A High-Resolution Atlas of the Infrared Spectrum of the Sun and the Earth Atmosphere from Space

Volume III. Key to Identification of Solar Features

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I. Introduction

During the period April 29 through May 2, 1985, the Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment was operated as part of the Spacelab-3 (SL-3) payload on the shuttle Challenger. The instrument, a Fourier transform spectrometer, recorded over 2000 infrared solar spectra from an altitude of 360 km. Detailed descriptions of the scientific background of the ATMOS experiment, of the instrument’s design and observation technique, and of the SL-3 mission, as well as of the instrument itself, are given by Farmer et al.¹ and Farmer².

Although the majority of the spectra were taken through the limb of the Earth’s atmosphere in order to better understand its composition, several hundred of the “high-sun” spectra³ were completely free from telluric absorption. These high-sun spectra recorded from space are, at the present time, the only high-resolution infrared spectra ever taken of the Sun free from absorptions due to constituents in the Earth’s atmosphere. Volumes I and II of this series⁴ provide a compilation of these spectra arranged in a hard copy format suitable for quick-look reference purposes and are the first record of the continuous high-resolution infrared spectrum of the Sun and the Earth’s atmosphere from space.

In the past, a number of infrared solar atlases⁵ have been published that have presented “solar-telluric” spectra containing lines originating in both the Sun and the Earth’s atmosphere derived from observations made at ground-based sites or aircraft or balloon platforms. Thus, for the Sun itself, high-resolution infrared solar spectra were only available in intervals not marked by the strong absorption lines of constituents in the Earth’s atmosphere, the atmospheric spectral “windows.”

The spectral range covered by the ATMOS experiment was from 600 to 5000 cm⁻¹ (2 to 16 μm) at a resolution of 0.01 cm⁻¹. Within this interval lie the fundamental vibration-rotation bands of the solar molecular species NH, CH and OH, the Δν = 1 and Δν = 2 vibration-rotation series of CO and its isotopomers, and the pure rotational bands of OH and NH. No other molecular species have been identified to date. In addition to these molecular bands, fifteen different atomic species can be identified by their transitions.

The ability to analyze these many solar spectral features will ultimately lead to the determination of more accurate solar atomic abundances, isotopic ratios, and photospheric temperature structures and motions, and will serve as a basis for comparison with the atmospheric spectra and for future flights of ATMOS or similar instruments. As a precursor to the aforementioned goals, an assignment of the observed features is required. The present key, which reports line positions and absorption depths of nearly 16,000 features in the spectral range 622 to 4798 cm⁻¹, with assignments for more than 12,000 of these features, represents the first step in this process.

II. Frequency Calibration

From the earliest operation of the ATMOS instrument, it was clear that the spectra contained absorption-like features that were neither solar nor atmospheric in origin. In addition to those few “artifacts” as discussed in Volume I, there were many spectral lines superimposed on all of the spectra due to water vapor and CO₂. Supporting evidence that these gases were inside the instrument itself was provided by a rotational analysis consistent with a very low pressure (~ 10⁻¹ torr) and an ambient temperature of 301 ± 2 K, expected within the instrument enclosure. A subset of these “instrumental” H₂O and CO₂ lines was used by Norton⁶ to assign an absolute frequency scale to the spectra. The internal consistency for these residual gas instrumental lines has been determined to be ± 0.0003 cm⁻¹ or better. For the solar spectral lines, the observed frequencies are shifted from measured laboratory rest-frame reference frequencies by the Doppler corrections for the projection of the SL-3 orbital velocity onto the line of sight to the Sun, the radial velocity between the Earth and the Sun, and the Einstein gravitational redshift. The net effect of all of these corrections can be summarized in a single correction term for the sunset spectra⁷

\[
σ_{\text{LAB}} = σ_{\text{OBS}} (1 + Δ)
\]  

where \(σ_{\text{LAB}}\) is the measured laboratory frequency, \(σ_{\text{OBS}}\) is the observed frequency for ATMOS solar spectra, and \(Δ\) is the correction factor. An important caveat to bear in mind is that the final stated frequencies in the table are not to be considered as reference standards but merely as a guide for identification of features in the solar atmosphere.

To optimize the instrument performance in terms of signal-to-noise ratio and data sampling rates, the broadband frequency response was limited by selection of several narrower band optical filters. The frequency ranges of the most important of these filters were roughly 600 to 1200 cm⁻¹ for filter #1, 1100 to 2000 cm⁻¹ for filter #2, 1580 to 3400 cm⁻¹ for filter #3, and 3100 to 4800 cm⁻¹ for filter #4. Certain observed solar features for CO have had transition
Table 1. Correction Factors for the Four Filters.

<table>
<thead>
<tr>
<th>Filter #</th>
<th>Wavelength Range (cm⁻¹)</th>
<th>Correction Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>600 - 1200</td>
<td>2.488\times10^{-5}</td>
</tr>
<tr>
<td>2</td>
<td>1100 - 2000</td>
<td>2.488\times10^{-5}</td>
</tr>
<tr>
<td>3</td>
<td>1580 - 3400</td>
<td>2.474\times10^{-5}</td>
</tr>
<tr>
<td>4</td>
<td>3100 - 4800</td>
<td>2.402\times10^{-5}</td>
</tr>
</tbody>
</table>

frequencies measured under laboratory conditions to quite high accuracy. These were used to determine the frequency shift to be applied to the entire spectrum. A global fit of all such features using a single correction parameter, $\Delta$, proved less satisfactory than treating each spectral filter range separately. Therefore, in the present catalogue, we have used a separate correction factor for each of the four filters. For filter #4 we have chosen the (2-0) band of CO as measured in the laboratory by Pollock et al.⁸ (from $P_{29}$ at 4120.7287 cm⁻¹ to $R_{35}$ at 4350.7189 cm⁻¹) as the reference standard leading to a correction factor of $\Delta = 2.402 \times 10^{-5}$. For 53 lines compared with the Pollock et al. reference standard, we find a root mean square deviation of 0.0023 cm⁻¹. Using only the observed frequencies from a single occultation (the 55 averaged high-sun spectra denoted as SUN2 in Volume I), Norton⁹ obtained a correction factor for these same 53 lines of $\Delta = 2.407 \times 10^{-5}$ and a root mean square deviation of 0.0008 cm⁻¹. For filter #2 we have chosen as a reference standard the “strong” CO lines from the (1-0) band to the (7-6) band as measured by Schneider et al.⁹ The overall correction factor for 117 lines as compared with the Schneider et al. reference standard is $\Delta = 2.474 \times 10^{-5}$, with a root mean square error of 0.0009 cm⁻¹. There appears to be a small but smooth change in the correction factor as one goes from the (1-0) band to the (7-6) band, perhaps indicating that the lines are formed at different altitudes in the photosphere. The same CO lines of Schneider et al.⁹ have been used as a reference standard to determine a value of $\Delta = 2.488 \times 10^{-5}$ for the correction factor for filter #2, again with a root mean square error of 0.0009 cm⁻¹ from 49 lines. Finally, although no adequate reference standard exists to determine $\Delta$ for filter #1, there are five unblended, relatively strong, atomic lines that occur in the 1100 to 1180 cm⁻¹ overlap region between filter #1 and filter #2. Two are silicon lines at 1100.173 cm⁻¹ and 1166.743 cm⁻¹ and three are magnesium lines at 1125.290 cm⁻¹, 1125.932 cm⁻¹ and 1127.247 cm⁻¹. Using the same correction factor for filter #1 as for filter #2, $2.488 \times 10^{-6}$, the consistency between the measured frequency of these five lines is ± 0.001 cm⁻¹. The results for the correction factors for the four filters are summarized in Table 1.

III. Assignment of Observed Features

Before any solar feature was assigned, a line list had to be generated. This was accomplished in a two-step procedure. In the first phase, every panel of four wavenumbers’ width from Volume I was expanded by a factor of ten vertically and scanned manually for any feature that appeared above the noise in both the sunrise and sunset spectra. In many cases this was a judgment based on experience as to what constituted noise and what was a true solar feature. The observed position of the line (in cm⁻¹) and depth (in mm) were recorded. In the second phase, a computer-generated line list was obtained from the “raw” averaged high-sun spectra for each filter in the spacecraft rest velocity frame. Every feature, whether a true solar feature, noise, or an instrumental line with greater than 0.1% absorption, was listed. After applying the appropriate correction factor for every feature, as discussed in the preceding section, and using the fact that 100% absorption corresponds

2
Table 2. Depth of Catalogued Lines

<table>
<thead>
<tr>
<th>Depth of Line (mm)</th>
<th>Number of Lines</th>
<th>% of Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1 - 0.3</td>
<td>5419</td>
<td>34.2</td>
</tr>
<tr>
<td>0.4 - 0.6</td>
<td>2051</td>
<td>12.9</td>
</tr>
<tr>
<td>0.7 - 1.1</td>
<td>2075</td>
<td>13.1</td>
</tr>
<tr>
<td>1.2 - 1.6</td>
<td>900</td>
<td>5.7</td>
</tr>
<tr>
<td>1.7 - 2.1</td>
<td>687</td>
<td>4.3</td>
</tr>
<tr>
<td>2.2 - 2.8</td>
<td>646</td>
<td>4.1</td>
</tr>
<tr>
<td>2.9 - 9.9</td>
<td>2372</td>
<td>15.0</td>
</tr>
<tr>
<td>10.0 - 19.9</td>
<td>963</td>
<td>6.1</td>
</tr>
<tr>
<td>≥ 20</td>
<td>491</td>
<td>3.1</td>
</tr>
<tr>
<td>Unknown</td>
<td>244</td>
<td>1.5</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>15848</strong></td>
<td><strong>100.0</strong></td>
</tr>
</tbody>
</table>

to a line of about 81 mm$^2$ to convert the % absorption to a depth in millimeters, a second list of positions and depths was generated. After comparing the two lists and excluding from the second phase many lines that were either noise or instrumental in origin, a final list of 15,848 line positions and depths was obtained, as reported in the body of this work. In Table 2 we present the final total number of lines observed for a given range of depths. The line depths noted as "unknown" in Table 2 are due to broad features, blends, or lines that lie on the shoulders of other lines, making it difficult to obtain an exact depth.

After the assignments for all molecular and atomic species have been made (as will be discussed below), of the 15,848 catalogued lines, 12,098 lines (76.3%) have been assigned and 3,750 lines (23.7%) remain unidentified. The breakdown of the identification for all of the lines is given in Table 3. Approximately two-thirds of all catalogued lines are molecular in origin, about one-tenth are atomic in origin, and less than one-quarter (assumed to be atomic) are unidentified.

A. Molecular Species

**CO**: As discussed in the preceding section, a small number of the strong CO lines have been used to determine the correction factor for each filter. The total number of CO lines observed for the $\Delta v = 1$ series, i.e., from the (1-0) band (with a maximum observed J-value of 135 in both the P and R branches of $^{12}$C$^{16}$O) to the (20-19) band, is 6,490. This number includes lines observed for the isotopes $^{12}$C$^{16}$O, $^{13}$C$^{16}$O, $^{12}$C$^{18}$O and $^{12}$C$^{17}$O. The number of lines observed for the $\Delta v = 2$ series (the isotope $^{12}$C$^{16}$O only) is 2,394. The maximum depth observed for the (1-0) band of $^{12}$C$^{16}$O is 27.5 mm for the $R_{29}$ through $R_{36}$ members (34% absorption) and for the (2-1) band of $^{12}$C$^{16}$O it is 26.1 mm for the $R_{27}$ through $R_{36}$ members (32% absorption). The maximum depth observed for the (2-0) band of $^{12}$C$^{16}$O is 7.9 mm for $R_{32}$ (10% absorption) and for the (3-1) band of $^{12}$C$^{16}$O it is 11 mm for $R_{29}$ and $R_{30}$ (13% absorption)$^{10}$. The totality of CO lines accounts for 56.0% of all catalogued lines. A summary of the $\Delta v = 1$ series is given for each isotope of CO in Table 4. The highest observed J-value is given for the P and R branches for each band from (1-0) to (20-19).
Table 3. Number of Catalogued Lines and Their Identification.

<table>
<thead>
<tr>
<th>Identification</th>
<th>Number of Lines</th>
<th>% of Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular</td>
<td>10389</td>
<td>65.5</td>
</tr>
<tr>
<td>(\text{CO}^* (\Delta v = 1))</td>
<td>6490</td>
<td>40.9</td>
</tr>
<tr>
<td>(\text{CO}^{**} (\Delta v = 2))</td>
<td>2394</td>
<td>15.1</td>
</tr>
<tr>
<td>OH</td>
<td>743</td>
<td>4.7</td>
</tr>
<tr>
<td>CH</td>
<td>581</td>
<td>3.7</td>
</tr>
<tr>
<td>NH</td>
<td>181</td>
<td>1.1</td>
</tr>
<tr>
<td>Atomic</td>
<td>1709</td>
<td>10.8</td>
</tr>
<tr>
<td>Unidentified</td>
<td>3750</td>
<td>23.7</td>
</tr>
<tr>
<td>TOTAL</td>
<td>15848</td>
<td>100.0</td>
</tr>
</tbody>
</table>

* - Includes isotopic variants \(^{12}\text{C}^{16}\text{O}, ^{13}\text{C}^{16}\text{O}, ^{12}\text{C}^{18}\text{O}\) and \(^{12}\text{C}^{17}\text{O}\).

** - The isotope \(^{12}\text{C}^{16}\text{O}\) only.

Similar results for the \(\Delta v = 2\) series for CO are given in Table 5 for the bands (2-0) to (16-14). In a recent paper by Farrenq et al.,\(^1\) the Dunham coefficients for all isotopes of CO have been improved based on about 4,500 of these high-J lines observed by ATMOs, plus an additional selected set of about 14,000 accurate laboratory measurements. A comparison of the line positions for more than 2,550 CO transitions of the \(\Delta v = 1\) series (all transitions reported to three decimal places in the main table with a depth of greater than or equal to 0.5 mm) determined by the constants of Farrenq et al.,\(^1\) with those from the line list modified by the correction factors given in Table 1 leads to a root mean square deviation of the residuals of \(\pm 0.0016\) cm\(^{-1}\). The corresponding root mean square deviation of the residuals for more than 4,250 transitions of CO and its isotopomers of the \(\Delta v = 1\) series (all transitions reported to three decimal places in the main table) is \(\pm 0.0024\) cm\(^{-1}\).

