Characterization of OCS-HCCCH and N₂O-HCCCCH dimers: Theory and experiment

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Abstract

The infrared spectra of the weakly-bound dimers OCS-HCCCCH, in the region of the $\nu_1$ fundamental band of OCS (2050 cm$^{-1}$), and N$_2$O-HCCCCH, in the region of the $\nu_1$ fundamental band of N$_2$O (2200 cm$^{-1}$), were observed in a pulsed supersonic slit jet expansion probed with tunable diode/QCL lasers. Both OCS-HCCCCH and N$_2$O-HCCCCH were found to have planar structure with side-by-side monomer units having nearly parallel axes. These bands have hybrid rotational structure which allows for estimates of the orientation of OCS and N$_2$O in the plane of their respective dimers. Analogous bands for OCS-DCCCCD and N$_2$O-DCCCCD were also observed and found to be consistent with the normal isotopologues. Various levels of ab initio calculations were performed to find stationary points on the potential energy surface, optimized structures and interaction energies. Four stable geometries were found for OCS-HCCCCH and three for N$_2$O-HCCCCH. The rotational parameters at CCSD(T*)-F12c level of theory give results in very good agreement with those obtained from the observed spectra. In both dimers, the experimental structure corresponds to the lowest energy isomer.
Introduction

Acetylene is a prototype molecule for examining weak intermolecular forces involving carbon-carbon triple bond. Pure and mixed acetylene clusters have been studied extensively both theoretically and experimentally [1, 2, 3, 4]. In particular, mixed dimers containing OCS and N$_2$O with acetylene are well characterized using microwave and infrared spectroscopy. To date, only one isomer of N$_2$O-HCCH has been observed in the gas phase [3, 5, 6]. This isomer, which is almost certainly the most stable structure, is planar with near parallel monomer units. For OCS-HCCH two isomers have been detected; a planar near-parallel structure analogous to the observed N$_2$O-HCCH and a T-shaped isomer having C$_{2v}$ symmetry, with OCS forming the stem of the T, and the S atom in the inner position pointing to the triple bond of C$_2$H$_2$ [3, 7, 8].

The longer counterpart of acetylene, diacetylene, provides a simple system with multiple triple-bond sites; thus clusters containing diacetylene potentially display much richer-structured energy surfaces. For example, theoretical calculations in Ref. [9] identify three structural isomers, a Y-shaped π-type hydrogen-bonded structure with C$_S$ symmetry, a parallel slipped structure with C$_{2h}$ symmetry, and a cross shaped structure with D$_{2d}$ symmetry. Since this dimer has not been observed experimentally, nor has its complete intermolecular potential surface been investigated with high-level ab initio calculations, it is unclear what type of tunneling dynamics exist in (HCCCCH)$_2$ and if there are out of plane paths via the cross-shaped structure, or the situation is similar to acetylene dimer where the large amplitude tunneling takes place in the plane of the dimer.

There are relatively few gas phase studies of mixed dimers containing diacetylene. The first of these is a microwave study of NH$_3$-HCCCCH and H$_2$O-HCCCCH by Matsumura et al. [10]. Here, NH$_3$-HCCCCH was found to be an axially symmetric complex where a diacetylene hydrogen bonds to the nitrogen in ammonia to form a symmetric top and H$_2$O-HCCCCH has a
planar symmetry where a diacetylene hydrogen bonds to the oxygen of water. The structural similarities with NH$_3$-HCCH and H$_2$O-HCCH suggest that diacetylene closely parallels acetylene in complexes with other bases. On the other hand a dissimilar behavior might be expected when acetylene and diacetylene act as bases in complexes with acids.

A study by Yang et al. [11] of HCN-HCCCCCH in the infrared region found only a linear configuration despite the fact that both linear and T-shaped structures are observed in HCN- HCCH and the T-shaped isomer is strongly favored in the molecular beam expansion of HCN- HCCH. Although, this observation seems to confirm the dissimilar behavior between acetylene and diacetylene when they act as bases, Yang et al. [11] attributed the absence of the T-shaped isomer in their experiment to the very asymmetric top character of the HCN-HCCCCCH which disperses its spectra and gives rise to an unfavorable partition function and consequently low signal to noise ratio.

