New infrared spectra of CO₂ – Ne: fundamental for CO₂ –²²Ne isotopologue and symmetry breaking of the intramolecular CO₂ bend

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Abstract

The infrared spectrum of the weakly-bound CO₂-Ne complex is studied in the region of the carbon dioxide ν₃ fundamental vibration (≈2350 cm⁻¹), using a tunable OPO laser source to probe a pulsed supersonic slit jet expansion. For the fundamental CO₂ transition (ν₁, ν₂, ν₃) = (00₁0) ← (00₀0), both CO₂-²⁰Ne and CO₂-²²Ne are assigned and analyzed in combination with available microwave data to obtain the best currently available molecular parameters. For the hot band CO₂ transition, (01₁1) ← (01₁₀), detection of the weak CO₂-Ne spectrum reveals the symmetry breaking of the CO₂ ν₂ bending mode induced by the Ne atom, with the out-of-plane component determined to lie 0.057 cm⁻¹ higher in energy than the in-plane component.
1. Introduction

The simplicity of the CO$_2$-rare gas clusters makes them ideal as the probe of the angular anisotropy of the intermolecular potential and test cases for improved theoretical models with the goal of rigorous fully dimensional and fully coupled intra- and inter-molecular rovibrational calculation, which we hope is realized soon. This task becomes amenable after the development of full-dimensional potential energy surface, 5D in the case of CO$_2$-rare gases. Towards this end, we have made new infrared observations for CO$_2$-Ar,$^1$ CO$_2$-Xe,$^2$ and CO$_2$-Kr.$^3$ Here we report new IR observations for CO$_2$-Ne.

The first high-resolution spectroscopic results on the weakly-bound CO$_2$-Ne complex were reported in 1988 by Randall et al.$^4$ and by Fraser et al.$^5$ In the former paper, the infrared spectrum of the dimer was observed in the region of the $v_3$ fundamental band of CO$_2$ near 2350 cm$^{-1}$. In the latter paper, pure rotational microwave spectra were observed as well as infrared spectra in the CO$_2$ $v_1 + v_3$ (3710 cm$^{-1}$) and $2v_2 + v_3$ (3610 cm$^{-1}$) regions. Subsequently, there has been a more extensive microwave study$^6$ of CO$_2$-Ne involving a number of isotopologues, and a further infrared study$^7$ involving the $v_3$ band of $^{12}$C$^{18}$O$_2$ (2314 cm$^{-1}$). On the theoretical side, a couple of detailed potential energy surfaces have been reported for the CO$_2$-Ne interaction.$^8,^9$ The latter paper includes the dependence of the potential on the CO$_2$ $v_3$ (asymmetric stretch) vibration in order to better represent infrared spectra, and further results using this potential were reported in two follow-up papers.$^{10,11}$

The minimum energy structure of CO$_2$-Ne (and the other CO$_2$-Rg dimers) is T-shaped, having the Ne atom located “beside” the linear CO$_2$ molecule with an effective C to Ne distance of about 3.29 Å. As a result, the $a$-inertial axis connects C and Ne, the $b$-axis is parallel to the O-
C-O axis, and the $c$-axis is perpendicular to the CO$_2$-Ne plane. Nuclear spin statistics allow only even values of $K_a$ for the ground state of dimers containing $^{16}$O$_2$ (or $^{18}$O$_2$).

In the present paper, we reexamine the spectrum of CO$_2$-Ne in the CO$_2$ $\nu_3$ region. Coverage of the fundamental band of CO$_2$-Ne is extended, and CO$_2$-$^{22}$Ne is observed in natural abundance and analyzed. A weak spectrum of CO$_2$-Ne is also detected in the region of the CO$_2$ $(01^11) – (01^10)$ hot band near 2337 cm$^{-1}$. This provides a determination of the splitting of the degenerate CO$_2$ $\nu_2$ bending vibration into two modes (in-plane and out-of-plane) induced by the presence of the nearby Ne atom.
Fig. 1. Observed and simulated (T = 2 K) spectra of CO$_2$-Ne in the region of the CO$_2$ $v_3$ band.
Gaps in the observed spectrum correspond to regions of CO$_2$ monomer or CO$_2$-He absorption, and the simulation also shows CO$_2$ dimer, which becomes significant above about 2350 cm$^{-1}$. 
Table 1. Molecular parameters for the fundamental band of CO$_2$-Ne (in cm$^{-1}$)\textsuperscript{a}

|                | CO$_2$-$^{20}$Ne Ground State | CO$_2$-$^{20}$Ne Excited State | CO$_2$-$^{22}$Ne Ground State | CO$_2$-$^{22}$Ne Excited State |
|----------------|-------------------------------|--------------------------------|-------------------------------|--------------------------------|
| $\nu_0$        |                               | 2349.2796(1)                   |                               | 2349.2819(1)                   |
| $A$            | 0.402339 (19)                 | 0.399171(17)                   | 0.402061(12)                  | 0.398786(10)                   |
| $B$            | 0.11537499(75)               | 0.1151810(28)                  | 0.10831698(41)                | 0.1081390(24)                  |
| $C$            | 0.08772499(76)               | 0.0874331(18)                  | 0.08358319(42)                | 0.0833061(21)                  |
| $10^5 \times \Delta K$ | -6.39(14)                  | [-6.39]                        | -7.592 (81)                   | [-7.592]                       |
| $10^5 \times \Delta \epsilon K$ | 7.36430(78)                 | [7.36430]                      | 6.56697(38)                   | [6.56697]                      |
| $10^6 \times \Delta J$ | 4.5224(48)                  | [4.5224]                       | 4.0004(24)                    | [4.0004]                       |
| $10^5 \times \delta K$ | 5.2279(104)                 | [5.2279]                       | 4.6096(58)                    | [4.6096]                       |
| $10^6 \times \delta J$ | 1.0605(53)                  | [1.0605]                       | 0.8893(29)                    | [0.8893]                       |
| $10^{10} \times H_J$ | -10.0(17)                   | [-10.0]                        | -7.28(84)                     | [-7.28]                        |

\textsuperscript{a} Quantities in parentheses correspond to 1\sigma from the least-squares fit, in units of the last quoted digit. The ground and excited state centrifugal distortion parameters were constrained to be equal.
2. Results

Spectra were recorded as described previously.\textsuperscript{12-14} A pulsed supersonic slit jet expansion was probed by a rapid-scan optical parametric oscillator source. The gas expansion mixture contained about 0.04\% carbon dioxide plus 0.9\% neon in helium carrier gas with a jet backing pressure of about 13 atmospheres. Wavenumber calibration was carried out by simultaneously recording signals from a fixed etalon and a CO\textsubscript{2} reference gas cell. Simulation and fitting were carried out using PGOPHER software.\textsuperscript{15}