**OH:** The optimum molecular constants and term values for OH have been given by Coxon\(^1\), based on his work and the earlier work of Maillard et al.\(^1\). From these constants, Pickett\(^1\) has performed a series of calculations for position and intensity of the pure rotational lines of OH to be expected in the solar photosphere at wavenumbers up to 1100 cm\(^{-1}\). In this catalogue, 370 pure rotational OH lines are reported between 622 and 1095 cm\(^{-1}\) for the strong (0-0) band to a few questionable lines of the very weak (4-4) band. In addition, 373 vibration-rotation lines of OH are observed for the P branch of the (1-0), (2-1), (3-2) and (4-3) bands between 1986 and 3508 cm\(^{-1}\). A comparison between 108 unblended pure rotational (0-0) OH lines compared with Pickett\(^1\) on the one hand and 53 unblended vibration-rotation lines of the (1-0) band compared with Maillard et al.\(^1\) on the other leads to a root mean square deviation of 0.005 cm\(^{-1}\).

**CH:** For CH, the most recent analyses of the vibration-rotation spectrum are by Mélen et al.\(^1\) and by Bernath\(^1\). In the present catalogue, 581 CH vibration-rotation lines for both the P and R branches
Table 4. Highest J-Values Observed for P and R Branches of CO: $\Delta v = 1$ Series

<table>
<thead>
<tr>
<th>Band</th>
<th>CO</th>
<th>13CO</th>
<th>18CO</th>
<th>17CO</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P</td>
<td>R</td>
<td>P</td>
<td>R</td>
</tr>
<tr>
<td>(1–0)</td>
<td>135</td>
<td>135</td>
<td>96</td>
<td>100</td>
</tr>
<tr>
<td>(2–1)</td>
<td>135</td>
<td>132</td>
<td>100</td>
<td>97</td>
</tr>
<tr>
<td>(3–2)</td>
<td>129</td>
<td>124</td>
<td>95</td>
<td>96</td>
</tr>
<tr>
<td>(4–3)</td>
<td>126</td>
<td>128</td>
<td>95</td>
<td>92</td>
</tr>
<tr>
<td>(5–4)</td>
<td>126</td>
<td>129</td>
<td>89</td>
<td>81</td>
</tr>
<tr>
<td>(6–5)</td>
<td>122</td>
<td>119</td>
<td>89</td>
<td>90</td>
</tr>
<tr>
<td>(7–6)</td>
<td>117</td>
<td>116</td>
<td>82</td>
<td>84</td>
</tr>
<tr>
<td>(8–7)</td>
<td>118</td>
<td>109</td>
<td>84</td>
<td>76</td>
</tr>
<tr>
<td>(9–8)</td>
<td>112</td>
<td>110</td>
<td>75</td>
<td>56</td>
</tr>
<tr>
<td>(10–9)</td>
<td>110</td>
<td>105</td>
<td>42</td>
<td>45</td>
</tr>
<tr>
<td>(11–10)</td>
<td>105</td>
<td>105</td>
<td>29</td>
<td>39</td>
</tr>
<tr>
<td>(12–11)</td>
<td>103</td>
<td>98</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(13–12)</td>
<td>97</td>
<td>90</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(14–13)</td>
<td>89</td>
<td>90</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(15–14)</td>
<td>83</td>
<td>82</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(16–15)</td>
<td>82</td>
<td>80</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(17–16)</td>
<td>76</td>
<td>74</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(18–17)</td>
<td>65</td>
<td>52</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(19–18)</td>
<td>57</td>
<td>52</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(20–19)</td>
<td>35</td>
<td>45</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Total number of observed lines: 3891, 1584, 853, 162

of the (1–0), (2–1), (3–2), and (4–3) bands have been observed, as well as a few Q branch lines of the (1–0) band. A small sampling of the strongest unblended lines compared with the above two references leads to a root mean square deviation of 0.005 cm$^{-1}$. No pure rotational lines of CH have been observed, although they are to be expected, based on their calculated intensities$^{14}$, below 622 cm$^{-1}$.

**NH:** Finally, for NH, 36 pure rotational lines have been observed by Geller et al.$^{17}$ for the (0–0) band, including a few lines of the (1–1) band, between 626
Table 5. Highest J-Values Observed for P and R Branches of CO: Δν = 2 Series

<table>
<thead>
<tr>
<th>Band</th>
<th>P</th>
<th>R</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-0</td>
<td>100</td>
<td>102</td>
</tr>
<tr>
<td>3-1</td>
<td>104</td>
<td>106</td>
</tr>
<tr>
<td>4-2</td>
<td>102</td>
<td>108</td>
</tr>
<tr>
<td>5-3</td>
<td>98</td>
<td>108</td>
</tr>
<tr>
<td>6-4</td>
<td>98</td>
<td>107</td>
</tr>
<tr>
<td>7-5</td>
<td>93</td>
<td>97</td>
</tr>
<tr>
<td>8-6</td>
<td>86</td>
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<td>9-7</td>
<td>86</td>
<td>90</td>
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<td>10-8</td>
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<td>85</td>
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<td>11-9</td>
<td>73</td>
<td>80</td>
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<td>12-10</td>
<td>72</td>
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<tr>
<td>13-11</td>
<td>64</td>
<td>81</td>
</tr>
<tr>
<td>14-12</td>
<td>51</td>
<td>68</td>
</tr>
<tr>
<td>15-13</td>
<td>44</td>
<td>55</td>
</tr>
<tr>
<td>16-14</td>
<td>32</td>
<td>35</td>
</tr>
</tbody>
</table>

Total number of observed lines 2394

The number of these observed atomic lines from hydrogen through nickel. In addition to fifteen different observed atoms in the ground neutral state, a few lines are reported for magnesium, aluminum, silicon and calcium in their first ionization state.

The primary sources for the energy levels from which these transitions were derived are Moore²¹,²² for H and C and the continuing series of compilations of energy levels in the Journal of Physical and Chemical Reference Data on Na (Martin and Zalubas²³), Mg (Martin and Zalubas²⁴), Al (Martin and Zalubas²⁵), Si (Martin and Zalubas²⁶), S (Martin, Zalubas and Musgrove²⁷), K (Corliss and Sugar²⁸), Ca (Sugar and Corliss²⁹), Sc (Sugar and Corliss³⁰), Ti (Corliss and Sugar³¹), Cr (Sugar and Corliss³²), Fe (Reader and Sugar³³), Co (Sugar and Corliss³⁴) and Ni (Corliss and Sugar³⁵).

As the work on identification of the atomic transitions progressed, it became clear that further calculations of the atomic energy levels had to be performed. As an example, in the 2450 to 2600 cm⁻¹ range, there are more than 680 observed features: only about 140 features are molecular in origin, approximately 80 features are atomic transitions that could be derived from the known energy levels, and the remaining 460 features were unidentified. Similar large groupings of atomic lines, many of which were unassigned, have been observed near 3808 cm⁻¹, 1340 cm⁻¹ and 808 cm⁻¹. These regions correspond to the hydrogen atom (4-5) transition at 2467.75 cm⁻¹, the (4-6) transition at 3808.26 cm⁻¹, the (5-6) and (6-8) transitions at 1340.50 cm⁻¹ and 1332.90 cm⁻¹, respectively, and the (6-7) and (7-9) transitions at 808.29 cm⁻¹ and 884.27 cm⁻¹, respectively, suggesting that many of the unidentified lines are atomic Rydberg-like transitions, as was later found to be the case. Chang³⁶ had noted that for low angular momentum states (L ≤ 3), we should expect to see only absorption-like features. Thus, as already noted for the 2450 to 2600 cm⁻¹ interval, a large number of the previously unidentified absorption features are atomic 4f-5g Rydberg-like transitions corresponding to the hydrogen atom (4-5) transition. As the L-value increases to L = 4 (g states), we begin to see Rydberg transitions with emission peaks in addition to the absorption troughs corresponding to the hydrogen atom (5-6) transition. A particularly striking example is the Mg 5g - 6h transition at 1356.19 cm⁻¹ with a strong central emission peak surrounded by two deep absorption troughs. Finally, at higher L-values (L ≥ 5), we see strong emission peaks, in some cases straddled by absorption troughs, corresponding to the hydrogen atom (6-7) and (7-9) transitions. Two examples, again due to Mg, are at 811.58 cm⁻¹ (6h - 7i) and 896 cm⁻¹. In addition, 145 vibration-rotation R branch lines of the (1-0) and (2-1) bands between 2919 and 3460 cm⁻¹ are catalogued. The identification for these lines comes from the works of Bernath and Amano¹⁸, Boudjadar et al.¹⁹ and Grevesse et al.²⁰

B. Atomic Species

As previously noted, 1,709 atomic lines have been identified. Table 6 represents the breakdown of
Table 6. Identified Atomic Features.

<table>
<thead>
<tr>
<th>Atom</th>
<th>Number of Identified Lines</th>
<th>Abundance*</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>13**</td>
<td>12.00</td>
</tr>
<tr>
<td>C</td>
<td>115</td>
<td>8.56</td>
</tr>
<tr>
<td>Na</td>
<td>37</td>
<td>6.33</td>
</tr>
<tr>
<td>Mg</td>
<td>176**</td>
<td>7.58</td>
</tr>
<tr>
<td>Mg II</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Al</td>
<td>61</td>
<td>6.47</td>
</tr>
<tr>
<td>Al II</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Si</td>
<td>481</td>
<td></td>
</tr>
<tr>
<td>Si II</td>
<td>2</td>
<td>7.55</td>
</tr>
<tr>
<td>S</td>
<td>28</td>
<td>7.21</td>
</tr>
<tr>
<td>K</td>
<td>16</td>
<td>5.12</td>
</tr>
<tr>
<td>Ca</td>
<td>97</td>
<td></td>
</tr>
<tr>
<td>Ca II</td>
<td>7</td>
<td>6.26</td>
</tr>
<tr>
<td>Sc</td>
<td>9</td>
<td>3.04</td>
</tr>
<tr>
<td>Ti</td>
<td>31</td>
<td>4.99</td>
</tr>
<tr>
<td>Cr</td>
<td>18</td>
<td>5.67</td>
</tr>
<tr>
<td>Fe</td>
<td>610</td>
<td>7.67</td>
</tr>
<tr>
<td>Co</td>
<td>1</td>
<td>4.92</td>
</tr>
<tr>
<td>Ni</td>
<td>5</td>
<td>6.25</td>
</tr>
</tbody>
</table>

TOTAL 1709


** See text Section III.B for additional H and Mg lines observed.
and 818.06 cm\(^{-1}\) (6g - 7h). Similar types of absorption troughs plus emission peaks are also found for hydrogen, silicon and aluminum. That these high-L states are populated and produce observable transitions may provide some clues to the mechanism of formation of these lines—whether formed in the upper photosphere or lower chromosphere, if charge exchange with hydrogen or \(n, \ell\) changing collisions play a role and if the emission features are expected to be more pronounced at the solar limb and in the region below 600 cm\(^{-1}\). Many recent papers have reported and discussed these emission features.\(^{37}\)

The basic theory for obtaining the line positions of these Rydberg transitions is the core-polarization approach\(^{38}\) in which

\[
E = E_0 - \frac{\text{Ryd}}{n^2} - \alpha P(n, \ell) + E_{J,K}^{\text{core}}(n, \ell)
\]

where \(E\) is the energy of an atom in a given state characterized by the quantum numbers \(n, \ell, J, K\), and \(E_0\) is the ionization potential; Ryd is the Rydberg constant for the given atomic species; \(\alpha\) is the dipole polarizability (in atomic units) of the atomic core; \(P(n, \ell)\) is a theoretically derived function of the quantum numbers \(n\) and \(\ell\) arising from the expectation value of the inverse fourth power of the hydrogenic radius, \(\langle r^{-4}\rangle_H\), given by

\[
P(n, \ell) = \frac{\text{Ryd} (3n^2 - \ell (\ell + 1))}{2n^5 (\ell - 1/2) \ell (\ell + 1/2) (\ell + 1) (\ell + 3/2)}
\]

and \(E_{J,K}^{\text{core}}(n, \ell)\) is a term representing quadrupole interactions and core-polarization and penetration effects. Using this approach, Chang\(^{39}\) has made detailed calculations on the (6-7) transitions in Si; Schoenfeld, Geller and Chang\(^{40}\) have made extensive calculations for the 4f - 5g, 4f - 6g and 5f - 6g transitions in Fe; and Geller\(^{41}\) has made preliminary calculations for C, Mg, Al, Si and Ca.

For C, in addition to those energy levels taken from Moore\(^{22}\), new energy levels have been derived\(^{41}\) as given in Table 7. The expected uncertainty in the levels is 0.05 cm\(^{-1}\) or less, except for the 5g [4 1/2] \(_{4,5}\) level, which has an uncertainty of about 0.10 cm\(^{-1}\), and the 5g [2 1/2] \(_{2,3}\) level, which has an uncertainty better than 0.2 cm\(^{-1}\).

The primary source for the energy levels of Mg\(^{24}\) has been supplemented by recent important papers\(^{42}\) by Biemont and Brault, Lemoine et al. and Kaufman and Martin, besides those papers by Chang, Jefferies, and Lemoine et al. cited in Reference 37. In addition to those features noted (in the main table of identifications that follows) as being due to magnesium, there are several regions that show a broad absorption that can also be ascribed to magnesium. In Table 8, we give the approximate central frequencies to (0.1 cm\(^{-1}\)) of these features and the corresponding transition multiplet, and classify the depth qualitatively as deep (D), medium (M) or shallow (S). As an example, in Figure 1 we show an enlargement of a portion of the “raw” uncorrected spectrum in the region around 3108 cm\(^{-1}\). Except for the feature at 3108.022 cm\(^{-1}\) (with a corrected frequency of 3108.099 cm\(^{-1}\), as given in the main table), which is ascribed to C(?), and the two narrow instrumental lines, the deep broad trough arises from the 5f - 9g multiplet of magnesium. Three similar features for hydrogen, not included in the main table, are the (5-10) transition (M) at 3290.3 cm\(^{-1}\), the (5-11) transition (S) at 3480.7 cm\(^{-1}\), and the (6-9) transition (M) at 1692.5 cm\(^{-1}\).

### Table 7. New Carbon Energy Levels.

<table>
<thead>
<tr>
<th>Term (cm(^{-1}))</th>
<th>Level (cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>5g [3 1/2] (_{3,4})</td>
<td>86426.76</td>
</tr>
<tr>
<td>5g [4 1/2] (_{4,5})</td>
<td>86427.25</td>
</tr>
<tr>
<td>5g [2 1/2] (_{2,3})</td>
<td>86498.5</td>
</tr>
<tr>
<td>5g [3 1/2] (_{3,4})</td>
<td>86489.62</td>
</tr>
<tr>
<td>5g [4 1/2] (_{4,5})</td>
<td>86485.56</td>
</tr>
<tr>
<td>5g [5 1/2] (_{5,6})</td>
<td>86495.26</td>
</tr>
<tr>
<td>6g [4 1/2] (_{4,5})</td>
<td>87769.96</td>
</tr>
<tr>
<td>6h [4 1/2] (_{4,5})</td>
<td>87771.65</td>
</tr>
<tr>
<td>6h [5 1/2] (_{5,6})</td>
<td>87771.65</td>
</tr>
</tbody>
</table>
Table 8. Additional Magnesium Features Observed in ATMOS.