In the present paper, we observe and analyze the spectra of OCS-HCCCCCH and OCS- DCCCCCD, in the region of the $v_1$ fundamental of OCS, and N$_2$O-HCCCCCH and N$_2$O-DCCCCCD, in the region of the $v_1$ fundamental of N$_2$O. Both dimers were found to have planar C$_5$ symmetry with monomer axes nearly parallel to each other. Furthermore, the spectra have hybrid a-, b-type rotational structure which allow for good estimates of the orientation of OCS and N$_2$O in their dimers. The four independent structural constants obtained from the analysis of spectra for OCS- HCCCCCH and OCS-DCCCCCD are insufficient for accurate determination of an experimental structure. The same can be said in the case of N$_2$O-HCCCCCH. Therefore, we carried out various levels of \textit{ab initio} calculations in support of our experimental findings. Counterpoise-corrected binding energy calculations indicate that the observed structures are the most stable isomers. In addition, three less energetically favorable structures were found for OCS-HCCCCCH and two for
N$_2$O-HCCCCH. Experimental rotational constants are in excellent agreement with the rotational constants at the CCSD(T*)-F12c level of theory. Our results closely parallel mixed acetylene complexes with OCS and N$_2$O.

1. **Computational details**

To support our experimental analysis, as well as to characterize the stationary points on the potential energy surface (PES) of these complexes, we performed several *ab initio* calculations.

As a first step, we searched the potential energy surface (PES) of both OCS-HCCCCH and N$_2$O-HCCCCH by means of density functional theory (DFT). Two different functionals, namely B3LYP [12, 13] and B2PLYP [14], were used employing the DFT-D3 dispersion corrections proposed by Grimme [15], in conjunction with the maug-cc-pVTZ basis set [16]. The inclusion of these corrections is mandatory since, even if DFT methods are nowadays widely employed for treating a wide variety of chemical problems, ranging from spectroscopic analysis to molecular complexes and adsorption processes (see for example Refs. [17, 18, 19, 20, 21, 22, 23, 24, 25], the role of dispersion contributions is fundamental for modeling correctly the energetics of van der Waals adducts [26, 27, 28]. The structures of the stationary points for both OCS-HCCCCH and N$_2$O-HCCCCH were first optimized at B3LYP-D3 level of theory and then refined using the B2PLYP-D3 functional. Calculations carried out with both functionals led to identification of four stationary points for OCS-HCCCCH and three for N$_2$O-HCCCCH; subsequent hessian calculations carried out on these optimized structures, corrected by the basis set superposition error (BSSE) using the counterpoise correction (CP) as proposed by Boys and Bernardi [29], confirmed that they correspond to true minima on the PES. These isomers are
shown in Fig. 1 for OCS-HCCCCH and in Fig. 2 for N₂O-HCCCCH. We computed the corresponding counterpoise corrected (CP) values of both binding and interaction energies (hereafter labeled as BE and IE, respectively) at the B2PLYP-D3 level of theory for all of the structures. We corrected these BE values by also taking into account the zero-point vibrational (ZPV) correction for each species, defined as

\[ \Delta E = \frac{1}{2} \sum_n \omega_n \]  

(1)

where the harmonic frequencies \( \omega_n \) (the index \( n \) labels the \( n \)-th vibrational mode) were obtained at B2PLYP-D3/maug-cc-pVTZ level. To determine a better estimate of the binding energy for all the structures, we performed additional single-point calculations on each of these optimized geometries at the coupled-cluster level of theory using the singles and doubles approximation augmented by a perturbative treatment of triple excitations, CCSD(T) [30, 31, 32], within the frozen core (fc) approximation. By using the correlation consistent basis sets cc-pVnZ basis set [33, 34, 35] both the Hartree-Fock self-consistent-field (HF-SCF) energies and the CCSD(T) correlation energies were extrapolated at the complete basis set (CBS) limit (at which the BSSE error vanishes), and then combined to correct for the error due to the basis-set truncation. CBS energies at HF-SCF level were evaluated using cc-pVnZ (\( n = T, Q \) and 5) basis sets, and employing the \( e^{-cn} \) formula [36], while the CCSD(T) correlation contributions were computed using the \( n^{-3} \) expression [37] with the cc-pVTZ and cc-pVQZ basis sets. Subsequent corrections due to core-valence (CV) correlation effects were calculated as the difference between CCSD(T) energies (in conjunction with the cc-pCVTZ basis set [38]) obtained by correlating all electrons and within the fc approximation. Inclusion of the ZPV corrections yielded the best estimate values for the binding energies reported in the present work, which therefore were then used to identify the most stable isomer for both OCS-HCCCCH and N₂O-HCCCCH complexes. The
results for rotational constants, interaction and binding energies are summarized in Table 1.