2.1. Fundamental band, CO\textsubscript{2} (00\textsuperscript{01}) $\leftrightarrow$ (00\textsuperscript{00})

The observed spectrum in the central part of the fundamental band is shown in Fig. 1. This is a perpendicular $b$-type band ($\Delta K_a = \pm 1$) with only $K_a =$ even levels in the ground state and $K_a =$ odd in the excited state. In Fig. 1 we see $K_a = 1 \leftrightarrow 0$ and $1 \leftrightarrow 2$ subbands with $Q$-branches at about 2349.6 and 2348.4 cm\textsuperscript{-1}, respectively. Further below and above the region shown in the figure, we also observed $K_a = 3 \leftrightarrow 4$ and $3 \leftrightarrow 2$ transitions. The natural abundance of $^{22}$Ne is about 9\%, and it was reasonably straightforward to assign some transitions of CO\textsubscript{2}-$^{22}$Ne in addition to those of the dominant CO\textsubscript{2}-$^{20}$Ne isotopologue. Ultimately we assigned 68 transitions of CO\textsubscript{2}-$^{20}$Ne, and 32 of CO\textsubscript{2}-$^{22}$Ne, which were analyzed to obtain the parameters listed in Table 1. The analyses also included 8 pure rotational microwave transitions for each isotopologue, taken from the paper by Xu and Jäger\textsuperscript{6} and weighted to reflect their higher precision. These microwave data essentially determined the ground state parameters except for $A$, to which they are not very sensitive. Excellent fits were obtained by constraining the ground and excited state centrifugal distortion parameters to be equal. The infrared root mean square errors were 0.00019 and 0.00010 cm\textsuperscript{-1}, for CO\textsubscript{2}-$^{20}$Ne and CO\textsubscript{2}-$^{22}$Ne, respectively, and the microwave rms errors were 1.2 and 0.1 kHz. Observed and calculated line positions are given as Supplementary Information.
The parameters for CO$_2$-$^{20}$Ne in Table 1 agree quite well with those of Randall et al., but they are more accurate thanks to the wider range of infrared data and the inclusion of microwave data. The parameters for CO$_2$-$^{22}$Ne are new, particularly those for the excited state. We see that the band origin of CO$_2$-$^{22}$Ne is slightly (0.002 cm$^{-1}$) higher than that of CO$_2$-$^{20}$Ne, so that the vibrational blue shift relative to the free CO$_2$ molecule increases from 0.1363 to 0.1386 cm$^{-1}$. This change can be explained by noting that the average intermolecular distance is slightly smaller for CO$_2$-$^{22}$Ne due to the anharmonicity of the van der Waals bond. This allows $^{22}$Ne to get slightly closer to CO$_2$ which induces a larger shift in the CO$_2$ vibration.

![Observed and simulated spectra of CO$_2$-Ne in the region of the CO$_2$ (01'1) $\leftrightarrow$ (01'0) hot band. Gaps in the observed spectrum correspond to regions of CO$_2$ monomer absorption. The simulated spectrum includes both the i-p and o-p modes, which are highly mixed by the Coriolis interaction.](image)

Fig. 2. Observed and simulated spectra of CO$_2$-Ne in the region of the CO$_2$ (01'1) $\leftrightarrow$ (01'0) hot band. Gaps in the observed spectrum correspond to regions of CO$_2$ monomer absorption. The simulated spectrum includes both the i-p and o-p modes, which are highly mixed by the Coriolis interaction.
2.2. Hot band, CO$_2$ (01$^1$1) $\leftrightarrow$ (01$^1$0)

Part of the observed spectrum in the region of the CO$_2$ (01$^1$1) – (01$^1$0) hot band is shown in Fig. 2. Observation of this weak spectrum is possible because a small fraction of CO$_2$ molecules remain “trapped” in the (01$^1$0) vibrational state following the supersonic jet expansion. The presence of the Ne atom breaks the symmetry of the doubly degenerate CO$_2$ v$_2$ bending mode into in-plane (i-p) and out-of-plane (o-p) components. As outlined previously for CO$_2$-Ar,$^1$ in the C$_{2v}$ point group these i-p and o-p modes have A$_1$ and B$_1$ symmetry, respectively, for the lower (01$^1$0) vibrational state, and B$_2$ and A$_2$ symmetry for the upper (01$^1$1) state. The hot band spectrum has $b$-type selection rules, the same as the fundamental. The i-p component is $B_2 \leftrightarrow A_1$ with $K_a =$ odd $\leftrightarrow$ even, and the o-p component is $A_2 \leftrightarrow B_1$ with $K_a =$ even $\leftrightarrow$ odd. There is strong $b$-type Coriolis mixing between the i-p and o-p modes, characterized by the matrix element

$$\langle \text{i-p, } J, k|H|\text{o-p, } J, k \pm 1 \rangle = \frac{1}{2} \zeta_b \times [J(J+1) - k(k \pm 1)]^{1/2},$$

where $k$ is signed $K_a$ and $\zeta_b$ is the Coriolis parameter, related to the usual dimensionless zeta parameter and the $B$ rotational constant by $\zeta_b = 2B \zeta$. In the present case, we expect $\zeta_b \approx 1$, as was found for CO$_2$-Ar.$^1$
Table 2. Molecular parameters for the (01\(^1\)1) ← (01\(^1\)0) hot band of CO\(_2\) – Ne (in cm\(^{-1}\)).\(^a\)

|                  | (01\(^1\)0) i-p | (01\(^1\)0) o-p | (01\(^1\)1) i-p | (01\(^1\)1) o-p |
|------------------|-----------------|-----------------|-----------------|-----------------|
| \(\sigma_0\)     | \(X^b\)         | \(0.05659(42)+X\) | 2336.7749(3)+X  | 2336.8240(5)+X  |
| \(A\)            | 0.401628(100)   | 0.400808(106)   | 0.398302(77)    | 0.397531(104)   |
| \(B\)            | 0.115030(33)    | 0.115500(51)    | 0.114550(39)    | 0.115332(28)    |
| \(C\)            | 0.088046(38)    | 0.087962(26)    | 0.087695(34)    | 0.088011(40)    |
| \(10^5 \Delta K\) | [-6.39]         | [-6.39]         | [-6.39]         | [-6.39]         |
| \(10^5 \Delta J_K\) | 5.29(40)       | 7.29(62)        | [5.29]          | [7.29]          |
| \(10^6 \Delta I\) | 5.80(44)        | 4.36(41)        | [5.80]          | [4.36]          |
| \(10^5 \delta K\) | [4.5224]        | [4.5224]        | [4.5224]        | [4.5224]        |
| \(10^6 \delta J\) | [5.2279]        | [5.2279]        | [5.2279]        | [5.2279]        |
| \(\xi_0\)        | 0.235640(60)    |                  | 0.235307(55)    |                  |

\(^a\) Quantities in parentheses correspond to 1\(\sigma\) from the least-squares fit, in units of the last quoted digit. The ground and excited state centrifugal distortion parameters \(\Delta K\) and \(\Delta J\) were constrained to be equal as indicated. Other centrifugal distortion parameters were fixed at ground state values (Table 1).