<table>
<thead>
<tr>
<th>Central Frequency (cm(^{-1}))</th>
<th>Transition Multiplet</th>
<th>Depth*</th>
</tr>
</thead>
<tbody>
<tr>
<td>2746.6</td>
<td>5f – 8g</td>
<td>D</td>
</tr>
<tr>
<td>3108.1</td>
<td>5f – 9g</td>
<td>D</td>
</tr>
<tr>
<td>3052.1</td>
<td>5g – 9h</td>
<td>M</td>
</tr>
<tr>
<td>3594.4</td>
<td>5d – 10f</td>
<td>M</td>
</tr>
<tr>
<td>3366.5</td>
<td>5f – 10g</td>
<td>M</td>
</tr>
<tr>
<td>3309.9</td>
<td>5g – 10h</td>
<td>S</td>
</tr>
<tr>
<td>3557.6</td>
<td>5f – 11g</td>
<td>S</td>
</tr>
<tr>
<td>1736.8</td>
<td>6f – 9g</td>
<td>M</td>
</tr>
<tr>
<td>1704.1</td>
<td>6g – 9h</td>
<td>M</td>
</tr>
<tr>
<td>1995.2</td>
<td>6f – 10g</td>
<td>S</td>
</tr>
<tr>
<td>1144.3</td>
<td>7h – 10i</td>
<td>S</td>
</tr>
<tr>
<td>1143.0</td>
<td>7i – 10k</td>
<td>S</td>
</tr>
</tbody>
</table>

* The notation for the depth represents qualitatively whether the broad trough is deep (D), medium (M) or shallow (S).

For Al, in addition to the primary source\(^{25}\), see the recent papers by Biemont and Brau,\(^{43}\) and Chang\(^{43}\). From the recent analysis by Chang\(^{39}\) on Si, several of the higher energy levels, although not explicitly stated, can be derived\(^{41}\) and are shown in Table 9. The expected uncertainty is 0.01 cm\(^{-1}\) for the 5g levels, 0.02 cm\(^{-1}\) for the 6g and 6h levels (except for the 6h [3 1/2] level, which is probably only good to 0.1 cm\(^{-1}\)) and 0.1 cm\(^{-1}\) for the 7g, 7h and 7i levels. As shown in Table 6, Si is the second most frequently occurring atomic species in the infrared solar spectrum, with nearly 500 transitions being observed. For Ca, several new levels have been found\(^{41}\) by the approach using equations (2) and (3). These energy levels are given in Table 10. The expected uncertainty for the 5g, 6g and 7g levels is 0.03 cm\(^{-1}\) and for the 6h and 7h levels it is 0.1 cm\(^{-1}\). Chang\(^{44}\) had earlier placed the 5g \(^1G_4\) level at 44874.5 ± 0.2 cm\(^{-1}\), in good agreement with the result shown in Table 10.

Iron is the dominant atomic species observed in the infrared solar spectrum, with over 600 lines being identified or characterized. Recently, Biemont et al.\(^{45}\) have made a study of iron in the infrared solar spectrum, without identifications, and Johansson and Learner\(^{46}\) have completed a thorough laboratory analysis of the lowest 3d to 4f transition supermultiplet. Using these experimentally determined 4f levels as a starting point, Schoenfeld, Geller and Chang\(^{40,47}\) have calculated, based on equations (2) and (3), the energy levels of the 5f, 5g, 6g and 6h levels of Fe. From this analysis, nearly two hundred previously unidentified solar lines have been accurately assigned. In Table 11 we present the
complete array of 5g levels with an estimated accuracy of \( \pm 0.01 \text{ cm}^{-1} \). The notation used for the levels is \([J'']_K\) where \(J''\) is the \(J\)-value of the parent \(6D\) core, \(K = \ell + J\) (\(\ell = 4\) corresponds to the g-levels) and \(J = K \pm 1/2\). We have also determined a value of \(63737.75 \pm 0.10 \text{ cm}^{-1}\) for the ionization potential and a value of \(28.2 \pm 0.2\) for \(\alpha\), the dipole polarizability of the FeII core.

We also note the useful papers by Biemont et al. for Cr\(^{49}\), for the iron group elements\(^{50}\) and for the lighter elements up to \(Z = 20\)\(^{51}\).

There is as yet no evidence for transitions of other atomic species than are presented in Table 6, although they cannot be ruled out at the present time. In Table 12 we show the twelve “strongest” identified atomic features with a depth of 27 mm or greater, corresponding to an absorption of 33% or more.

Figure 1. Two tracings of a portion of the ATMOS spectrum around 3108 cm\(^{-1}\) showing the Mg 5f-9g multiplet. The lower tracing has been expanded in the vertical scale by a factor of ten.

<table>
<thead>
<tr>
<th>Term</th>
<th>Level (cm(^{-1}))</th>
<th>Term</th>
<th>Level (cm(^{-1}))</th>
<th>Term</th>
<th>Level (cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>5g ([3_1/2])</td>
<td>61346.46</td>
<td>5g ([4_1/2])</td>
<td>61346.79</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5g ([2_1/2])</td>
<td>61654.31</td>
<td>5g ([3_1/2])</td>
<td>61629.54</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5g ([4_1/2])</td>
<td>61619.18</td>
<td>5g ([5_1/2])</td>
<td>61644.32</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6g ([3_1/2])</td>
<td>62692.54</td>
<td>6g ([4_1/2])</td>
<td>62692.43</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6g ([2_1/2])</td>
<td>62991.19</td>
<td>6g ([3_1/2])</td>
<td>62976.35</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6g ([4_1/2])</td>
<td>62970.58</td>
<td>6g ([5_1/2])</td>
<td>62985.32</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6g ([5_1/2])</td>
<td>63503.60</td>
<td>6h ([4_1/2])</td>
<td>63507.07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7g ([3_1/2])</td>
<td>63503.50</td>
<td>7h ([4_1/2])</td>
<td>63506.70</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7g ([2_1/2])</td>
<td>63797.74</td>
<td>7h ([3_1/2])</td>
<td>63796.23</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7g ([3_1/2])</td>
<td>63788.50</td>
<td>7h ([4_1/2])</td>
<td>63792.44</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7g ([4_1/2])</td>
<td>63784.93</td>
<td>7h ([5_1/2])</td>
<td>63790.74</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7g ([5_1/2])</td>
<td>63794.4</td>
<td>7h ([6_1/2])</td>
<td>63795.59</td>
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<td></td>
</tr>
</tbody>
</table>

Table 9. New Silicon Energy Levels.
### Table 10. New Calcium Energy Levels.

<table>
<thead>
<tr>
<th>Term (cm⁻¹)</th>
<th>Level (cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5g (^3)G(_{3,4,5})</td>
<td>44874.83</td>
</tr>
<tr>
<td>5g (^1)G(_4)</td>
<td>44874.42</td>
</tr>
<tr>
<td>6g (^3)G(_{3,4,5})</td>
<td>46231.03</td>
</tr>
<tr>
<td>6g (^1)G(_4)</td>
<td>46231.70</td>
</tr>
<tr>
<td>6h (^1)^{3}H</td>
<td>46249.14</td>
</tr>
<tr>
<td>7g (^1)G(_4)</td>
<td>47048.89</td>
</tr>
<tr>
<td>7h (^1)^{3}H</td>
<td>47060.5</td>
</tr>
</tbody>
</table>

### Table 11. New Iron 5g Energy Levels.

<table>
<thead>
<tr>
<th>Term</th>
<th>Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>5g (9/2) ([8_{1/2}])</td>
<td>59335.72</td>
</tr>
<tr>
<td>5g (9/2) ([7_{1/2}])</td>
<td>59331.26</td>
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<tr>
<td>5g (9/2) ([6_{1/2}])</td>
<td>59329.63</td>
</tr>
<tr>
<td>5g (9/2) ([5_{1/2}])</td>
<td>59329.88</td>
</tr>
<tr>
<td>5g (9/2) ([4_{1/2}])</td>
<td>59331.28</td>
</tr>
<tr>
<td>5g (9/2) ([3_{1/2}])</td>
<td>59333.25</td>
</tr>
<tr>
<td>5g (9/2) ([2_{1/2}])</td>
<td>59335.31</td>
</tr>
<tr>
<td>5g (9/2) ([1_{1/2}])</td>
<td>59337.07</td>
</tr>
<tr>
<td>5g (9/2) ([1_{2}])</td>
<td>59338.24</td>
</tr>
<tr>
<td>5g (7/2) ([7_{1/2}])</td>
<td>59717.93</td>
</tr>
<tr>
<td>5g (7/2) ([6_{1/2}])</td>
<td>59717.07</td>
</tr>
<tr>
<td>5g (7/2) ([5_{1/2}])</td>
<td>59716.79</td>
</tr>
<tr>
<td>5g (7/2) ([4_{1/2}])</td>
<td>59716.93</td>
</tr>
<tr>
<td>5g (7/2) ([3_{1/2}])</td>
<td>59717.31</td>
</tr>
<tr>
<td>5g (7/2) ([2_{1/2}])</td>
<td>59717.75</td>
</tr>
<tr>
<td>5g (7/2) ([1_{1/2}])</td>
<td>59718.15</td>
</tr>
<tr>
<td>5g (7/2) ([1_{2}])</td>
<td>59718.36</td>
</tr>
<tr>
<td>5g (5/2) ([6_{1/2}])</td>
<td>59999.20</td>
</tr>
<tr>
<td>5g (5/2) ([5_{1/2}])</td>
<td>60001.33</td>
</tr>
<tr>
<td>5g (5/2) ([4_{1/2}])</td>
<td>60001.57</td>
</tr>
<tr>
<td>5g (5/2) ([3_{1/2}])</td>
<td>60000.71</td>
</tr>
<tr>
<td>5g (5/2) ([2_{1/2}])</td>
<td>59999.39</td>
</tr>
<tr>
<td>5g (5/2) ([1_{1/2}])</td>
<td>59998.12</td>
</tr>
<tr>
<td>5g (3/2) ([5_{1/2}])</td>
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<td>60197.93</td>
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<tr>
<td>5g (3/2) ([3_{1/2}])</td>
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<td>60192.14</td>
</tr>
<tr>
<td>5g (1/2) ([4_{1/2}])</td>
<td>60309.69</td>
</tr>
<tr>
<td>5g (1/2) ([3_{1/2}])</td>
<td>60309.70</td>
</tr>
</tbody>
</table>

### C. Unidentified Lines

From Table 3 we recall that there are a total of 3,750 unidentified lines accounting for 23.7% of the total of 15,848 lines. The breakdown of the depth of these unidentified lines, in mm, is given in Table 13. Only 533 lines, corresponding to 14.2% of the unidentified lines or 3.4% of the total number of lines, have an absorption of 0.8% or more (greater than 0.6 mm in depth). The totality of these 533 "large" unidentified features is given in Table 14 and in Figure 2 we present a histogram of these "large" unidentified features in blocks of 100 cm⁻¹. At present, only 29 unidentified lines have an absorption greater than 6%. The ten deepest lines from Table 14 are given in Table 15. Note that only three out of the total of 1,454 lines with depth \(\geq 10.0\) mm remain unidentified.

If and when a thorough analysis is made of the higher angular momentum levels in the third row atoms, Ca through Zn, and their corresponding Rydberg transitions, the number of "large" unidentified features is expected to drop markedly. Based on the solar atomic abundances of Cr (5.67), Mn (5.39), Co (4.92) and Ni (6.25) and the paucity of experimental energy levels, these four atomic species are highly likely candidates for a number of the unidentified features.
Table 12. Strongest Identified Atomic Features.

<table>
<thead>
<tr>
<th>Frequency (cm(^{-1}))</th>
<th>Depth (mm)</th>
<th>Identification</th>
</tr>
</thead>
<tbody>
<tr>
<td>4021.336</td>
<td>35.0</td>
<td>Mg 4p – 5s</td>
</tr>
<tr>
<td>4028.081</td>
<td>32.4</td>
<td>Mg 4p – 5s</td>
</tr>
<tr>
<td>4681.636</td>
<td>32</td>
<td>Si 4p – 5s</td>
</tr>
<tr>
<td>4532.583</td>
<td>30.6</td>
<td>Na 4s – 4p</td>
</tr>
<tr>
<td>4531.301</td>
<td>29.4</td>
<td>Si 3d – 4f</td>
</tr>
<tr>
<td>4723.760</td>
<td>29.2</td>
<td>Al 4p – 5s</td>
</tr>
<tr>
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Table 13. Breakdown of Unidentified Lines.

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Figure 2. Histogram of a number of “large” unidentified features (with depth ≥ 0.7 mm) in blocks of 100 cm\(^{-1}\) width. Data taken from Table 14.
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Table 14. "Large" Unidentified Features.
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\(^{12}\)C\(^{16}\)O, \(^{13}\)C\(^{16}\)O, \(^{12}\)C\(^{18}\)O and \(^{12}\)C\(^{17}\)O, the notations CO, C\(13\)O16, C\(12\)O18 and C\(12\)O17 are used, respectively. The remaining molecular species are OH, CH and NH. Standard atomic designations are used throughout. Tentative identifications are marked with a species name plus a question mark, such as "Fe(?)." A question mark in the second column indicates that the line is unidentified. The third and fourth columns represent the assigned transition, such as OH (1-1) R\(\lambda\)E 27.5, indicating the R\(\lambda\)e 27.5 transition of the (1-1) pure rotational band of molecular OH, or Si 4p \(^3\)D\(_1\) - \(^3\)F\(_{0}\), corresponding to the silicon transition from the even state characterized by \(1s\(^2\)2s\(^2\)2p\(^6\)3s\(^2\)3p\(^4\)p\(^3\)D\(_1\)\) to the odd state \(1s\(^2\)2s\(^2\)2p\(^6\)3s\(^2\)3p3d \(^3\)F\(_{0}\)\). The fifth column gives the depth of the line in millimeters, at the scale of the published spectra in Volume I, usually to one decimal place. In some cases, usually for a small line, the notations "<" ("less than") or "<<" ("much less than") are also used. Depths as small as 0.1 mm can be discerned for filters #1, #2 and #3, where the noise level is small. For filter #4, the noise level increases, particularly from about 4600 cm\(^{-1}\) on. Since an absorption of 100% is represented in the spectra by a line of about 81 mm in depth, a depth of 0.7 mm corresponds to about 0.8% absorption. Also included in this column is a notation to indicate whether the line is a blend (b) or lies on the shoulder(s) of another line (s). The final column repeats the question mark if the line is unidentified. A few comments have been included, such as "broad" (self-evident) and "Abs + Emission" (if the line manifests emission features plus an absorption trough(s)). Most of these latter comments occur between 806 and 912 cm\(^{-1}\) and between 1342 and 1358 cm\(^{-1}\).

