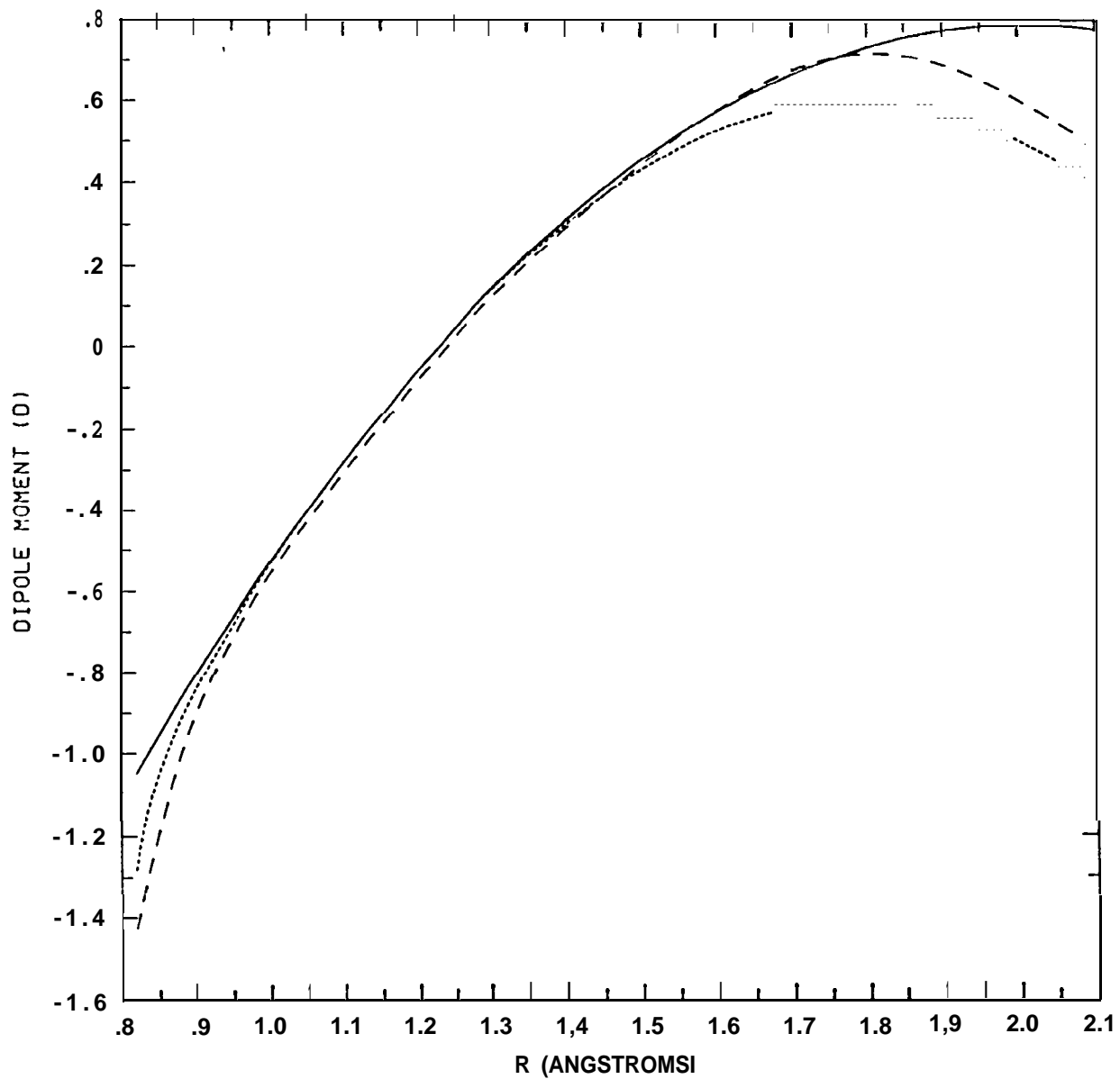


Fig. 3.