\(^b\) \(X\) is equal to the free CO\(_2\) \(v_2\) frequency (667.380 cm\(^{-1}\)) plus or minus a (small) unknown vibrational shift.
The strongest feature in the hot band spectrum is a partly resolved $Q$-branch around 2336.78 cm$^{-1}$ (Fig. 2), which is accompanied by a weaker and more widely spaced $Q$-branch about 0.05 cm$^{-1}$ lower in wavenumber. The proximity of these $Q$-branches is a clue that the splitting between the i-p and o-p modes is quite small. Once we established the correct splitting by trial and error, it was possible to get a good simulation of the spectrum using PGOPHER. We assigned a total of 112 transitions of CO$_2$-$^{20}$Ne in the band and fitted them with an rms error of 0.00048 cm$^{-1}$ to obtain the parameters listed in Table 2. It was also possible to assign 26 transitions of CO$_2$-$^{22}$Ne, but these were not sufficient to obtain any really new information. Basically the CO$_2$-$^{22}$Ne spectrum could be very well reproduced by simply scaling the rotational constants from $^{20}$Ne to $^{22}$Ne using the fundamental band ratios (Table 1) and by assuming the same small change in the vibrational shift as for the fundamental. Line positions for both isotopologues are given as Supplementary Information.

The i-p to o-p splitting was determined to be 0.057 cm$^{-1}$ in the lower state, (01$^1$0), and 0.049 cm$^{-1}$ in the upper state, (01$^1$1), with o-p lying above i-p. These compare to previously reported splittings of 0.877 cm$^{-1}$ for CO$_2$-Ar, $^{1}$ 2.140 cm$^{-1}$ for CO$_2$-Xe, $^{2}$ and 2.307 cm$^{-1}$ for CO$_2$-N$_2$. $^{16}$ The values of $\xi_b$ in Table 2 correspond to $\xi_b \approx 1.02$, depending slightly on what value is used for $B$, similar to what was observed for CO$_2$-Ar, -Xe, and -N$_2$. In the present case, the i-p to o-p splitting for CO$_2$-Ne is very small compared to the $K_a$ rotational level spacing, so Coriolis mixing is virtually complete. Complete mixing means that the quantum labels i-p or o-p, $K_a$, and $K_c$, are not very meaningful. For example, the transitions in the strong $Q$-branch at 2336.78 cm$^{-1}$ are best labeled as $K_a = 0$ (o-p) $\leftrightarrow$ 0 (i-p), even though such transitions would be forbidden in the absence of Coriolis mixing. Similarly, the weaker $Q$-branch is nominally $K_a = 1$ (i-p) $\leftrightarrow$ 1 (o-p).
The CO$_2$-Ne band origins from Table 2 represent vibrational shifts of +0.142 and +0.134 cm$^{-1}$ for the i-p and o-p modes, respectively, relative to the (01$^1$1) ← (01$^1$0) hot band origin of the free CO$_2$ molecule, which is 2336.633 cm$^{-1}$. These are very similar to the blue shift of +0.136 cm$^{-1}$ as determined above for the fundamental band. Although the hot band spectrum reveals the i-p to o-p splitting, it does not yield the actual CO$_2$ v$_2$ bending frequency for CO$_2$-Ne. This frequency is represented by X in Table 2, and it will probably be quite close (< 0.5 cm$^{-1}$?) to the free CO$_2$ value of 667.38 cm$^{-1}$. Our predicted CO$_2$-Ne spectrum in the CO$_2$ v$_2$ region for a temperature of 2 K is shown in Fig. 3. Here the i-p and o-p modes, which have a- and c-type selection rules, are shown separately. But, as mentioned above, they are highly mixed so these labels are only approximate. The strongest features in the predicted spectrum are Q-branches with $K_a = 0$ (i-p) ← 0 and $K_a = 1$ (o-p) ← 0 (the former would of course be forbidden in the absence of Coriolis mixing).

The observed CO$_2$ bending mode splittings in CO$_2$-Rg complexes are compared in Fig. 4 by plotting them as a function of Rg atomic polarizability, as is commonly done for vibrational shifts. There is an almost perfect linear relationship for Ne, Ar, and Kr, while the splitting observed for CO$_2$-Xe is a bit smaller than expected on the basis of linear extrapolation. A vertical line indicates the polarizability of He, and we see that extrapolation of the Ne-Ar-Kr line suggests that for CO$_2$-He we might expect a negative splitting (that is, with the o-p mode below the i-p mode). Unfortunately, we have so far been unable to detect the CO$_2$-He spectrum in the hot band region.
Fig. 3. Predicted spectrum of CO$_2$-Ne in the region of the CO$_2$ v$_2$ fundamental band for a temperature of 2K. Here it is assumed that the unknown vibrational shift relative to the free CO$_2$ molecule is zero. So the actual spectrum, not yet observed, will be shifted up or down from this simulation (probably by less than 0.5 cm$^{-1}$).
Fig. 4. In-plane / out-of-plane mode splittings for CO₂-Rg complexes in the v₂ bending state of CO₂ as a function of atomic polarizability. Splitting values: Ne (present work), Ar¹, Kr³ (to be published), and Xe.² Note the almost perfect linear relationship for Ne-Ar-Kr. The polarizability of He is indicated by the vertical red line, and extrapolation (in red) suggests that the splitting for CO₂-He (not yet determined) might be negative (i-p above o-p).
3. Conclusions

In conclusion, the infrared spectrum of the weakly-bound complex CO$_2$-Ne has been studied in the region of the CO$_2$ v$_3$ asymmetric stretch, using a tunable optical parametric oscillator source to probe a pulsed slit jet supersonic expansion. The fundamental band has been assigned for both CO$_2$-$^{20}$Ne and CO$_2$-$^{22}$Ne and fitted including available microwave data. The resulting molecular parameters (Table 1) should be the best currently available. In addition, the relatively weak hot band corresponding to the CO$_2$ (01$^1$1) – (01$^1$0) transition has been detected for CO$_2$-Ne. Its analysis yields a measurement of the symmetry breaking of the degenerate CO$_2$ v$_2$ bend into in-plane and out-of-plane components, which turns out to have a magnitude of about 0.057 cm$^{-1}$ in the (01$^1$0) state, with o-p above i-p. This splitting is a sensitive probe of vibrational dynamics, and we have now published determinations for CO$_2$ with Ne, Ar and Xe.$^{1,2}$ In this context, CO$_2$-He$^{18,19}$ would be especially interesting: could the ordering of the i-p and o-p modes be reversed, as suggested by Fig. 4?

Supplementary Information

Supplementary Information includes tables giving observed and fitted line positions for CO$_2$-Ne.