IV. Description of the Table of Identifications

In the Table of Identifications, which constitutes the main body of this volume, each block of eight wavenumbers is given a separate heading and corresponds to a page of two panels in Volume I of this series. In addition, three separate blocks of data available from ATMOS from 622–630 cm\(^{-1}\), 630–638 cm\(^{-1}\) and 638–646 cm\(^{-1}\), excluded from Volume I because of the low signal-to-noise ratio, have been included due to the certain identification of several OH and NH transitions. In the first column of the table, the corrected frequency (see Table 1) is given, usually to three decimal figures if warranted by the data. In the case of blends, lines on the shoulders of other lines, noise, or background continuum, only two decimal figures are reported. The second column identifies the species. For the molecular species

V. Corrections and Additions

In an undertaking such as this, it is inevitable that errors will persist in the tables. It would be greatly appreciated if any corrections, additions or identifications were brought to the author's attention. The ultimate aim is to completely identify every observable feature in the infrared solar spectrum.

VI. Acknowledgements

This catalogue and identification key would not have been possible had not Barney Farmer, the late Bob Norton, and Rudy Schindler spent many years of their lives bringing the ATMOS experiment to fruition. The author especially thanks Barney Farmer for continuing encouragement and discussions and for providing a pre-publication copy of the spectra
early in 1989. Special thanks go to Nicolas Grevesse and Jacques Sauval for a comprehensive preliminary molecular line list and invaluable conversations, and to Bob Kurucz for supplying a useful expanded version of the ATMOS data. Acknowledgements are also given to Linda Brown, Ed Chang, John Jefferies, Bob Norton, Herb Pickett and Geoff Toon for many useful, stimulating and informative discussions. Finally, the publication of this identification key would have been a lot more difficult without the continuing aid, advice and support of Mike Gunson.
References


3. The term "high-sun" spectra has been taken to mean all spectra whose minimum ray height above the surface of the Earth is greater than 165 km.


6. The late Bob Norton, in a private communication, had made a thorough analysis of all the effects involved in retrieving a "true" frequency scale from the observed frequencies both for the instrumental lines and for the solar lines.

7. Slightly different correction factors Δ' are obtained from the sunrise spectra where the correction term is given by sLab = sObs (1 - Δ').


10. The corresponding maximum depth for the R branch of the (1-0) and (2-1) bands in ¹²C¹⁸O is about 5 mm (6% absorption), in ¹³C¹⁸O about 1.2 mm (1.5% absorption) and in ¹²C¹⁷O about 0.2 mm (0.2% absorption).


14. The author wishes to thank Herb Pickett for performing calculations for the position and intensity for the pure rotational transitions in OH and CH.


36. E. Chang, private discussion held at JPL in October 1990.


40. Schoenfeld, W., Geller, M., and Chang, E. S., "High Angular Momentum Energy Levels in Fe, Calculation and Comparison with ATMOS Data," to be published in Astrophys. J.

41. Detailed analysis and results of these calculations will be reported elsewhere.


47. Private communication from Nicolas Grevesse and Sven Johansson. By combining an experimental study with the results of the ATMOS experiment, they have succeeded in unraveling the 4f - 5g multiplet.

48. Although the ionization potential is given in Reference 33 as 63480 cm\(^{-1}\) with no error limits, we have noted a paper by E. P. Worden et al. in J. Opt. Soc. Amer. 81, 314 (1984), where the ionization potential is given as 63737 ± 1 cm\(^{-1}\), in excellent agreement with our findings.


Supplementary Note

After completion of this work, a thorough check of the main table uncovered several errors, which we note in the following supplementary table. In addition, a final literature search conducted by the author brought to light several papers on Fe, which has allowed many previously unassigned lines (some already correctly identified as being due to Fe) to be classified. In particular, we note the paper by Zhu and Knight, which gives several new even-parity levels of Fe. From the eleven new levels that we present below, refined from Zhu and Knight’s preliminary estimate, more than sixty identifications have been made, including the three “largest” unidentified lines at 3403.279, 3463.247 and 3483.381 cm⁻¹. Similarly, the paper by Brown, Ginter, Johansson and Tilford presents new odd-parity energy levels from which more than thirty transitions have been identified. Other recent important Fe papers are by Johansson and Cowley, who discuss the present status of the iron group elements in the neutral and first and second ionization states, and by O’Brien, Wickliffe, Lawler, Whaling and Brault, who give lifetimes, transition probabilities, and an accurate updated listing of the known Fe I energy levels but not including those reported in Refs. S1 and S2. Most of the new Ni identifications presented in this supplementary table are taken from Biemont, Brault, Delbouille and Roland. Two entries in Table 14 should be corrected to 2925.390 from 2925.190 cm⁻¹ and 3313.15 from 3313.13 cm⁻¹.

In the supplementary table, the first and fourth columns correspond to the frequency in wavenumbers and the depth in millimeters as given in the main table. The second and third columns are the species identification and transition, if known. The last column notes what the previous identification was: “?” indicates that the line was unidentified, “Fe-No” indicates that the line was identified as Fe but without an assigned transition, and the remaining comments—“Add,” “Corr” (correction), and “Delete”—are self-evident. We have used a shorthand notation for most of the Fe transitions, in which A, B, C and D represent the core:

A 3d⁶(²D)4s(⁶D)
B 3d⁶(²D)4s(⁴D)
C 3d⁷(⁴F)
D 3d⁷(⁴F)

The eleven new even-parity energy levels, based on the work of Zhu and Knight, but refined due to the observed transitions, are:

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<td>A5d ⁵D₄</td>
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<td></td>
<td></td>
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</tr>
<tr>
<td>C6s ⁵F₅</td>
<td>56113.90</td>
<td>A5d ⁵F₅ (?)</td>
</tr>
</tbody>
</table>

All of these energy levels, in wavenumbers, are expected to be accurate to ±0.02 cm⁻¹. We expect that as more of the A5d multiplet for Fe becomes known (in the range 56000-57000 cm⁻¹), many more of the unidentified lines will be identified. At present, only 51 lines remain unidentified in the range 2.2–2.8 mm and 52 lines remain unidentified with a depth greater than 2.8 mm, a total of 103 unidentified lines with an absorption greater than 2.5%. We note finally that six of the ten “largest” lines from Table 15 have all been identified as Fe with assigned transitions.
Supplementary References


Supplementary Table

| Mass       | Element | Symbol | 
|------------|---------|--------|        |
| 1342.177   | C       | 5p     |         |
| 1376.769   | C       | 5p     | 3\(^3\)D\(_3\) - 5d 3\(^3\)F\(_3\) 0.2 |        |
| 1382.276   | C       | 5p     | 3\(^3\)D\(_2\) - 5d 3\(^3\)F\(_2\) 0.1 |        |
| 1384.64    | C       | 5p     | 3\(^3\)D\(_1\) - 5d 3\(^3\)F\(_1\) 0.1 |        |
| 1649.937   | Fe      | C6s    | 5\(^5\)F\(_5\) - B5p 5\(^5\)D\(_4\) 0.4 |        |
| 1803.326   | Fe      | C6s    | 5\(^5\)F\(_5\) - B5p 3\(^3\)F\(_2\) 0.2 |        |
| 1926.947   | Fe      | A4d    | f\(^3\)F\(_4\) - C5p 5\(^5\)F\(_5\) 0.4 |        |
| 1966.172   | Fe      | A4d    | f\(^3\)F\(_5\) - C5p 5\(^5\)G\(_6\) 0.4 |        |
| 1984.690   | Fe      | A5p    | t\(^3\)D\(_4\) - C4d g\(^5\)F\(_5\) 0.4 |        |
| 2078.517   | Fe      | A5p    | t\(^3\)D\(_4\) - C4d h\(^3\)D\(_4\) 0.5 |        |
| 2095.531   | Fe      | A6s    | 5\(^3\)D\(_1\) - A6p 5\(^3\)D\(_1\) 0.2 |        |
| 2114.003   | Fe      | A6s    | g\(^5\)D\(_4\) - A6p 5\(^5\)D\(_4\) 0.9 |        |
| 2124.834   | Fe      | A4d    | f\(^3\)F\(_4\) - C5p 5\(^5\)G\(_5\) 0.2 |        |
| 2182.676   | Fe      | C4p    | y\(^3\)D\(_1\) - X 3\(^3\)P\(_1\) 1.5 |        |
| 2199.516   | Fe      | A6s    | 5\(^3\)D\(_3\) - A6p 5\(^3\)F\(_4\) 5.3 |        |
| 2200.999   | Fe      | A5p    | t\(^3\)D\(_2\) - C4d g\(^5\)T\(_3\) 0.1 |        |
| 2209.650   | Fe      | A6s    | 5\(^3\)D\(_2\) - A6p 5\(^3\)F\(_4\) 1.0 |        |
| 2227.384   | Fe      | A6s    | 5\(^3\)D\(_4\) - A6p 5\(^3\)F\(_4\) 5.7 |        |
| 2252.437   | Fe      | A6s    | 5\(^3\)D\(_4\) - A6p 5\(^3\)D\(_4\) 5.2 |        |
| 2266.882   | Fe      | A6s    | 5\(^3\)D\(_1\) - A6p 5\(^3\)F\(_4\) bs 0.3 |        |
| 2285.450   | Fe      | A4d    | f\(^3\)F\(_5\) - C5p 5\(^3\)F\(_4\) 1.7 |        |
| 2303.691   | Fe      | A6s    | 5\(^3\)D\(_3\) - A6p 5\(^3\)D\(_3\) 2.5 |        |
| 2319.481   | Fe      | A6s    | g\(^5\)D\(_5\) - A6p 5\(^5\)D\(_5\) 8.9 |        |
| 2367.418   | Fe      | C6s    | 5\(^3\)F\(_4\) - B5p 5\(^3\)F\(_4\) 0.4 |        |
| 2378.215   | Fe      | A6s    | g\(^5\)D\(_4\) - A6p 5\(^5\)F\(_5\) 7.3 |        |
| 2380.925   | Fe      | A4d    | e\(^5\)G\(_5\) - C5p 5\(^5\)F\(_5\) 1.0 |        |
| 2391.444   | Fe      | A6s    | 5\(^3\)D\(_3\) - A6p 5\(^3\)P\(_3\) b 2.7 Add |        |
| 2399.422   | Fe      | A6s    | g\(^7\)D\(_3\) - A6p 7\(^7\)F\(_4\) 6.1 Fe-No |        |
| 2408.524   | Fe      | A6s    | 3\(^3\)D\(_4\) - A6p 7\(^3\)P\(_3\) 1.9 |        |
| 2409.228   | Ni      |        | 1.4 |        |
| 2415.281   | Fe      | A6s    | g\(^7\)D\(_2\) - A6p 7\(^3\)F\(_3\) 5.5 Fe-No |        |
| 2416.859   | Fe      | A6s    | g\(^3\)D\(_4\) - A6p 7\(^3\)P\(_4\) 6.4 Fe-No |        |
| 2429.641   | Fe      | A5p    | t\(^3\)D\(_1\) - C4d g\(^5\)F\(_2\) 0.4 |        |
| 2435.843   | Fe      | A6s    | 5\(^3\)D\(_1\) - A6p 5\(^3\)P\(_1\) 0.8 |        |
| 2437.883   | Fe      | A6s    | g\(^5\)D\(_5\) - A6p 5\(^5\)D\(_4\) 7.6 Fe-No |        |
| 2438.341   | Fe      | A6s    | 5\(^3\)D\(_2\) - A6p 5\(^3\)F\(_2\) 1.0 |        |
| 2444.65    | Fe      | A5p    | t\(^3\)D\(_0\) - C4d g\(^5\)F\(_1\) 0.1 |        |
| 2447.824   | Fe      |        | v\(^3\)P\(_2\) - A4d e\(^3\)P\(_3\) 0.3 |        |
| 2460.135   | Fe      | A6s    | g\(^3\)D\(_5\) - A6p 7\(^3\)F\(_5\) 10.2 Fe-No |        |
| 2469.585   | Fe      | A5p    | t\(^3\)D\(_3\) - C4d g\(^5\)F\(_3\) 0.3 |        |
| 2478.988   | Fe      | A6s    | 5\(^3\)D\(_3\) - A6p 5\(^3\)F\(_3\) b Add |        |
| 2483.649   | Fe      | A6s    | g\(^5\)D\(_3\) - A6p 7\(^3\)P\(_3\) 4.0 Fe-No |        |
| 2500.375   | Fe      | C4p    | y\(^3\)D\(_2\) - X 3\(^3\)P\(_1\) 5.7 Fe-No |        |
| 2506.059   | Ni      |        | 1.8 |        |
| 2506.498   | Ni      |        | 1.8 |        |
| 2508.697   | Fe      |        | v\(^3\)P\(_3\) - A4d e\(^3\)P\(_4\) 3.6 Fe-No |        |
|---------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 2548.41 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2348.795|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2576.67 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2577.932|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2625.41 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2668.62 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2692.415|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2725.72 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2754.376|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2785.89 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2827.36 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2852.65 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2875.61 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2886.87 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2860.09 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2858.06 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2865.82 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2869.30 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2890.24 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2904.97 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2905.25 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2905.04 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 2909.22 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 3004.50 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 3044.53 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 3098.49 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 3125.18 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 3182.86 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 3195.38 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 3195.04 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 3234.34 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |

Supplementary Table (continued)
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### 630-638 cm⁻¹

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### 670–678 cm⁻¹

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### 718-726 cm\(^{-1}\)

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<td>720.379</td>
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### 726-734 cm\(^{-1}\)

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### 734-742 cm\(^{-1}\)

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<td>734.763</td>
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<td>734.819</td>
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<td>735.237</td>
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### 742-750 cm\(^{-1}\)

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### 750-758 cm\(^{-1}\)

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### 758-766 cm⁻¹

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<td>758.577</td>
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<td>758.994</td>
<td>OH (1-1)</td>
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<td>761.095</td>
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<td>762.004</td>
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<td>763.983</td>
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<td>764.487</td>
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<td>764.534</td>
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<td>765.058</td>
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<td>Si 5d ⁸P⁰ -5f [4½]’s</td>
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### 766-774 cm⁻¹