36

ME9341 08/26/97  
Frame # 1

PP22J=124.5 v=11 solid .13 det ,pred dash) 1/2

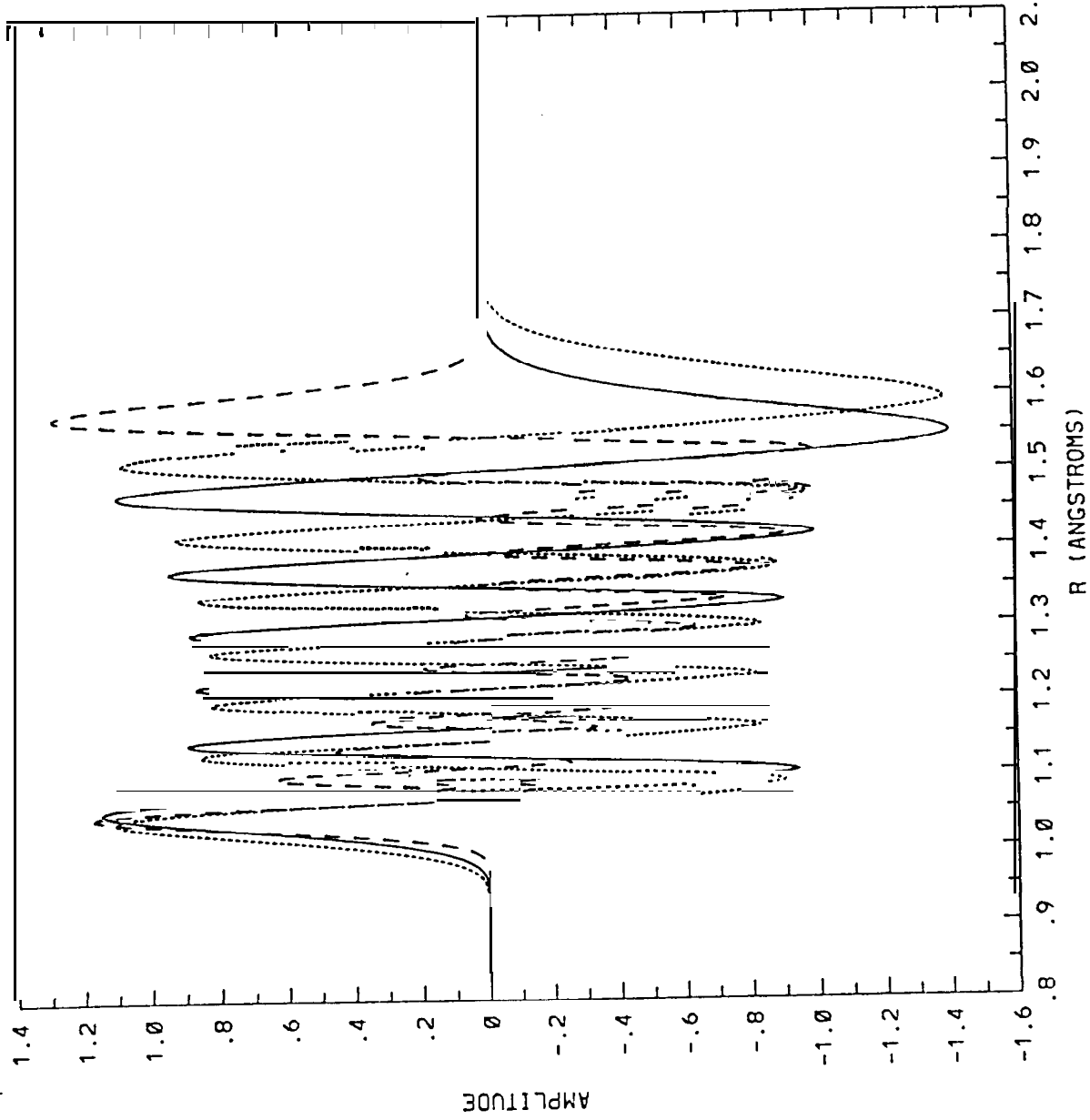


Fig. 4.