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Appendix to:

New infrared spectra of CO2-Ne:

Fundamental for CO2-22Ne isotopologue, intermolecular bend, and symmetry breaking of the intramolecular CO2 bend

Table A-1. Observed transitions of the fundamental band of CO2-20Ne (units of 1/cm)

| J' Ka' Kc' | J" Ka" Kc" | Observed    | Calc       | Obs-Calc | Obs-Calc |
|------------|------------|-------------|------------|----------|----------|
| 8 3 6      | 9 4 5      | 2345.3551   | 2345.3549  | 0.0003   |
| 8 3 5      | 9 4 6      | 2345.3919   | 2345.3914  | 0.0004   |
| 7 3 5      | 8 4 4      | 2345.5514   | 2345.5516  | -0.0002  |
| 7 3 4      | 8 4 5      | 2345.5684   | 2345.5684  | 0.0001   |
| 6 3 4      | 7 4 3      | 2345.7472   | 2345.7473  | -0.0001  |
| 6 3 3      | 7 4 4      | 2345.7540   | 2345.7540  | -0.0000  |
| 4 3 1      | 5 4 2      | 2346.1399   | 2346.1406  | -0.0007  |
| 4 3 2      | 5 4 1      | 2346.1399   | 2346.1400  | -0.0002  |
|            | Blend      | 2346.1403   | -0.0004    |          |
| 3 3 0      | 4 4 1      | 2346.3382   | 2346.3379  | 0.0002   |
| 3 3 1      | 4 4 0      | 2346.3382   | 2346.3379  | 0.0003   |
|            | Blend      | 2346.3379   | 0.0003     |          |
| 6 1 6      | 7 2 5      | 2346.4741   | 2346.4741  | -0.0000  |
| 5 1 5      | 6 2 4      | 2346.8384   | 2346.8385  | -0.0001  |
| 7 1 6      | 8 2 7      | 2347.1294   | 2347.1295  | -0.0000  |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 3 | 1 |   |   |   | 4 | 4 | 0 | 2347.1454 | 2347.1456 | -0.0002 |
| 4 | 3 | 2 |   |   |   | 4 | 4 | 1 | 2347.1454 | 2347.1451 | 0.0004 |
|   |   |   |   |   |   | Blend | 2347.1453 | 0.0001 |
| 6 | 3 | 4 |   |   |   | 6 | 4 | 3 | 2347.1555 | 2347.1556 | -0.0002 |
| 6 | 1 | 5 |   |   |   | 7 | 2 | 6 | 2347.2430 | 2347.2429 | 0.0001 |
| 5 | 1 | 4 |   |   |   | 6 | 2 | 5 | 2347.3657 | 2347.3656 | 0.0001 |
| 3 | 1 | 3 |   |   |   | 4 | 2 | 2 | 2347.4549 | 2347.4549 | 0.0000 |
| 4 | 1 | 3 |   |   |   | 5 | 2 | 4 | 2347.4999 | 2347.4998 | 0.0001 |
| 8 | 1 | 8 |   |   |   | 9 | 0 | 9 | 2347.6324 | 2347.6326 | -0.0002 |
| 3 | 1 | 2 |   |   |   | 4 | 2 | 3 | 2347.6467 | 2347.6468 | -0.0001 |
| 2 | 1 | 2 |   |   |   | 3 | 2 | 1 | 2347.7157 | 2347.7158 | -0.0001 |
| 2 | 1 | 1 |   |   |   | 3 | 2 | 2 | 2347.8075 | 2347.8075 | 0.0000 |
| 7 | 1 | 7 |   |   |   | 8 | 0 | 8 | 2347.8316 | 2347.8316 | 0.0000 |
| 1 | 1 | 1 |   |   |   | 2 | 2 | 0 | 2347.9529 | 2347.9529 | 0.0000 |
| 1 | 1 | 0 |   |   |   | 2 | 2 | 1 | 2347.9823 | 2347.9823 | 0.0000 |
| 5 | 1 | 6 |   |   |   | 7 | 0 | 7 | 2348.0388 | 2348.0386 | 0.0002 |
| 6 | 1 | 6 |   |   |   | 6 | 2 | 5 | 2348.0736 | 2348.0735 | 0.0001 |
| 5 | 1 | 5 |   |   |   | 5 | 2 | 4 | 2348.1604 | 2348.1604 | 0.0000 |
| 4 | 1 | 4 |   |   |   | 4 | 2 | 3 | 2348.2326 | 2348.2324 | 0.0001 |
| 5 | 1 | 5 |   |   |   | 6 | 0 | 6 | 2348.2544 | 2348.2543 | 0.0001 |
| 3 | 1 | 3 |   |   |   | 3 | 2 | 2 | 2348.2895 | 2348.2896 | -0.0001 |
| 2 | 1 | 2 |   |   |   | 2 | 2 | 1 | 2348.3319 | 2348.3320 | -0.0002 |
| 2 | 1 | 1 |   |   |   | 2 | 2 | 0 | 2348.4126 | 2348.4127 | -0.0001 |
| 3 | 1 | 2 |   |   |   | 3 | 2 | 1 | 2348.4451 | 2348.4453 | -0.0002 |
|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| 4 | 1 | 4 | 5 | 0 | 5 | 2348.4784 | 2348.4777 | 0.0007 |
| 4 | 1 | 3 | 4 | 2 | 2 | 2348.4784 | 2348.4794 | -0.0010 |
|   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |
| Blend |   |   |   |   |   | 2348.4784 | -0.0001 |
| 5 | 1 | 4 | 5 | 2 | 3 | 2348.5079 | 2348.5080 | -0.0001 |
| 7 | 1 | 6 | 7 | 2 | 5 | 2348.5201 | 2348.5202 | -0.0000 |
| 6 | 1 | 5 | 6 | 2 | 4 | 2348.5237 | 2348.5237 | -0.0001 |
| 3 | 1 | 3 | 4 | 0 | 4 | 2348.7060 | 2348.7059 | 0.0001 |
| 3 | 1 | 3 | 2 | 2 | 0 | 2348.8947 | 2348.8948 | -0.0001 |
| 2 | 1 | 2 | 3 | 0 | 3 | 2348.9347 | 2348.9346 | 0.0001 |
| 3 | 1 | 2 | 2 | 2 | 1 | 2349.0613 | 2349.0615 | -0.0002 |
| 5 | 1 | 5 | 4 | 2 | 2 | 2349.1400 | 2349.1400 | 0.0000 |
| 1 | 1 | 1 | 2 | 0 | 2 | 2349.1589 | 2349.1589 | 0.0000 |
| 6 | 1 | 6 | 5 | 2 | 3 | 2349.2157 | 2349.2158 | -0.0002 |
| 4 | 1 | 3 | 3 | 2 | 2 | 2349.3141 | 2349.3141 | 0.0000 |
| 1 | 1 | 0 | 1 | 0 | 1 | 2349.5907 | 2349.5906 | 0.0001 |
| 2 | 1 | 1 | 2 | 0 | 2 | 2349.6188 | 2349.6187 | 0.0001 |
| 3 | 1 | 2 | 3 | 0 | 3 | 2349.6642 | 2349.6641 | 0.0001 |
| 4 | 1 | 3 | 4 | 0 | 4 | 2349.7306 | 2349.7304 | 0.0002 |
| 1 | 1 | 1 | 0 | 0 | 0 | 2349.7662 | 2349.7662 | -0.0000 |
| 5 | 1 | 4 | 5 | 0 | 5 | 2349.8217 | 2349.8214 | 0.0003 |
| 6 | 1 | 5 | 5 | 2 | 4 | 2349.8458 | 2349.8456 | 0.0001 |
| 2 | 1 | 2 | 1 | 0 | 1 | 2349.9403 | 2349.9403 | -0.0000 |
| 3 | 1 | 3 | 2 | 0 | 2 | 2350.1008 | 2350.1007 | 0.0001 |
| 4 | 1 | 4 | 3 | 0 | 3 | 2350.2499 | 2350.2497 | 0.0002 |
5 1 5 4 0 4 2350.3910 2350.3911 -0.0001
6 1 6 5 0 5 2350.5293 2350.5293 0.0001
6 3 3 6 2 4 2350.6547 2350.6548 -0.0001
7 1 7 6 0 6 2350.6684 2350.6684 -0.0000
5 3 2 5 2 3 2350.6987 2350.6987 -0.0000
4 3 1 4 2 2 2350.7284 2350.7285 -0.0001
3 3 0 3 2 1 2350.7464 2350.7464 0.0000
8 1 8 7 0 7 2350.8114 2350.8113 0.0001
9 1 9 8 0 8 2350.9591 2350.9590 0.0001
3 3 0 2 2 1 2351.3615 2351.3626 -0.0010
3 3 1 2 2 0 2351.3615 2351.3606 0.0009