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<td>770.437</td>
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### 774-782 cm⁻¹

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<td>776.986</td>
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### 782–790 cm\(^{-1}\)

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### 790–798 cm\(^{-1}\)

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<td>795.122</td>
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### 798–806 cm\(^{-1}\)

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<tr>
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<td>OH</td>
<td>(1-1)</td>
<td>R2F 24.5</td>
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<tr>
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Abs. + Emission
### 806-814 cm\(^{-1}\) (Continued)

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### 814-822 cm\(^{-1}\)

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### 822–830 cm⁻¹

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### 830–838 cm⁻¹

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### 838–846 cm⁻¹

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* Best estimates place the lines at

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<td>848.061</td>
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### 854-862 cm⁻¹

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<td>861.303</td>
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<td>861.794</td>
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### 862-870 cm⁻¹

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### 870-878 cm⁻¹

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### 878-886 cm⁻¹

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### 886-894 cm⁻¹

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### 894-902 cm⁻¹

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<td>901.634</td>
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<td>901.882</td>
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### 902-910 cm⁻¹

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### 910-918 cm\(^{-1}\)

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### 918-926 cm\(^{-1}\)

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<tbody>
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<tr>
<td>919.029</td>
<td>OH</td>
<td>(1-1) R1E 31.5</td>
<td>1.3</td>
</tr>
<tr>
<td>919.513</td>
<td>Si</td>
<td>6p (\frac{3}{2}, \frac{5}{2}) - 7s (\frac{3}{2}, \frac{1}{2})^o</td>
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<td>OH</td>
<td>(0-0) R1E 29.5</td>
<td>3.4</td>
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<tr>
<td>924.681</td>
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<td>(0-0) R2E 28.5</td>
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</tr>
<tr>
<td>925.035</td>
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<td>(0-0) R1F 29.5</td>
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<tr>
<td>925.326</td>
<td>Fe</td>
<td>5p (^{7}P^o) - (e) (^{7}G_6)</td>
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### 926-934 cm\(^{-1}\)

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<tbody>
<tr>
<td>926.866</td>
<td>?</td>
<td></td>
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<tr>
<td>927.351</td>
<td>?</td>
<td></td>
<td>0.1</td>
</tr>
<tr>
<td>928.172</td>
<td>OH</td>
<td>(2-2) R2F 34.5</td>
<td>0.2</td>
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<tr>
<td>928.349</td>
<td>OH</td>
<td>(2-2) R1E 35.5</td>
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<tr>
<td>928.720</td>
<td>OH</td>
<td>(2-2) R2E 34.5</td>
<td>0.2</td>
</tr>
<tr>
<td>928.925</td>
<td>OH</td>
<td>(2-2) R1F 35.5</td>
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### 934–942 cm\(^{-1}\)

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<tbody>
<tr>
<td>934.472</td>
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<td>(1-1)</td>
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<tr>
<td>934.673</td>
<td>OH</td>
<td>(1-1)</td>
<td>R1E 32.5</td>
<td>1.2</td>
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<tr>
<td>935.23</td>
<td>?</td>
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<td></td>
<td>bs 0.2</td>
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<td>938.147</td>
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<td>R2F 35.5</td>
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<td>938.810</td>
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### 942–950 cm\(^{-1}\)

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<td>R2E 29.5</td>
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<tr>
<td>943.866</td>
<td>OH</td>
<td>(0-0)</td>
<td>R1F 30.5</td>
<td>3.1</td>
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<tr>
<td>944.224</td>
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<td></td>
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<td>946.946</td>
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<td>R2F 36.5</td>
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<td>946.984</td>
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<td>947.100</td>
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<tr>
<td>947.514</td>
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<tr>
<td>949.831</td>
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### 950–958 cm\(^{-1}\)

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<th>Comment</th>
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<tbody>
<tr>
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<td>OH</td>
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<td>R1F 33.5</td>
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<tr>
<td>951.496</td>
<td>?</td>
<td></td>
<td></td>
<td>0.1</td>
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<tr>
<td>954.535</td>
<td>OH</td>
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<tr>
<td>954.682</td>
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<tr>
<td>954.866</td>
<td>OH</td>
<td>(2-2)</td>
<td>R2E 37.5</td>
<td>0.1</td>
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<tr>
<td>955.007</td>
<td>OH</td>
<td>(2-2)</td>
<td>R1F 38.5</td>
<td>0.1</td>
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<tr>
<td>957.906</td>
<td>Mg</td>
<td>6d (^{1,3}D_{1,2,3})  (- ) 7f (^{1,3}P_{2,3,4})</td>
<td>1.1</td>
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\(4 \text{ lines}\)
### 958–966 cm\(^{-1}\)

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<th>R1E</th>
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<tbody>
<tr>
<td>959.165</td>
<td>Ca</td>
<td>(4p^2 , ^1D_2 - 4s , ^1P_1)</td>
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<tr>
<td>960.427</td>
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<tr>
<td>960.629</td>
<td>OH</td>
<td>(0-0)</td>
<td>R1E 31.5</td>
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<tr>
<td>960.760</td>
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<td>960.89</td>
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<tr>
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<td>R1E 39.5</td>
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<tr>
<td>961.133</td>
<td>OH</td>
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<td>R2E 38.5</td>
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</tr>
<tr>
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<tr>
<td>963.298</td>
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<tr>
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<td>965.14</td>
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### 966–974 cm\(^{-1}\)

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<th>R1E</th>
</tr>
</thead>
<tbody>
<tr>
<td>966.933</td>
<td>Si</td>
<td>(6p , (\frac{3}{2}, \frac{3}{2})_1 - 7s , (\frac{3}{2}, \frac{3}{2})_2)</td>
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<td></td>
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<tr>
<td>972.051</td>
<td>?</td>
<td></td>
<td></td>
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<tr>
<td>972.957</td>
<td>?</td>
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</tr>
<tr>
<td>973.783</td>
<td>Si</td>
<td>(7p , ^3P_0 - 7s , ^3P_1)</td>
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### 974–982 cm\(^{-1}\)

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<th>R1E</th>
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</thead>
<tbody>
<tr>
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<tr>
<td>975.006</td>
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<td>R2F 34.5</td>
<td>0.6</td>
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<tr>
<td>975.165</td>
<td>OH</td>
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<td>975.660</td>
<td>OH</td>
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<td>975.868</td>
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<td>0.6</td>
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<td>976.899</td>
<td>Ca</td>
<td>(7s , ^3S_1 - 7p , ^3P_0)</td>
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<tr>
<td>977.236</td>
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<td>977.421</td>
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<td>978.132</td>
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<td>R2E 31.5</td>
<td>2.4</td>
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<tr>
<td>978.406</td>
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<tr>
<td>981.001</td>
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<td>(7s , ^3S_1 - 7p , ^3P_2)</td>
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### 982–990 cm⁻¹

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<tbody>
<tr>
<td>982.500</td>
<td>Mg</td>
<td>7d 3D₁,₂,₃ - 9f 3P₂,₃,₄</td>
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<td>983.956</td>
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<td></td>
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<tr>
<td>985.305</td>
<td>Si</td>
<td>6p ½ (½, ½)₁ - 5d 3P₂</td>
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</tr>
<tr>
<td>986.311</td>
<td>OH</td>
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<td>R2F 35.5</td>
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<td>986.459</td>
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<td>R1E 36.5</td>
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<td>986.905</td>
<td>OH</td>
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<td>R2E 35.5</td>
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<td>987.093</td>
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<td>R1F 36.5</td>
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<tr>
<td>988.572</td>
<td>Ca</td>
<td>4s 6s 3S₀ - 3d 4p 1P₁</td>
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<tr>
<td>989.785</td>
<td>Fe</td>
<td>5p 7D₀ - e 7F₆</td>
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### 990–998 cm⁻¹

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<tr>
<td>992.983</td>
<td>OH</td>
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<td>R2F 32.5</td>
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<tr>
<td>993.153</td>
<td>OH</td>
<td>(0-0)</td>
<td>R1E 33.5</td>
</tr>
<tr>
<td>993.835</td>
<td>OH</td>
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<td>R2E 32.5</td>
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<td>994.086</td>
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<td>R1F 33.5</td>
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<tr>
<td>996.483</td>
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<td>996.57</td>
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<tr>
<td>996.621</td>
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<td>997.011</td>
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<td>997.180</td>
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### 998–1006 cm⁻¹

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<tbody>
<tr>
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<td>Si</td>
<td>5d 1P₂ - 5f [2½],</td>
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<tr>
<td>1002.734</td>
<td>Fe</td>
<td>5p 1P₁ - 7D₄</td>
<td>0.2</td>
</tr>
<tr>
<td>1003.442</td>
<td>Si</td>
<td>5p 1D₀ - 4d 1P₁</td>
<td>0.3</td>
</tr>
<tr>
<td>1004.191</td>
<td>Si</td>
<td>5p 1D₂ - 5f [3½],</td>
<td>0.3</td>
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<tr>
<td>1005.502</td>
<td>OH</td>
<td>(1-1)</td>
<td>R2F 37.5</td>
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<td>1005.634</td>
<td>OH</td>
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<td>R1E 38.5</td>
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<td>1005.962</td>
<td>OH</td>
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<td>R2E 37.5</td>
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### 1006-1014 cm$^{-1}$

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<td>1007.61</td>
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<tr>
<td>1007.654</td>
<td>OH</td>
<td>(0-0)</td>
<td>R2F 33.5</td>
</tr>
<tr>
<td>1007.810</td>
<td>OH</td>
<td>(0-0)</td>
<td>R1E 34.5</td>
</tr>
<tr>
<td>1008.459</td>
<td>OH</td>
<td>(0-0)</td>
<td>R2E 33.5</td>
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<td>1008.687</td>
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<td>(0-0)</td>
<td>R1F 34.5</td>
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<tr>
<td>1011.792</td>
<td>?</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1013.352</td>
<td>OH</td>
<td>(1-1)</td>
<td>R2F 38.5</td>
</tr>
<tr>
<td>1013.472</td>
<td>OH</td>
<td>(1-1)</td>
<td>R1E 39.5</td>
</tr>
<tr>
<td>1013.734</td>
<td>OH</td>
<td>(1-1)</td>
<td>R2E 38.5</td>
</tr>
<tr>
<td>1013.866</td>
<td>OH</td>
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<td>R1F 39.5</td>
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### 1014-1022 cm$^{-1}$

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<tbody>
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<td>1020.001</td>
<td>OH</td>
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<td>R2F 39.5</td>
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<td>1020.118</td>
<td>OH</td>
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<td>R1E 40.5</td>
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<td>1020.307</td>
<td>OH</td>
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<td>R2E 39.5</td>
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<td>1020.422</td>
<td>OH</td>
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<td>R1F 40.5</td>
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<tr>
<td>1021.237</td>
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<td>(0-0)</td>
<td>R2F 34.5</td>
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<td>1021.381</td>
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<tr>
<td>1021.56</td>
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<td>1021.989</td>
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### 1022-1030 cm$^{-1}$

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<tr>
<td>1025.434</td>
<td>OH</td>
<td>(1-1)</td>
<td>R2F 40.5</td>
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<tr>
<td>1025.56</td>
<td>OH</td>
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<td>R1E 41.5</td>
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<td>1025.562</td>
<td>Fe</td>
<td>5$p^7_3^D_5 - f^7_3^D_4$</td>
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<tr>
<td>1025.653</td>
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<td>1025.751</td>
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<td>1026.008</td>
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<td>1027.49</td>
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<td>1028.127</td>
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<td>6$s^1^1S_0 - 6p^1^1P_0$</td>
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<tr>
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<td>1029.824</td>
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### 1030-1038 cm\(^{-1}\)

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<tr>
<td>1032.609</td>
<td>?</td>
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</tr>
<tr>
<td>1033.718</td>
<td>OH (0-0)</td>
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<tr>
<td>1033.852</td>
<td>OH (0-0)</td>
<td>R1E 36.5</td>
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<tr>
<td>1034.414</td>
<td>OH (0-0)</td>
<td>R2E 35.5</td>
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<td>1034.602</td>
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### 1038-1046 cm\(^{-1}\)

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<td>1039.580</td>
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<tr>
<td>1042.808</td>
<td>?</td>
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<tr>
<td>1044.864</td>
<td>?</td>
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<tr>
<td>1045.086</td>
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<td>1045.210</td>
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<td>1045.721</td>
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### 1046-1054 cm\(^{-1}\)

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<td>1050.526</td>
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<tr>
<td>1050.930</td>
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<td>0.2</td>
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<tr>
<td>1052.524</td>
<td>Fe 5p (^7D^o_4) (-\rightarrow) (^7P'_3)</td>
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### 1054-1062 cm\(^{-1}\)

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<td>1055.328</td>
<td>OH (0-0)</td>
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<td>1055.377</td>
<td>?</td>
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<tr>
<td>1055.444</td>
<td>OH (0-0)</td>
<td>R1E 38.5</td>
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<td>1055.897</td>
<td>OH (0-0)</td>
<td>R2E 37.5</td>
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<td>1056.052</td>
<td>OH (0-0)</td>
<td>R1F 38.5</td>
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<td>1056.06</td>
<td>Fe 5p (^7D^o_3) (-\rightarrow) (^7P'_2)</td>
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<td>1056.355</td>
<td>Ca 3d 4p (^1P^o_1) (-\rightarrow) 4s 6d (^1D^2)</td>
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<td>1056.556</td>
<td>Fe 5p (^7D^o_3) (-\rightarrow) (^7D_3)</td>
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<tr>
<td>1058.534</td>
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## 1062-1070 cm⁻¹

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<td>1064.431</td>
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<td>1064.931</td>
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<td>1069.900</td>
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## 1070-1078 cm⁻¹

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## 1078-1086 cm⁻¹

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<td>1079.51</td>
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## 1086-1094 cm⁻¹

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<td>1092.438</td>
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<td>R1E 44.5</td>
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<td>1092.438</td>
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### 1094-1102 cm\(^{-1}\)

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<tbody>
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<td>1094.105</td>
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<td>1094.285</td>
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<td>1094.326</td>
<td>OH(?)</td>
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<td>1094.375</td>
<td>OH(?)</td>
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<td>1095.281</td>
<td>Si</td>
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<td>1096.469</td>
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<td>1099.068</td>
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<td>1099.703</td>
<td>Na</td>
<td>3d (^2)D(<em>{5/2}) - 4p (^2)P(</em>{3/2})</td>
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<td>1099.750</td>
<td>Na</td>
<td>3d (^2)D(<em>{3/2}) - 4p (^2)P(</em>{3/2})</td>
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<tr>
<td>1100.096</td>
<td>Al</td>
<td>5d (^2)D(<em>{5/2}) - 6p (^2)P(</em>{3/2})</td>
<td>0.2</td>
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<td>1100.173</td>
<td>Si</td>
<td>4p (^3)S(_1) - 3d (^2)P(_2)</td>
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<td>1101.303</td>
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### 1102-1110 cm\(^{-1}\)