Blend 2351.3616 -0.0001
4 3 2 3 2 1 2351.5535 2351.5535 0.0000
4 3 1 3 2 2 2351.5631 2351.5632 -0.0001
5 3 3 4 2 2 2351.7378 2351.7377 0.0002
5 3 2 4 2 3 2351.7669 2351.7669 0.0001
6 3 4 5 2 3 2351.9088 2351.9088 -0.0000
6 3 3 5 2 4 2351.9766 2351.9767 -0.0001
7 3 4 6 2 5 2352.1968 2352.1967 0.0001
8 3 6 7 2 5 2352.1968 2352.1981 -0.0013

Blend 2352.1971 -0.0002
8 3 5 7 2 6 2352.4317 2352.4322 -0.0005
5 5 0 4 4 1 2352.9136 2352.9134 0.0002
5 5 1 4 4 0 2352.9136 2352.9134 0.0002
Blend 2352.9134 0.0002

6 5 1 5 4 2 2353.1009 2353.1014 -0.0004
6 5 2 5 4 1 2353.1009 2353.1014 -0.0004

Blend 2353.1014 -0.0004

6 3 4 5 0 5 2353.2226 2353.2223 0.0004
7 5 2 6 4 3 2353.2870 2353.2866 0.0005
7 5 3 6 4 2 2353.2870 2353.2865 0.0006

Blend 2353.2865 0.0005

7 3 5 6 0 6 2353.4784 2353.4788 -0.0004

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Table A-2. Observed transitions in the microwave spectrum of CO2-20Ne

MW data from: Y. Xu and W. Jäger, J. Mol. Spectrosc. 192, 435-440 (1998).

| J' Ka' Kc' | J" Ka" Kc" | Obs(MHz) | Calc(MHz) | Obs-Calc(MHz) |
|------------|------------|----------|-----------|---------------|
| 1 0 1      | 0 0 0      | 6088.2440| 6088.2413 | 0.0027        |
| 2 0 2      | 1 0 1      | 12117.9430| 12117.9444| -0.0014       |
| 3 0 3      | 2 0 2      | 18032.3303| 18032.3309| -0.0006       |
| 4 0 4      | 3 0 3      | 23782.8865| 23782.8861| 0.0004        |
| 3 2 2      | 2 2 1      | 18198.6807| 18198.6791| 0.0016        |
| 3 2 1      | 2 2 0      | 18418.0132| 18418.0146| -0.0014       |
| 4 2 3      | 3 2 2      | 24211.8532| 24211.8539| -0.0007       |
| 4 2 2      | 3 2 1      | 24749.1378| 24749.1372| 0.0006        |
Table A-3. Observed transitions of the fundamental band of CO2-22Ne (units of 1/cm)

| J' Ka' Kc' | J" Ka" Kc" | Observed | Calc | Obs-Calc | Obs-Calc |
|------------|------------|----------|------|----------|----------|
| 4 3 1      | 5 4 2      | 2346.1594 | 2346.1598 | -0.0003 |
| 4 3 2      | 5 4 1      | 2346.1594 | 2346.1594 | 0.0000   |
| Blend      |            | 2346.1596 | -0.0002   |
| 3 3 0      | 4 4 1      | 2346.3469 | 2346.3466 | 0.0003   |
| 3 3 1      | 4 4 0      | 2346.3469 | 2346.3465 | 0.0003   |
| Blend      |            | 2346.3466 | 0.0003    |
| 4 1 4      | 5 2 3      | 2347.2324 | 2347.2325 | -0.0001 |
| 6 1 5      | 7 2 6      | 2347.2772 | 2347.2771 | 0.0001   |
| 5 1 4      | 6 2 5      | 2347.3967 | 2347.3966 | 0.0001   |
| 4 1 3      | 5 2 4      | 2347.5269 | 2347.5267 | 0.0002   |
| 3 1 2      | 4 2 3      | 2347.6684 | 2347.6684 | -0.0001 |
| 2 1 2      | 3 2 1      | 2347.7413 | 2347.7414 | -0.0001 |
| 2 1 1      | 3 2 2      | 2347.8225 | 2347.8225 | 0.0000   |
| 1 1 1      | 2 2 0      | 2347.9630 | 2347.9630 | 0.0000   |
| 1 1 0      | 2 2 1      | 2347.9891 | 2347.9891 | 0.0000   |
| 6 1 6      | 6 2 5      | 2348.0915 | 2348.0915 | 0.0000   |
| 6 1 6      | 7 0 7      | 2348.1212 | 2348.1212 | 0.0000   |
| 5 1 5      | 5 2 4      | 2348.1689 | 2348.1691 | -0.0002 |
| 2 1 2      | 2 2 1      | 2348.3221 | 2348.3223 | -0.0001 |
| 2 1 1      | 2 2 0      | 2348.3948 | 2348.3947 | 0.0001   |
|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 2 | 3 | 2 | 1 | 2348.4245 | 2348.4247 | -0.0002 |
| 4 | 1 | 3 | 4 | 2 | 2 | 2348.4573 | 2348.4573 | -0.0000 |
| 5 | 1 | 4 | 5 | 2 | 3 | 2348.4866 | 2348.4868 | -0.0002 |
| 4 | 1 | 4 | 5 | 0 | 5 | 2348.541 | 2348.5441 | -0.0000 |
| 3 | 1 | 3 | 4 | 0 | 4 | 2348.7617 | 2348.7616 | 0.0001 |
| 2 | 1 | 2 | 3 | 0 | 3 | 2348.9783 | 2348.9782 | 0.0000 |
| 1 | 1 | 1 | 2 | 0 | 2 | 2349.1899 | 2349.1899 | 0.0000 |
| 1 | 1 | 0 | 1 | 0 | 1 | 2349.5968 | 2349.5967 | 0.0000 |
| 4 | 1 | 3 | 4 | 0 | 4 | 2349.7195 | 2349.7195 | 0.0001 |
| 5 | 1 | 4 | 5 | 0 | 5 | 2349.7986 | 2349.7984 | 0.0001 |
| 3 | 1 | 3 | 2 | 0 | 2 | 2350.0838 | 2350.0835 | 0.0003 |
| 5 | 1 | 5 | 4 | 0 | 4 | 2350.3619 | 2350.3619 | -0.0000 |
| 7 | 1 | 7 | 6 | 0 | 6 | 2350.6245 | 2350.6244 | 0.0001 |
| 4 | 3 | 2 | 4 | 2 | 3 | 2350.7837 | 2350.7835 | 0.0001 |
| 3 | 3 | 1 | 3 | 2 | 2 | 2350.7837 | 2350.7843 | -0.0007 |
|   |   |   |   |   |   |   |   |   |
| Blend | 2350.7839 | -0.0003 |
|   |   |   |   |   |   |   |   |   |
| 4 | 3 | 2 | 3 | 2 | 1 | 2351.5395 | 2351.5398 | -0.0003 |
| 5 | 5 | 0 | 4 | 4 | 1 | 2352.9090 | 2352.9087 | 0.0003 |
| 5 | 5 | 1 | 4 | 4 | 0 | 2352.9090 | 2352.9087 | 0.0003 |
|   |   |   |   |   |   |   |   |   |
| Blend | 2352.9087 | 0.0003 |
|   |   |   |   |   |   |   |   |   |
| 6 | 5 | 1 | 5 | 4 | 2 | 2353.0871 | 2353.0872 | -0.0001 |
| 6 | 5 | 2 | 5 | 4 | 1 | 2353.0871 | 2353.0872 | -0.0001 |
|   |   |   |   |   |   |   |   |   |
| Blend | 2353.0872 | -0.0001 |
|   |   |   |   |   |   |   |   |   |
| 7 | 5 | 2 | 6 | 4 | 3 | 2353.2632 | 2353.2634 | -0.0001 |
|   7   |   5   |   3   |   6   |   4   |   2   | 2353.2632 | 2353.2633 | -0.0001 |
|-----|-----|-----|-----|-----|-----|----------|----------|--------|
| Blend | 2353.2633 | -0.0001 |
| 3   |   1   |   3   |   4   |   0   |   4   | 2348.7617 | 2348.7616 | 0.0001 |

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Table A-4. Observed transitions in the microwave spectrum of CO$_2$-22Ne

MW data from: Y. Xu and W. Jäger, J. Mol. Spectrosc. 192, 435-440 (1998).

| J' K'a' Kc' | J" K'a" Kc" | Obs(MHz)   | Calc(MHz)   | Obs-Calc(MHz) |
|-------------|--------------|-------------|-------------|---------------|
| 1 0 1       | 0 0 0        | 5752.5423   | 5752.5425   | -0.0002       |
| 2 0 2       | 1 0 1        | 11458.7128  | 11458.7126  | 0.0002        |
| 3 0 3       | 2 0 2        | 17073.2426  | 17073.2428  | -0.0002       |
| 3 2 2       | 2 2 1        | 17198.8324  | 17198.8323  | 0.0001        |
| 3 2 1       | 2 2 0        | 17371.6715  | 17371.6716  | -0.0001       |
| 4 0 4       | 3 0 3        | 22556.0274  | 22556.0273  | 0.0001        |
| 4 2 3       | 3 2 2        | 22888.5325  | 22888.5325  | -0.0000       |
| 4 2 2       | 3 2 1        | 23313.7122  | 23313.7122  | 0.0000        |
Table A-5. Observed transitions of the combination band of CO2-20Ne (units of 1/cm)

| J'  | Ka' | Kc' | J"  | Ka" | Kc" | Observed   | Calc   | Obs-Calc |
|-----|-----|-----|-----|-----|-----|------------|--------|----------|
| 6   | 2   | 4   | 7   | 2   | 5   | 2365.3207  | 2365.3190 | 0.0017   |
| 6   | 0   | 6   | 7   | 0   | 7   | 2365.3716  | 2365.3707 | 0.0009   |
| 5   | 0   | 5   | 6   | 0   | 6   | 2365.6291  | 2365.6290 | 0.0000   |
| 5   | 2   | 3   | 6   | 2   | 4   | 2365.6546  | 2365.6547 | -0.0002  |
| 5   | 2   | 4   | 6   | 2   | 5   | 2365.7207  | 2365.7200 | 0.0007   |
| 4   | 0   | 4   | 5   | 0   | 5   | 2365.8779  | 2365.8770 | 0.0009   |
| 4   | 2   | 2   | 5   | 2   | 3   | 2365.9698  | 2365.9702 | -0.0004  |
| 4   | 2   | 3   | 5   | 2   | 4   | 2366.0086  | 2366.0093 | -0.0007  |
| 3   | 0   | 3   | 4   | 0   | 4   | 2366.1183  | 2366.1177 | 0.0006   |
| 3   | 2   | 1   | 4   | 2   | 2   | 2366.2622  | 2366.2624 | -0.0002  |
| 3   | 2   | 2   | 4   | 2   | 3   | 2366.2817  | 2366.2820 | -0.0003  |
| 2   | 0   | 2   | 3   | 0   | 3   | 2366.3517  | 2366.3515 | 0.0002   |
| 2   | 2   | 0   | 3   | 2   | 1   | 2366.5305  | 2366.5302 | 0.0003   |
| 2   | 2   | 1   | 3   | 2   | 2   | 2366.5381  | 2366.5379 | 0.0002   |
| 1   | 0   | 1   | 2   | 0   | 2   | 2366.5764  | 2366.5773 | -0.0009  |
| 0   | 0   | 0   | 1   | 0   | 1   | 2366.7915  | 2366.7929 | -0.0014  |
| 5   | 2   | 4   | 5   | 2   | 3   | 2366.8627  | 2366.8624 | 0.0002   |
| 5   | 2   | 3   | 5   | 2   | 4   | 2366.9764  | 2366.9766 | -0.0002  |
| 4   | 2   | 3   | 4   | 2   | 2   | 2366.9883  | 2366.9889 | -0.0006  |
| 4   | 2   | 2   | 4   | 2   | 3   | 2367.0381  | 2367.0385 | -0.0004  |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|   |   |   |   |   |   |   |
| 3 2 2 | 3 2 1 | 2367.0801 | 2367.0805 | -0.0004 |
| 3 2 1 | 3 2 2 | 2367.0969 | 2367.0971 | -0.0001 |
| 2 2 1 | 2 2 0 | 2367.1438 | 2367.1431 | 0.0007 |
| 2 2 0 | 2 2 1 | 2367.1469 | 2367.1464 | 0.0005 |
| 1 0 1 | 0 0 0 | 2367.1842 | 2367.1846 | -0.0004 |
| 2 0 2 | 1 0 1 | 2367.3575 | 2367.3573 | 0.0002 |
| 3 0 3 | 2 0 2 | 2367.5134 | 2367.5125 | 0.0009 |
| 4 0 4 | 3 0 3 | 2367.6503 | 2367.6491 | 0.0011 |
| 3 2 2 | 2 2 1 | 2367.6971 | 2367.6967 | 0.0004 |
| 3 2 1 | 2 2 0 | 2367.7029 | 2367.7023 | 0.0006 |
| 5 0 5 | 4 0 4 | 2367.7669 | 2367.7660 | 0.0009 |
| 4 2 3 | 3 2 2 | 2367.8243 | 2367.8236 | 0.0006 |
| 4 2 2 | 3 2 1 | 2367.8374 | 2367.8369 | 0.0005 |
| 6 0 6 | 5 0 5 | 2367.8601 | 2367.8616 | -0.0015 |
| 5 2 4 | 4 2 3 | 2367.9293 | 2367.9307 | -0.0014 |
| 7 0 7 | 6 0 6 | 2367.9318 | 2367.9345 | -0.0027 |
| 5 2 3 | 4 2 2 | 2367.9544 | 2367.9563 | -0.0019 |
| 8 0 8 | 7 0 7 | 2367.9843 | 2367.9830 | 0.0012 |
| 6 2 5 | 5 2 4 | 2368.0190 | 2368.0171 | 0.0018 |
| 6 2 4 | 5 2 3 | 2368.0596 | 2368.0608 | -0.0012 |