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<tbody>
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<td>1103.642</td>
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<td>6p ((1/2, 3/2)) (^3)S(_1) - 5d (^3)P(_0)</td>
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<td>1104.02</td>
<td>?</td>
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<tr>
<td>1106.771</td>
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<td>1107.185</td>
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<td>1107.727</td>
<td>Si</td>
<td>6s ((1/2, 1/2)) (^0) - 6p ((1, 1)) (^1)</td>
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<td>1108.712</td>
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<td>1109.748</td>
<td>Mg</td>
<td>7p (^1)P(_0) - 8d (^1)D(_2)</td>
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### 1110-1118 cm\(^{-1}\)

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<tbody>
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<td>1114.437</td>
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<td>0.2</td>
</tr>
<tr>
<td>1114.535</td>
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<tr>
<td>1115.609</td>
<td>?</td>
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<tr>
<td>1115.651</td>
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### 1118-1126 cm\(^{-1}\)

<table>
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<th>Element</th>
<th>Transition</th>
<th>Value (cm(^{-1}))</th>
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</thead>
<tbody>
<tr>
<td>1119.027</td>
<td>Si</td>
<td>6P(<em>{1/2}) ((1/2, 3/2)), 7s(</em>{1/2}) ((1/2, 3/2)) (^0)</td>
<td>0.7</td>
</tr>
<tr>
<td>1120.197</td>
<td>Si</td>
<td>6P(<em>{1/2}) ((1/2, 1/2)), 5d (^3)P(</em>{1/2})</td>
<td>0.1</td>
</tr>
<tr>
<td>1122.944</td>
<td>Fe</td>
<td>5p (^1)P(_0) - e (^7)P(_4)</td>
<td>0.4</td>
</tr>
<tr>
<td>1125.290</td>
<td>Mg</td>
<td>6s (^3)S(_1) - 6p (^3)P(_0)</td>
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<tr>
<td>1125.557</td>
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<tr>
<td>1125.932</td>
<td>Mg</td>
<td>6s (^3)S(_1) - 6p (^3)P(_1)</td>
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## 1126-1134 cm⁻¹

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<tbody>
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<td>1126.862</td>
<td>Mg</td>
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<td>1127.081</td>
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<td>1127.247</td>
<td>Mg</td>
<td>6s ³S₁ - 6p ³p°₂</td>
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<td>1127.43</td>
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## 1134-1142 cm⁻¹

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<td>1137.408</td>
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<td>1138.668</td>
<td>Fe</td>
<td>⁵D₂ - ⁵D₀</td>
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<td>1140.323</td>
<td>Fe</td>
<td>⁵D₀ - ⁷F₃</td>
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<td>1140.393</td>
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## 1142-1150 cm⁻¹

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<td>1144.345</td>
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<td>1145.13</td>
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<td>1145.535</td>
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<td>1146.289</td>
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### 1158-1166 cm⁻¹

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<tr>
<td>1160.198</td>
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<td>1160.284</td>
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<td>1160.52</td>
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<td>1160.586</td>
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### 1166-1174 cm⁻¹

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<tbody>
<tr>
<td>1166.743</td>
<td>Si</td>
<td>3p 4p ³S₁ - 3p 3d ³P⁰₁</td>
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<tr>
<td>1169.97</td>
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<td>7f 1.3P⁰ - 9g 1.3G</td>
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<tr>
<td>1171.360</td>
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<td>1171.40</td>
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<td>1172.147</td>
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<td>1172.371</td>
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<tr>
<td>1173.120</td>
<td>Si</td>
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### 1174-1182 cm⁻¹

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<td>1175.184</td>
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<td>1175.894</td>
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<tr>
<td>1176.347</td>
<td>Fe</td>
<td>5p ⁷P⁰₅ - e ⁷G₅</td>
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<td>1176.732</td>
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<td>4p ³P⁰₂ - 4d ³D₂</td>
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<tr>
<td>1177.503</td>
<td>Fe</td>
<td>w ⁵D⁰₄ - e ⁴D₄</td>
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<tr>
<td>1177.55</td>
<td>K(?)</td>
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<tr>
<td>1178.435</td>
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### 1182-1190 cm⁻¹

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<tbody>
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<td>1182.332</td>
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53
### 1190-1198 cm⁻¹

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<th>Transition</th>
<th>Intensity</th>
</tr>
</thead>
<tbody>
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<td>Al</td>
<td>6s²S½ - 6p²p²0/2</td>
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<tr>
<td>1190.892</td>
<td>Si</td>
<td>4f [2½]₃ - 5d³D₀ₐ</td>
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<td>1192.130</td>
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<td>1192.319</td>
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<td>1192.569</td>
<td>Ca</td>
<td>6d¹D₂ - 6f¹F₀</td>
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<tr>
<td>1192.97</td>
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<td>1193.355</td>
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<td>1193.429</td>
<td>Ca</td>
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<tr>
<td>1193.481</td>
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<td>6s²S₁/₂ - 6p²P₀³/₂</td>
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<td>1194.05</td>
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<tr>
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### 1198-1206 cm⁻¹

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<th>Intensity</th>
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<tbody>
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### 1206-1214 cm⁻¹

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<td>1209.677</td>
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### 1214-1222 cm⁻¹

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<tbody>
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<td>$6s \left( \frac{1}{2}, \frac{1}{2} \right)_1 - 6p \left( \frac{1}{2}, \frac{1}{2} \right)_2$</td>
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<tr>
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### 1254-1262 cm⁻¹

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### 1262-1270 cm⁻¹

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## 1326-1334 cm\(^{-1}\)

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- Values for 1613.038 and 1613.141 are unspecified.
- CO transition at 1613.273 cm⁻¹ is 0.5 with a source of P69.
- CO transition at 1613.328 cm⁻¹ is 0.1 with a source of P36.
- C13O16 transition at 1613.505 cm⁻¹ is 0.1 with a source of P96.
- CO transition at 1613.732 cm⁻¹ is 5.5 with a source of P81.
- C13O16 transition at 1613.79 cm⁻¹ is 0.2 with a source of P73.
- C13O16 transition at 1613.798 cm⁻¹ is 0.2 with a source of P81.
- Value for 1613.887 cm⁻¹ is unspecified.
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**Notes:**
- b indicates a blended line.
- bs indicates a blended system.

Refer to the table for detailed assignments and wavenumbers.
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bs 1

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**Notes:**
- CO refers to carbon monoxide.
- The values represent wave numbers in cm\(^{-1}\).
- The references (R62, P43, etc.) are to specific spectra or literature entries.
- The < symbol indicates a lower limit.
- The b symbol indicates a blended line.
- The "bs" symbol indicates a blended series.

**Legend:**
- **CO** indicates carbon monoxide.
- **C13016** indicates a specific isotope of carbon dioxide.
- **R62, P43, etc.** refer to specific references or values in the literature.
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Wavenumber range: 2142-2150 cm⁻¹

Key:
- CO: Carbon Monoxide
- ?: Uncertain or unknown

Wavenumbers in MHz:
- 16.8
- 9.6
- 9.4
- 4.5
- 3.8
- 2.3
- 1.6
- 0.8
- 0.3
- 0.2
- 0.1
- 0.01
- 0.001

Time in years:
- 22.4
- 10.7
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| 13.8       |         |            |
| 4          |         |            |
| 0.1        |         |            |
| 16.8       |         |            |
| 9          |         |            |
| 0.3        |         |            |
| 0.1        |         |            |
| 2.0        |         |            |
| 0.1        |         |            |
| 3.8        |         |            |
| 9.0        |         |            |
| 4.3        |         |            |
| 1          |         |            |
| 0.2        |         |            |
| 0.7        |         |            |
| 0.1        |         |            |
| 0.2        |         |            |
| 0.2        |         |            |
| 0.2        |         |            |
| 0.4        |         |            |
| 0.4        |         |            |
| 0.4        |         |            |
| 0.8        |         |            |
| 1          |         |            |
| 2.3        |         |            |
| 1          |         |            |
| 23.3       |         |            |
| 0.2        |         |            |
| 8          |         |            |
| 0.1        |         |            |
| 2.4        |         |            |
| 7.8        |         |            |

Broad
| Wavenumber (cm⁻¹) | OH, C 13016, CO, C 12018, C 13016 | P(E) 26.5 | 0.2  
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### 2390-2398 cm⁻¹

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### 2470-2478 cm⁻¹

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### 2614-2622 cm⁻¹

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### 2646-2654 cm\(^{-1}\)

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303
### 2774–2782 cm\(^{-1}\)

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| 2830.310 | Si | 4f [3\(\frac{1}{2}\)]\(_4\) - 5g [4\(\frac{1}{2}\)]' | 3.4 | 0.1 | 2.5 | 0.3 | \\hline
| 2830.459 | ? |  | 1.0 | 0.9 | 0.1 | 0.3 | \\hline
| 2830.510 | CH | (2-1) | R1F 10.5 | 2.1 | 0.9 | 0.2 | \\hline
| 2830.685 | CH | (2-1) | R2E 9.5 | 0.3 | 0.3 | 0.2 | \\hline
| 2830.996 | ? |  |  | 2.6 | 3.9 | \\hline
| 2831.073 | CH | (2-1) | R1E 10.5 | 0.5 | 0.5 | 0.5 | \\hline
| 2831.260 | CH | (2-1) | R2F 9.5 |  |  |  | \\hline
| 2831.85 | ? |  |  |  |  |  | \\hline
| 2831.893 | ? |  |  |  |  |  | \\hline
| 2832.330 | Si | 4f [3\(\frac{1}{2}\)]\(_5\) - 5g [4\(\frac{1}{2}\)]' | 2.5 | 0.1 |  |  | \\hline
| 2832.449 | ? |  | 2.6 | 0.2 |  |  | \\hline
| 2833.854 | ? |  |  |  |  |  | \\hline
| 2834.56 | ? |  |  |  |  |  | \\hline
| 2834.694 | ? |  | 3.9 |  |  |  | \\hline
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| 2835.220 | CH | (1-0) | R1E 3.5 | 0.5 |  |  | \\hline
| 2835.312 | ? |  | 1.4 | 0.1 |  |  | \\hline
| 2835.378 | ? |  | 1.2 |  |  |  | \\hline
| 2835.651 | ? |  | 0.1 |  |  |  | \\hline
| 2836.118 | CH | (1-0) | R2E 2.5 | 0.4 |  |  | \\hline
| 2836.225 | ? |  | 0.3 |  |  |  | \\hline
| 2836.387 | CH | (1-0) | R2F 2.5 | 0.4 |  |  | \\hline
| 2837.433 | OH | (1-0) | P1F 16.5 | 0.3 |  |  | \\hline
| 2837.66 | ? |  | 2.1 |  |  |  | \\hline
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### 2950-2958 cm⁻¹

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### 2958-2966 cm⁻¹

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### 2966-2974 cm\(^{-1}\)

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### 2974-2982 cm\(^{-1}\)

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321
### 2982–2990 cm\(^{-1}\)

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### 2990–2998 cm\(^{-1}\)

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### 3006–3014 cm⁻¹

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### 3062-3070 cm\(^{-1}\)

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### 3078-3086 cm\(^{-1}\)

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### 3086-3094 cm⁻¹

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### 3094-3102 cm⁻¹

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### 3110-3118 cm⁻¹

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### 3118-3126 cm⁻¹

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### 3126-3134 cm⁻¹

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### 3166-3174 cm\(^{-1}\)

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### 3174-3182 cm⁻¹

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### 3182-3190 cm⁻¹

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### 3198–3206 cm\(^{-1}\)

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### 3206-3214 cm⁻¹

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### 3214-3222 cm⁻¹

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### 3246-3254 cm⁻¹

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<td>3257.191</td>
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### 3262–3270 cm⁻¹

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### 3270-3278 cm⁻¹

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339
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<td>NH</td>
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<td>R2 6</td>
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### 3318–3326 cm⁻¹

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### 3326-3334 cm⁻¹

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### 3350–3358 cm⁻¹

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b: Unspectroscopic
### 3374–3382 cm\(^{-1}\)

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3470–3478 cm$^{-1}$

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**4190-4198 cm⁻¹**
### 4198-4206 cm⁻¹

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### 4318-4326 cm⁻¹

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### 4350-4358 cm\(^{-1}\)

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### 4358-4366 cm\(^{-1}\)

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### 4366-4374 cm\(^{-1}\)

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### 4374-4382 cm\(^{-1}\)

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443
### 4414-4422 cm⁻¹

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### 4422-4430 cm⁻¹

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### 4430-4438 cm⁻¹

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### 4438-4446 cm⁻¹

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### 4454-4462 cm⁻¹

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<td>4458.022</td>
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<td>4458.115</td>
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### 4486-4494 cm⁻¹

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### 4526-4534 cm⁻¹

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### 4534-4542 cm⁻¹

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<td>0.4</td>
</tr>
<tr>
<td>4549.803</td>
<td>?</td>
<td>?</td>
<td>0.3</td>
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### 4550-4558 cm\(^{-1}\)

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<tbody>
<tr>
<td>4551.852</td>
<td>Si</td>
<td>5p (^1)D(_2) - 6d (^3)P(_0)</td>
<td></td>
<td>1</td>
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<tr>
<td>4552.82</td>
<td>Si</td>
<td>5p (^3)P(_1) - 7s ((\frac{3}{2}, \frac{3}{2}))</td>
<td></td>
<td>0.7</td>
</tr>
<tr>
<td>4553.777</td>
<td>?</td>
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<td>0.4</td>
</tr>
<tr>
<td>4555.024</td>
<td>K(?)</td>
<td>4d (^2)D(<em>{5/2}) - 6f (^2)P(</em>{5/2})</td>
<td></td>
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</tr>
<tr>
<td>4555.506</td>
<td>?</td>
<td></td>
<td></td>
<td>1.3</td>
</tr>
<tr>
<td>4556.09</td>
<td>K(?)</td>
<td>4d (^2)D(<em>{5/2}) - 6f (^2)P(</em>{7/2})</td>
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<tr>
<td>4556.706</td>
<td>?</td>
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### 4558-4566 cm\(^{-1}\)