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Table A-6. Observed transitions of the combination band of CO2-22Ne (units of 1/cm)

| J' Ka' Kc' | J" Ka" Kc" | Observed   | Calc   | Obs-Calc |
|------------|------------|------------|--------|----------|
| 5          | 0          | 5          | 6      | 0        | 5          | 62365.7069  | 2365.7079  | -0.0010  |
| 5          | 2          | 4          | 6      | 2        | 5          | 2365.8065  | 2365.8062  | 0.0003   |
| 4          | 0          | 4          | 5      | 0        | 5          | 2365.9455  | 2365.9458  | -0.0003  |
| 4          | 2          | 2          | 5      | 2        | 3          | 2366.0495  | 2366.0493  | 0.0002   |
| 4          | 2          | 3          | 5      | 2        | 4          | 2366.0805  | 2366.0810  | -0.0005  |
| 3          | 0          | 3          | 4      | 0        | 4          | 2366.1760  | 2366.1760  | 0.0000   |
| 3          | 2          | 1          | 4      | 2        | 2          | 2366.3224  | 2366.3232  | -0.0007  |
| 3          | 2          | 2          | 4      | 2        | 3          | 2366.3384  | 2366.3389  | -0.0005  |
| 2          | 0          | 2          | 3      | 0        | 3          | 2366.3988  | 2366.3986  | 0.0001   |
| 1          | 0          | 1          | 2      | 0        | 2          | 2366.6124  | 2366.6126  | -0.0003  |
| 0          | 0          | 0          | 1      | 0        | 1          | 2366.8163  | 2366.8164  | -0.0002  |
| 4          | 2          | 3          | 4      | 2        | 2          | 2367.0111  | 2367.0116  | -0.0005  |
| 4          | 2          | 2          | 4      | 2        | 3          | 2367.0500  | 2367.0502  | -0.0003  |
| 3          | 2          | 1          | 3      | 2        | 2          | 2367.1078  | 2367.1081  | -0.0002  |
| 2          | 2          | 0          | 2      | 2        | 1          | 2367.1540  | 2367.1550  | -0.0010  |
| 2          | 2          | 1          | 2      | 2        | 0          | 2367.1540  | 2367.1524  | 0.0016   |
| 2          | 0          | 2          | 1      | 0        | 1          | 2367.3505  | 2367.3504  | 0.0002   |
| 3          | 0          | 3          | 2      | 0        | 2          | 2367.4982  | 2367.4979  | 0.0003   |
| 4          | 0          | 4          | 3      | 0        | 3          | 2367.6286  | 2367.6282  | 0.0004   |
| 3          | 2          | 2          | 2      | 2        | 1          | 2367.6762  | 2367.6760  | 0.0002   |
| 3 | 2 | 1 | 2 | 2 | 0 | 2367.6808 | 2367.6803 | 0.0005 |
|---|---|---|---|---|---|------------|------------|--------|
| 5 | 0 | 5 | 4 | 0 | 4 | 2367.7409 | 2367.7401 | 0.0008 |
| 4 | 2 | 3 | 3 | 2 | 2 | 2367.7973 | 2367.7965 | 0.0008 |

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Table A-7. Observed transitions of the hot band of CO2-20Ne (units of 1/cm)

| J' Ka' Kc' | J"  Ka" Kc" | Observed | Calc      | Obs-Calc | Obs-Calc |
|------------|-------------|----------|-----------|----------|----------|
| 3 2 2      | 4 3         | 2334.4230 | 2334.4230 | 0.0001   |
| 3 2 1      | 4 3         | 2334.5275 | 2334.5279 | -0.0004  |
| 2 2 1      | 3 3         | 0 2334.6462 | 2334.6457 | 0.0005   |
| 2 2 0      | 3 3         | 1 2334.6697 | 2334.6695 | 0.0002   |
| 5 1 5      | 6 2         | 4 2334.9574 | 2334.9576 | -0.0002  |
| 2 1 2      | 3 2         | 1 2334.9886 | 2334.9877 | 0.0009   |
| 6 0 6      | 7 1         | 7 2335.0148 | 2335.0138 | 0.0010   |
| 4 0 4      | 5 2         | 4 2335.0991 | 2335.1001 | -0.0010  |
| 5 0 5      | 6 1         | 6 2335.1749 | 2335.1746 | 0.0003   |
| 4 2 3      | 4 3         | 2 2335.2316 | 2335.2319 | -0.0004  |
| 3 2 2      | 3 3         | 1 2335.2618 | 2335.2616 | 0.0002   |
| 3 1 2      | 4 2         | 3 2335.2951 | 2335.2949 | 0.0002   |
| 5 1 5      | 5 2         | 4 2335.3339 | 2335.3348 | -0.0009  |
| 4 1 3      | 5 1         | 5 2335.3537 | 2335.3541 | -0.0004  |
| 1 1 1      | 2 2         | 0 2335.3673 | 2335.3675 | -0.0001  |
| 2 1 1      | 3 2         | 2 2335.4476 | 2335.4470 | 0.0006   |
| 4 1 4      | 4 2         | 3 2335.4604 | 2335.4601 | 0.0003   |
| 3 1 3      | 4 2         | 2 2335.4712 | 2335.4714 | -0.0002  |
| 3 0 3      | 4 1         | 4 2335.5534 | 2335.5542 | -0.0008  |
| 1 1 0      | 2 2         | 1 2335.5581 | 2335.5584 | -0.0003  |
| 5 0 5 | 5 2 | 3 | 2335.5771 | 2335.5769 | 0.0002 |
| 3 1 3 | 3 2 | 2 | 2335.5916 | 2335.5910 | 0.0006 |
| 4 1 3 | 4 2 | 2 | 2335.6450 | 2335.6451 | -0.0001 |
| 2 1 2 | 2 2 | 1 | 2335.7166 | 2335.7168 | -0.0002 |
| 2 1 2 | 3 1 | 2 | 2335.7585 | 2335.7587 | -0.0001 |
| 3 0 3 | 3 1 | 2 | 2335.7655 | 2335.7661 | -0.0006 |
| 2 0 2 | 3 1 | 3 | 2335.7763 | 2335.7770 | -0.0006 |
| 2 0 2 | 2 1 | 1 | 2335.9547 | 2335.9550 | -0.0004 |
| 3 1 2 | 3 2 | 1 | 2335.9997 | 2335.9985 | 0.0012 |
| 1 0 1 | 2 1 | 2 | 2336.0224 | 2336.0229 | -0.0004 |
| 2 1 1 | 2 2 | 0 | 2336.0448 | 2336.0449 | -0.0001 |
| 1 1 1 | 2 1 | 1 | 2336.0779 | 2336.0783 | -0.0004 |
| 5 1 5 | 6 0 | 6 | 2336.1874 | 2336.1874 | -0.0001 |
| 1 0 1 | 1 1 | 0 | 2336.2012 | 2336.2012 | -0.0001 |
| 0 0 0 | 1 1 | 1 | 2336.2789 | 2336.2786 | 0.0002 |
| 2 1 1 | 3 1 | 3 | 2336.5778 | 2336.5777 | 0.0000 |
| 2 0 2 | 1 1 | 1 | 2336.5924 | 2336.5923 | 0.0001 |
| 4 1 4 | 4 1 | 4 | 2336.7220 | 2336.7228 | -0.0008 |
| 3 1 3 | 3 1 | 3 | 2336.7220 | 2336.7217 | 0.0003 |

**Blend**: 2336.7223 -0.0003

| 3 0 3 | 2 1 | 2 | 2336.7263 | 2336.7265 | -0.0002 |
| 1 1 0 | 1 1 | 0 | 2336.7395 | 2336.7390 | 0.0004 |
| 2 1 1 | 2 1 | 1 | 2336.7557 | 2336.7558 | 0.0000 |
| 5 0 5 | 5 0 | 5 | 2336.7768 | 2336.7766 | 0.0002 |
3 2 2 3 1 3 2337.9240 2337.9242 -0.0002
4 1 4 3 0 3 2337.9523 2337.9519 0.0004
2 2 1 1 1 0 2337.9836 2337.9829 0.0007
4 2 2 3 1 3 2338.0287 2338.0289 -0.0002
4 2 3 4 1 4 2338.0465 2338.0472 -0.0007
3 2 2 2 1 1 2338.1022 2338.1023 0.0000
3 3 0 3 2 1 2338.1282 2338.1275 0.0007
2 2 0 1 1 1 2338.1481 2338.1474 0.0007
5 1 5 4 0 4 2338.1481 2338.1476 0.0004
                  Blend        2338.1475  0.0006
5 1 4 4 2 3 2338.1549 2338.1553 -0.0004
5 2 4 5 1 5 2338.1625 2338.1632 -0.0007
4 3 2 4 2 3 2338.2550 2338.2552 -0.0002
4 2 3 3 1 2 2338.2588 2338.2590 -0.0003
5 2 3 4 1 4 2338.2970 2338.2974 -0.0004
6 1 6 5 0 5 2338.3224 2338.3220 0.0003
5 2 4 4 2 2 2338.4538 2338.4543 -0.0005
3 2 1 2 1 2 2338.5152 2338.5154 -0.0002
6 2 4 5 1 5 2338.5468 2338.5477 -0.0009
8 1 8 7 0 7 2338.6134 2338.6143 -0.0009
6 2 5 5 2 3 2338.6701 2338.6702 -0.0001
7 2 5 6 1 6 2338.7890 2338.7893 -0.0003
3 3 1 2 2 0 2338.8297 2338.8296 0.0001
3 3 0 2 2 1 2338.8563 2338.8566 -0.0003
| i | j | k | l | m | n | Value | Value | Difference |
|---|---|---|---|---|---|-------|-------|------------|
| 7 | 2 | 6 | 6 | 2 | 4 | 2338.8919 | 2338.8918 | 0.0001 |
| 4 | 3 | 2 | 3 | 2 | 1 | 2338.9591 | 2338.9588 | 0.0004 |
| 8 | 2 | 6 | 7 | 1 | 7 | 2339.0307 | 2339.0298 | 0.0009 |
| 5 | 3 | 3 | 4 | 1 | 3 | 2339.0511 | 2339.0508 | 0.0003 |
| 4 | 3 | 1 | 3 | 2 | 2 | 2339.0736 | 2339.0741 | -0.0005 |
| 4 | 1 | 4 | 5 | 2 | 3 | 2335.2076 | 2335.2080 | -0.0004 |
| 5 | 2 | 3 | 5 | 1 | 4 | 2335.6343 | 2335.6341 | 0.0003 |
| 2 | 2 | 1 | 3 | 1 | 2 | 2336.8448 | 2336.8442 | 0.0006 |
| 3 | 1 | 3 | 2 | 1 | 1 | 2336.8992 | 2336.8998 | -0.0006 |
| 4 | 0 | 4 | 3 | 2 | 2 | 2336.8992 | 2336.8982 | 0.0010 |
| 2 | 1 | 2 | 1 | 1 | 0 | 2336.8992 | 2336.8974 | 0.0018 |
|    |     |     |     |     |     |     |     | Blend   |
|    |     |     |     |     |     |     |     |         |
| 2336.8988 |         | 0.0004 |
| 4 | 1 | 4 | 3 | 1 | 2 | 2336.9349 | 2336.9347 | 0.0002 |
| 6 | 1 | 6 | 5 | 2 | 3 | 2337.1227 | 2337.1223 | 0.0004 |
| 4 | 2 | 2 | 3 | 2 | 2 | 2337.8202 | 2337.8204 | -0.0002 |
| 5 | 3 | 2 | 5 | 1 | 4 | 2337.9280 | 2337.9288 | -0.0008 |
| 6 | 2 | 4 | 6 | 0 | 6 | 2338.0121 | 2338.0128 | -0.0008 |
| 7 | 2 | 5 | 7 | 0 | 7 | 2338.0194 | 2338.0194 | 0.0000 |
| 4 | 3 | 1 | 4 | 1 | 3 | 2338.0229 | 2338.0225 | 0.0004 |
| 6 | 1 | 5 | 6 | 2 | 4 | 2338.1135 | 2338.1132 | 0.0003 |
| 3 | 3 | 1 | 3 | 2 | 2 | 2338.2318 | 2338.2317 | 0.0001 |
| 6 | 2 | 5 | 6 | 1 | 6 | 2338.2677 | 2338.2679 | -0.0002 |
| 2 | 2 | 0 | 2 | 0 | 2 | 2338.3443 | 2338.3442 | 0.0001 |
| 7 | 2 | 6 | 7 | 1 | 7 | 2338.3621 | 2338.3610 | 0.0011 |
2 2 1 1 0 1 2338.5812 2338.5819 -0.0006
8 2 7 7 2 5 2339.1111 2339.1103 0.0008
6 3 4 5 1 4 2339.1309 2339.1313 -0.0005

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