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<tr>
<td>4558.04</td>
<td>Cr</td>
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<tr>
<td>4559.755</td>
<td>Si</td>
<td>5d (^3)D(_3) - 7s ((\frac{1}{2}, \frac{3}{2}))</td>
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</tr>
<tr>
<td>4561.527</td>
<td>Fe</td>
<td>(\omega) (^5)P(_3) - f (^5)D(_2)</td>
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<td>2.0</td>
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<tr>
<td>4561.65</td>
<td>?</td>
<td></td>
<td></td>
<td>(bs) 0.3</td>
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<tr>
<td>4563.166</td>
<td>Cr</td>
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<td></td>
<td>0.3</td>
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<tr>
<td>4565.506</td>
<td>Ti</td>
<td>3d(^2)4s (^5)P(_2) - 3d(^2)4s(^4)p (^5)D(_0)</td>
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<td>3.5</td>
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<tr>
<td>4565.648</td>
<td>?</td>
<td></td>
<td></td>
<td>0.3</td>
</tr>
<tr>
<td>4565.87</td>
<td>Fe</td>
<td>(e) (^5)D(_4) - (w) (^3)P(_0)</td>
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<td>(bs) &lt;1</td>
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### 4566-4574 cm\(^{-1}\)

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<th>Value</th>
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</thead>
<tbody>
<tr>
<td>4566.017</td>
<td>Fe</td>
<td>5p (^7)P(_4) - g (^7)D(_4)</td>
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<tr>
<td>4566.563</td>
<td>Fe</td>
<td>(\omega) (^5)P(_0) - f (^5)D(_1)</td>
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<tr>
<td>4567.147</td>
<td>Fe</td>
<td>(\gamma) (^3)P(_2) - e (^3)D(_3)</td>
<td></td>
<td>0.8</td>
</tr>
<tr>
<td>4568.539</td>
<td>?</td>
<td></td>
<td></td>
<td>4.3</td>
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<tr>
<td>4568.96</td>
<td>Fe</td>
<td>(u) (^5)D(_2) - f (^5)F(_2)</td>
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<td>(bs) 1</td>
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<tr>
<td>4569.280</td>
<td>Si</td>
<td>3d (^3)D(_5) - 4f (^2)[(\frac{7}{2})]</td>
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<td>26</td>
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<tr>
<td>4569.593</td>
<td>?</td>
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<td>(s) 0.3</td>
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<tr>
<td>4569.647</td>
<td>?</td>
<td></td>
<td></td>
<td>(s) 0.3</td>
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<tr>
<td>4569.808</td>
<td>?</td>
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<td>(s) &lt;1</td>
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<tr>
<td>4570.357</td>
<td>Si</td>
<td>3d (^3)D(_5) - 4f (^2)[(\frac{7}{2})]</td>
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<td>11.2</td>
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<tr>
<td>4571.470</td>
<td>?</td>
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<td>4571.682</td>
<td>?</td>
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<tr>
<td>4572.511</td>
<td>Fe</td>
<td>(u) (^5)D(_4) - f (^5)F(_4)</td>
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<tr>
<td>4573.753</td>
<td>Fe</td>
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### 4574-4582 cm\(^{-1}\)

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<th>Energy (Å)</th>
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<tr>
<td>4575.122</td>
<td>Fe</td>
<td>b (^3\text{D}_3) - z (^3\text{P}^0_2)</td>
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<tr>
<td>4575.842</td>
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<tr>
<td>4576.26</td>
<td>?</td>
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<tr>
<td>4577.252</td>
<td>Fe</td>
<td>u (^5\text{D}^0_1) - f (^5\text{F}^1_1)</td>
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<tr>
<td>4577.925</td>
<td>Si</td>
<td>5p (^3\text{D}_2) - 7s ((\frac{1}{2}, \frac{1}{2})^0_1)</td>
<td>2.1</td>
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<tr>
<td>4578.987</td>
<td>Fe</td>
<td></td>
<td>2.8</td>
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<tr>
<td>4580.22</td>
<td>?</td>
<td></td>
<td>0.3</td>
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<tr>
<td>4581.090</td>
<td>?</td>
<td></td>
<td>0.3</td>
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<tr>
<td>4581.771</td>
<td>Si</td>
<td>3d (^3\text{D}^0_2) - 4f (^2[\frac{3}{2}]_1),</td>
<td>24.8</td>
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<td></td>
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<td>5s (^3\text{P}^0_2) - 4f (^2[\frac{3}{2}]_1),</td>
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### 4582-4590 cm\(^{-1}\)

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<tr>
<td>4582.169</td>
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<td>4582.418</td>
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<tr>
<td>4582.981</td>
<td>Fe</td>
<td>u (^5\text{D}^0_0) - f (^5\text{F}^1_1)</td>
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<tr>
<td>4584.742</td>
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<tr>
<td>4585.078</td>
<td>?</td>
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<td>0.6</td>
</tr>
<tr>
<td>4586.924</td>
<td>Fe</td>
<td>u (^5\text{D}^0_1) - f (^5\text{F}^1_1)</td>
<td>0.8</td>
</tr>
<tr>
<td>4587.777</td>
<td>?</td>
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<td>1.8</td>
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<tr>
<td>4587.987</td>
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<td></td>
<td>0.6</td>
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<tr>
<td>4588.23</td>
<td>?</td>
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<tr>
<td>4588.478</td>
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<tr>
<td>4589.492</td>
<td>Ti</td>
<td>3d(^2)4s (a) (^5\text{P}_3) - 3d(^2)4s4p (z) (^5\text{D}^0_4)</td>
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<tr>
<td>4589.930</td>
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<td>bs &lt;&lt; 1</td>
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### 4590-4598 cm\(^{-1}\)

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<tbody>
<tr>
<td>4590.181</td>
<td>Si</td>
<td>3d (^3\text{D}^0_1) - 4f (^2[\frac{3}{2}]_2)</td>
<td>27.5</td>
</tr>
<tr>
<td>4590.181</td>
<td>Fe</td>
<td>b (^3\text{D}_2) - z (^3\text{P}^0_2)</td>
<td>b</td>
</tr>
<tr>
<td>4590.990</td>
<td>Fe(?)</td>
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<tr>
<td>4591.159</td>
<td>?</td>
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<td>4592.339</td>
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<td>4593.023</td>
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<td>4594.48</td>
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<td>0.4</td>
</tr>
<tr>
<td>4594.99</td>
<td>Fe</td>
<td>5p (^3\text{D}^0_1) - g (^7\text{D}_1)</td>
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</tr>
<tr>
<td>4595.547</td>
<td>?</td>
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<td>1.7</td>
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<tr>
<td>4596.927</td>
<td>?</td>
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<tr>
<td>4597.428</td>
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### 4598-4606 cm⁻¹

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<th>Intensity</th>
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<tbody>
<tr>
<td>4599.529</td>
<td>Fe</td>
<td>5p 7D₃ → g 7D₂</td>
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<tr>
<td>4599.869</td>
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</tr>
<tr>
<td>4600.959</td>
<td>C</td>
<td>3d ³P₁ → 4f [2½]₂</td>
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<tr>
<td>4603.233</td>
<td>Fe</td>
<td>5p 7D₉ → g 7D₂</td>
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<tr>
<td>4605.090</td>
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<tr>
<td>4605.545</td>
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### 4606-4614 cm⁻¹

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<th>Intensity</th>
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<tbody>
<tr>
<td>4607.019</td>
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<tr>
<td>4608.740</td>
<td>?</td>
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<td>bs &lt;1</td>
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<tr>
<td>4608.793</td>
<td>C</td>
<td>3d ³P₂ → 4f [2½]₃</td>
<td>2.3</td>
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<tr>
<td>4609.701</td>
<td>?</td>
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<td>0.5</td>
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<tr>
<td>4611.377</td>
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<td>s 0.4</td>
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### 4614-4622 cm⁻¹

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</thead>
<tbody>
<tr>
<td>4614.076</td>
<td>Na(?)</td>
<td>4f ²P⁰₅/₂,₇/₂ → 7d ²D₃/₂,₅/₂</td>
<td>0.6</td>
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<tr>
<td>4616.56</td>
<td>H</td>
<td>(4-7) Very Broad</td>
<td>10⁺</td>
</tr>
<tr>
<td>4618.063</td>
<td>Fe</td>
<td>⁵G⁰₂ → ⁵F₃</td>
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### 4622-4630 cm⁻¹

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<tr>
<td>4623.727</td>
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<tr>
<td>4625.544</td>
<td>Si</td>
<td>5p ³D₃ → 7s (½, ½)₀</td>
<td>5</td>
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<tr>
<td>4629.569</td>
<td>?</td>
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<tr>
<td>4629.720</td>
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### 4630-4638 cm⁻¹

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</thead>
<tbody>
<tr>
<td>4634.318</td>
<td>Fe</td>
<td>5s e ³D₂ → 4s4p ν ³D₀₁</td>
<td>3.5</td>
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<tr>
<td>4634.800</td>
<td>Ni(?)</td>
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<td>1.7</td>
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<tr>
<td>4635.680</td>
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<tr>
<td>4636.763</td>
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### 4638-4646 cm\(^{-1}\)

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<td>4638.396</td>
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<tr>
<td>4638.81</td>
<td>?</td>
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<td>0.4</td>
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<tr>
<td>4640.87</td>
<td>?</td>
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<td>0.6</td>
</tr>
<tr>
<td>4641.378</td>
<td>?</td>
<td></td>
<td>1.0</td>
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<tr>
<td>4642.056</td>
<td>Mg</td>
<td>(4f , ^3P^0_{2,3,4} - 7d , ^3D_{1,2,3})</td>
<td>1.1</td>
</tr>
<tr>
<td>4643.92</td>
<td>Si</td>
<td>(5p , ^3D - 5d , ^3P^0)</td>
<td>0.7</td>
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<tr>
<td>4644.456</td>
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<td>4645.118</td>
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### 4646-4654 cm\(^{-1}\)

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<th>Value</th>
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<tbody>
<tr>
<td>4646.625</td>
<td>Fe</td>
<td>(z , ^5H_4 - e , ^5F_3)</td>
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<tr>
<td>4648.138</td>
<td>?</td>
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<tr>
<td>4651.476</td>
<td>?</td>
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<td>0.6</td>
</tr>
<tr>
<td>4652.132</td>
<td>?</td>
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<td>1.2</td>
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<tr>
<td>4652.283</td>
<td>?</td>
<td></td>
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</tr>
<tr>
<td>4652.531</td>
<td>Fe(?)</td>
<td>(y , ^3H_4 - e , ^3G_3)</td>
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<tr>
<td>4652.695</td>
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### 4654-4662 cm\(^{-1}\)

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<td>Fe</td>
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<tr>
<td>4656.521</td>
<td>?</td>
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<tr>
<td>4657.014</td>
<td>?</td>
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<td>0.4</td>
</tr>
<tr>
<td>4658.808</td>
<td>Mg</td>
<td>(5s , ^1S_0 - 6p , ^1P^0)</td>
<td>6.6</td>
</tr>
<tr>
<td>4658.81</td>
<td>Cr</td>
<td></td>
<td>b &lt;1</td>
</tr>
<tr>
<td>4660.228</td>
<td>Na(?)</td>
<td>(4d , ^2D_{3/2,5/2} - 7f , ^2P^0_{5/2,7/2})</td>
<td>bs 0.5</td>
</tr>
<tr>
<td>4660.355</td>
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### 4662-4670 cm\(^{-1}\)

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<th>Value</th>
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<tbody>
<tr>
<td>4662.40</td>
<td>Si</td>
<td>(4f , [4\frac{1}{2}]_4' - 7g , [5\frac{1}{2}]_4')</td>
<td>2</td>
</tr>
<tr>
<td>4663.84</td>
<td>?</td>
<td></td>
<td>0.5</td>
</tr>
<tr>
<td>4665.347</td>
<td>CaII</td>
<td>(4f , ^2P^0_{5/2} - 5d , ^2D_{3/2})</td>
<td>4</td>
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<tr>
<td>4665.584</td>
<td>Fe</td>
<td></td>
<td>3</td>
</tr>
<tr>
<td>4665.88</td>
<td>Si</td>
<td>(4f , [4\frac{1}{2}]_5' - 7g , [5\frac{1}{2}]_5')</td>
<td>2*</td>
</tr>
<tr>
<td>4667.17</td>
<td>?</td>
<td></td>
<td>0.5</td>
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</table>
### 4670-4678 cm⁻¹

<table>
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<tr>
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<th>Energy (cm⁻¹)</th>
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<tbody>
<tr>
<td>4672.171</td>
<td>?</td>
<td>?</td>
<td>0.6</td>
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<tr>
<td>4674.031</td>
<td>CaII</td>
<td>4f (^2)F(<em>{7/2}) - 5d (^2)D(</em>{5/2})</td>
<td>5.7</td>
</tr>
<tr>
<td>4674.571</td>
<td>?</td>
<td>bs</td>
<td>0.3</td>
</tr>
<tr>
<td>4674.641</td>
<td>Al(?)</td>
<td>5d (^2)D(<em>{5/2}) - 9f (^2)P(</em>{7/2})</td>
<td>2.9</td>
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<tr>
<td>4674.641</td>
<td>Fe(?)</td>
<td>b</td>
<td></td>
</tr>
<tr>
<td>4677.53</td>
<td>Si</td>
<td>4f ([2\frac{1}{2}])'(_2) - 7g ([3\frac{3}{2}])'</td>
<td>1.4</td>
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### 4678-4686 cm⁻¹

<table>
<thead>
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<th>Energy (cm⁻¹)</th>
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<tbody>
<tr>
<td>4678.436</td>
<td>Mg II</td>
<td>5s (^2)S(<em>{1/2}) - 5p (^2)P(</em>{3/2})</td>
<td>b 2.7</td>
</tr>
<tr>
<td>4678.436</td>
<td>Al(?)</td>
<td>5d (^2)D(<em>{3/2}) - 9f (^2)P(</em>{5/2})</td>
<td>b 2.7</td>
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<tr>
<td>4678.51</td>
<td>Si</td>
<td>4f ([2\frac{1}{2}])'(_3) - 7g ([3\frac{3}{2}])'</td>
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</tr>
<tr>
<td>4681.636</td>
<td>Si</td>
<td>4p (^1)D(_2) - 5s (^1)P(_1)</td>
<td>32</td>
</tr>
<tr>
<td>4682.06</td>
<td>?</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>4685.13</td>
<td>?</td>
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### 4686-4694 cm⁻¹

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<tr>
<td>4687.93</td>
<td>?</td>
<td>0.5</td>
</tr>
<tr>
<td>4691.66</td>
<td>?</td>
<td>0.7</td>
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### 4694-4702 cm⁻¹

<table>
<thead>
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<th>Energy (cm⁻¹)</th>
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<tbody>
<tr>
<td>4694.614</td>
<td>C</td>
<td>3d (^3)P(_1) - 4f ([2\frac{1}{2}])'(_2)</td>
<td>b 4.1</td>
</tr>
<tr>
<td>4694.67</td>
<td>Fe(?)</td>
<td>b</td>
<td></td>
</tr>
<tr>
<td>4695.393</td>
<td>?</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>4696.983</td>
<td>?</td>
<td>b 1.4</td>
<td></td>
</tr>
<tr>
<td>4697.013</td>
<td>Fe</td>
<td>c (^3)P(_1) - z (^5)P(_2)</td>
<td>b 1.4</td>
</tr>
<tr>
<td>4698.575</td>
<td>Fe</td>
<td>e (^5)P(_3) - 4s4f(\frac{3}{2}) ([3\frac{3}{2}])'</td>
<td>0.9</td>
</tr>
<tr>
<td>4701.139</td>
<td>Fe(?)</td>
<td>u (^5)D(_2) - e (^5)P(_3)</td>
<td>0.7</td>
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### 4702-4710 cm\(^{-1}\)

<table>
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<th>Value</th>
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<tbody>
<tr>
<td>4702.383</td>
<td>C</td>
<td>3d (^3P^0_2) - 4f ([2\frac{1}{2}]_2)'</td>
<td>10.6</td>
</tr>
<tr>
<td>4702.54</td>
<td>C</td>
<td>3d (^3P^0_2) - 4f ([2\frac{1}{2}]_2)'</td>
<td>bs &lt;1</td>
</tr>
<tr>
<td>4704.046</td>
<td>Fe</td>
<td>(\nu) (^3G^0) - e (^3H_4)</td>
<td>0.7</td>
</tr>
<tr>
<td>4704.83</td>
<td>Fe</td>
<td>4f (^1P^0_3) - 7g (^1G^0_4)</td>
<td>1.3</td>
</tr>
<tr>
<td>4705.307</td>
<td>Ca</td>
<td>(x) (^5D^0_3) - e (^5D^0_4)</td>
<td>1.0</td>
</tr>
<tr>
<td>4706.884</td>
<td>?</td>
<td>(x) (^5D^0_3) - e (^5D^0_4)</td>
<td>1.4</td>
</tr>
<tr>
<td>4707.156</td>
<td>Fe</td>
<td>(x) (^5D^0_3) - e (^5D^0_4)</td>
<td>13.3</td>
</tr>
<tr>
<td>4709.63</td>
<td>?</td>
<td>(x) (^5D^0_3) - e (^5D^0_4)</td>
<td>0.5</td>
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### 4710-4718 cm\(^{-1}\)

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</thead>
<tbody>
<tr>
<td>4710.011</td>
<td>Mg</td>
<td>5p (^3P^0_2) - 8s (^3S^1)</td>
<td>4.1</td>
</tr>
<tr>
<td>4710.30</td>
<td>?</td>
<td>(e) (^5P^0_2) - ((\frac{3}{2})) ([2\frac{1}{2}]_2)'</td>
<td>1.4</td>
</tr>
<tr>
<td>4712.06</td>
<td>Fe</td>
<td>(e) (^5P^0_2) - ((\frac{3}{2})) ([2\frac{1}{2}]_2)'</td>
<td>1.8</td>
</tr>
<tr>
<td>4712.666</td>
<td>Mg</td>
<td>5p (^3P^0_1) - 8s (^3S^1)</td>
<td>2.4</td>
</tr>
<tr>
<td>4713.13</td>
<td>C</td>
<td>3d (^3P^0_0) - 4f ([1\frac{1}{2}]_1)'</td>
<td>4.1</td>
</tr>
<tr>
<td>4713.875</td>
<td>Al</td>
<td>4f (^2P^0_{3/2,1/2}) - 7g (^2G^0_{1/2,3/2})</td>
<td>5</td>
</tr>
<tr>
<td>4713.905</td>
<td>Mg</td>
<td>5p (^3P^0_0) - 8s (^3S^1)</td>
<td>b 5</td>
</tr>
<tr>
<td>4714.71</td>
<td>Si</td>
<td>4f ([3\frac{1}{2}]_4) - 7g ([4\frac{1}{2}]_1)'</td>
<td>2.6</td>
</tr>
<tr>
<td>4714.99</td>
<td>Fe(?)</td>
<td>(u) (^5D^0_4) - f (^5P^0_3)</td>
<td>1</td>
</tr>
<tr>
<td>4715.578</td>
<td>Fe</td>
<td>(4f) ([3\frac{1}{2}]_3) - 7g ([4\frac{1}{2}]_1)'</td>
<td>1.5</td>
</tr>
<tr>
<td>4716.69</td>
<td>Fe</td>
<td>(4f) ([3\frac{1}{2}]_3) - 7g ([4\frac{1}{2}]_1)'</td>
<td>4.6</td>
</tr>
<tr>
<td>4717.52</td>
<td>C</td>
<td>3d (^3P^0_1) - 4f ([1\frac{1}{2}]_1)'</td>
<td>b 5</td>
</tr>
<tr>
<td>4717.64</td>
<td>C</td>
<td>3d (^3P^0_1) - 4f ([1\frac{1}{2}]_1)'</td>
<td>5</td>
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### 4718-4726 cm\(^{-1}\)

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<thead>
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<th>Wavenumber</th>
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<th>Transition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4720.556</td>
<td>Fe</td>
<td>(c) (^3P^0_2) - (2) (^5P^0_3)</td>
<td>2.0</td>
</tr>
<tr>
<td>4722.85</td>
<td>Fe</td>
<td>(c) (^3P^0_2) - (2) (^5P^0_3)</td>
<td>2.9</td>
</tr>
<tr>
<td>4723.760</td>
<td>Al</td>
<td>4p (^2P^0_{3/2}) - 5s (^3S^1_{1/2})</td>
<td>29.2</td>
</tr>
<tr>
<td>4724.147</td>
<td>Fe</td>
<td>(e) (^5P^0_2) - ((3)) ([1\frac{3}{2}]_1)'</td>
<td>2.5</td>
</tr>
<tr>
<td>4725.466</td>
<td>C</td>
<td>3d (^3P^0_2) - 4f ([1\frac{1}{2}]_1)'</td>
<td>1</td>
</tr>
<tr>
<td>4725.562</td>
<td>C</td>
<td>3d (^3P^0_2) - 4f ([1\frac{1}{2}]_1)'</td>
<td>2</td>
</tr>
<tr>
<td>4725.639</td>
<td>?</td>
<td>(3d) (^3P^0_2) - 4f ([1\frac{1}{2}]_1)'</td>
<td>0.9</td>
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### 4726-4734 cm\(^{-1}\)

<table>
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<th>Transition</th>
<th>Intensity</th>
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<tbody>
<tr>
<td>4726.995</td>
<td>?</td>
<td>?</td>
<td>0.7</td>
</tr>
<tr>
<td>4728.327</td>
<td>?</td>
<td>?</td>
<td>1.7</td>
</tr>
<tr>
<td>4729.147</td>
<td>?</td>
<td>?</td>
<td>1'</td>
</tr>
<tr>
<td>4729.69</td>
<td>?</td>
<td>?</td>
<td>1</td>
</tr>
<tr>
<td>4731.29</td>
<td>?</td>
<td>?</td>
<td>1.3</td>
</tr>
<tr>
<td>4732.41</td>
<td>Fe</td>
<td>(5^G^4 \rightarrow e^F_3)</td>
<td>2</td>
</tr>
<tr>
<td>4732.56</td>
<td>Fe</td>
<td>(5^G^4 \rightarrow e^F_3)</td>
<td>3</td>
</tr>
<tr>
<td>4732.687</td>
<td>Fe</td>
<td>(5^G^4 \rightarrow e^F_3)</td>
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### 4734-4742 cm\(^{-1}\)

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<th>Intensity</th>
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<tbody>
<tr>
<td>4736.895</td>
<td>?</td>
<td>(5^D^9 \rightarrow g^D_4)</td>
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<tr>
<td>4739.095</td>
<td>Fe</td>
<td>(5^D^9 \rightarrow g^D_4)</td>
<td>4</td>
</tr>
<tr>
<td>4739.603</td>
<td>Al</td>
<td>(4^P^9_{1/2} \rightarrow 5^S_{1/2})</td>
<td>25</td>
</tr>
<tr>
<td>4741.558</td>
<td>Cr(?)</td>
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### 4742-4750 cm\(^{-1}\)

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<tbody>
<tr>
<td>4742.297</td>
<td>?</td>
<td>(4f^3F_{2,3,4} \rightarrow 7g^3G_{3,4,5})</td>
<td>1.6</td>
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<tr>
<td>4745.090</td>
<td>?</td>
<td>(4f^3F_{2,3,4} \rightarrow 7g^3G_{3,4,5})</td>
<td>1.5</td>
</tr>
<tr>
<td>4746.80</td>
<td>Mg</td>
<td>(4f^3F_{2,3,4} \rightarrow 7g^3G_{3,4,5})</td>
<td>17</td>
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<tr>
<td>4747.108</td>
<td>Mg</td>
<td>(4f^3F_{2,3,4} \rightarrow 7g^3G_{3,4,5})</td>
<td>10</td>
</tr>
<tr>
<td>4747.86</td>
<td>Si</td>
<td>(4f^3F_{2,3,4} \rightarrow 7g^3G_{3,4,5})</td>
<td>2'</td>
</tr>
<tr>
<td>4749.91</td>
<td>Si</td>
<td>(4f^3F_{2,3,4} \rightarrow 7g^3G_{3,4,5})</td>
<td>2</td>
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### 4750-4758 cm\(^{-1}\)

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<tbody>
<tr>
<td>4752.38</td>
<td>Fe</td>
<td>(3p^1S_0 \rightarrow 3d^1P_1)</td>
<td>1</td>
</tr>
<tr>
<td>4755.36</td>
<td>C</td>
<td>(3p^1S_0 \rightarrow 3d^1P_1)</td>
<td>8'</td>
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### 4758-4766 cm\(^{-1}\)

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<tbody>
<tr>
<td>4758.27</td>
<td>?</td>
<td>(c^3P_1 \rightarrow y^3D_3)</td>
<td>1'</td>
</tr>
<tr>
<td>4762.64</td>
<td>Fe</td>
<td>(c^3P_1 \rightarrow y^3D_3)</td>
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### 4766-4774 cm⁻¹

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<tbody>
<tr>
<td>4766.64</td>
<td>Ca</td>
<td>4d (^3\text{D}_1) - 6p (^3\text{P}^0_0)</td>
<td>1</td>
</tr>
<tr>
<td>4766.84</td>
<td>Ca</td>
<td>4d (^3\text{D}_2) - 6p (^3\text{P}^0_0)</td>
<td>2</td>
</tr>
<tr>
<td>4768.52</td>
<td>Fe</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>4769.11</td>
<td>Fe</td>
<td></td>
<td>b</td>
</tr>
<tr>
<td>4769.11</td>
<td>Ca</td>
<td>4d (^3\text{D}_1) - 6p (^3\text{P}^0_2)</td>
<td>4</td>
</tr>
<tr>
<td>4770.52</td>
<td>Ca</td>
<td>4d (^3\text{D}_2) - 6p (^3\text{P}^0_1)</td>
<td>1</td>
</tr>
<tr>
<td>4772.41</td>
<td>Fe</td>
<td>5p (^5\text{D}^0_3) - (^7\text{D}_4)</td>
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### 4774-4782 cm⁻¹

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<th>Value</th>
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<tr>
<td>4774.72</td>
<td>Ca</td>
<td>4d (^3\text{D}^0_2) - 6p (^3\text{P}^0_2)</td>
<td>1</td>
</tr>
<tr>
<td>4777.41</td>
<td>Si</td>
<td>3d (^3\text{D}^0_3) - 4f (^2\text{[3\frac{1}{2}]}_3)</td>
<td>5</td>
</tr>
<tr>
<td>4779.46</td>
<td>Si</td>
<td>3d (^3\text{D}^0_3) - 4f (^2\text{[3\frac{1}{2}]}_4)</td>
<td>27</td>
</tr>
<tr>
<td>4779.46</td>
<td>Fe</td>
<td></td>
<td>b</td>
</tr>
<tr>
<td>4780.45</td>
<td>Fe</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>4781.39</td>
<td>Si</td>
<td>4d (^3\text{F}^0_3) - 7p ((\frac{1}{2}, \frac{3}{2})_2)</td>
<td>&lt;1</td>
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### 4782-4790 cm⁻¹

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<tr>
<td>4782.13</td>
<td>?</td>
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<td>2</td>
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<tr>
<td>4785.60</td>
<td>Si(?)</td>
<td>4p (^3\text{S}_1) - 3d (^3\text{P}^0_1)</td>
<td>8</td>
</tr>
<tr>
<td>4787.45</td>
<td>Fe</td>
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### 4790-4798 cm⁻¹

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<th>Value</th>
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<tbody>
<tr>
<td>4792.92</td>
<td>?</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>4794.69</td>
<td>?</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>4796.97</td>
<td>Fe</td>
<td>(e , 3\text{F}^0_3) - (^5\text{P}^0_4)</td>
<td>17</td>
</tr>
<tr>
<td>4797.10</td>
<td>Si(?)</td>
<td>5s (^3\text{P}^0_2) - 4f (^2\text{[2\frac{1}{2}]}_2)</td>
<td>bs 1</td>
</tr>
</tbody>
</table>

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A High-Resolution Atlas of the Infrared Spectrum of the Sun and the Earth Atmosphere from Space.
Vol. III. Key to Identification of Solar Features

Murray Geller

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California Institute of Technology
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Pasadena, California 91109-8099

National Aeronautics and Space Administration
Washington, D.C. 20546-0001

During the period April 29 to May 2, 1985, the Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment was operated as part of the Spacelab-3 payload of the shuttle Challenger. The principal purpose of this experiment was to study the distribution of the atmosphere's minor and trace molecular constituents. The instrument, a modified Michelson interferometer covering the frequency range from 600 to 5000 cm\(^{-1}\) at a spectral resolution of 0.01 cm\(^{-1}\), recorded infrared absorption spectra of the Sun and of the Earth's atmosphere at times close to entry into and exit from occultation by the Earth's limb. Spectra were obtained that are free from absorptions due to constituents of the atmosphere (i.e., they are "pure solar" spectra), as well as spectra of the atmosphere itself, covering line-of-sight tangent altitudes that span the range from the lower thermosphere to the bottom of the troposphere. Volume I gives the solar spectrum from 650 to 4800 cm\(^{-1}\), and Volume II covers the stratosphere and mesosphere for frequencies from 650 to 3350 cm\(^{-1}\). The present volume, Volume III, serves as a key to the identification of the nearly 16,000 solar features observed in Volume I.