For the most stable isomer of both OCS-HCCCCH and N₂O-HCCCCH complexes, we carried out additional geometry optimizations at both CCSD(T) and CCSD(T*)-F12c [39] levels of theory and in conjunction with the cc-pVTZ and cc-pVnZ-F12 [40] basis sets \((n = D, T)\), respectively; for the latter, both the appropriate auxiliary basis sets [41] and its complement auxiliary basis sets (CABS) [42] were used. Finally, for these two structures, within the framework of the vibrational second-order perturbation theory (VPT2 [43, 44]) we computed the vibrational corrections \(\Delta B_{\text{vib}}^i\) to the corresponding equilibrium rotational constants \(B_e^i\) by means of the following expression

\[
\Delta B_{\text{vib}}^i = -\frac{1}{2} \sum_n \alpha_n^i
\]  

where the \(\alpha_n^i\) are the vibration-rotation interaction constants \((i\) labels the inertial axis). These corrections were computed on the basis of the cubic force fields, which were calculated by using the maug-cc-pVTZ basis set and the B3PLYP functional (with the D3 corrections), in view of its good performance in modeling the anharmonic part of the potential [45], following the procedures established in previous works [46, 47].

We performed all DFT calculations employing the Gaussian suite of quantum chemical programs [48]; for both B3LYP and B2PLYP functionals, we employed the UltraFine grid available in Gaussian09 (corresponding to 99 radial and 590 angular points), because of its good results (see for example Refs. [18, 49]) for the calculations of anharmonic force field data. For the calculations carried out at coupled cluster levels of theory we used the MOLPRO program [50, 51] together with its appropriate software packages [52, 53, 54, 55, 56]. The optimized rotational parameters for the most stable isomers are given in Table 2.
Table 1. Theoretical molecular parameters for OCS-HCCCH and N₂O-HCCCH isomers optimized at DFT level of theory.\(^a\)

|                | OCS-HCCCH | N₂O-HCCCH |
|----------------|-----------|-----------|
|                | Isomer I  | Isomer II | Isomer III | Isomer IV | Isomer I | Isomer II | Isomer III |
|                | (S-in)    | (O-in)    | T-shaped   | Cross-shaped | (N-in)    | (O-in)    | Cross-shaped |
| \(A^a\)       | 2897      | 4088      | 4255       | 2629       | 4461      | 4401      | 3262       |
| \(B^a\)       | 1277      | 1000      | 795        | 1243       | 1446      | 1470      | 1754       |
| \(C^a\)       | 886       | 803       | 670        | 1139       | 1092      | 1102      | 1394       |
| \(\text{BE}_{\text{CP}}^b\) | -776      | -630      | -584       | -668       | -727      | -675      | -612       |
| \(\text{BE}_{\text{CP+ZPV}}^c\) | -562      | -313      | -403       | -352       | -495      | -285      | -406       |
| \(\text{IE}_{\text{CP}}^d\) | -780      | -633      | -584       | -668       | -727      | -679      | -612       |
| \(\text{BE}_{\text{CBS}}^e\) | -682      | -560      | -504       | -567       | -700      | -611      | -570       |
| \(\text{BE}_{\text{CBS+CV}}^f\) | -694      | -569      | -513       | -577       | -705      | -617      | -577       |
| \(\text{BE}_{\text{CBS+CV+ZPV}}^g\) | -479      | -252      | -332       | -384       | -472      | -227      | -371       |

\(^a\)Equilibrium rotational constants (in MHz) obtained from optimized geometries obtained with B2PLYP-D3 in conjunction with maug-cc-pVTZ basis set. Binding energies (BE) and interaction energies (IE) reported in cm\(^{-1}\).

\(^b\)Counterpoise-corrected binding energy computed at B2PLYP-D3/maug-cc-pVTZ level of theory.

\(^c\)Binding energy including zero-point vibrational contribution evaluated at B2PLYP-D3/maug-cc-pVTZ level of theory.

\(^d\)Counterpoise-corrected interaction energy computed at B2PLYP-D3/maug-cc-pVTZ level of theory.

\(^e\)Binding energy obtained from extrapolated energies to the CBS limit at CCSD(T) level of theory.

\(^f\)Binding energy obtained from extrapolated energies to the CBS limit at CCSD(T) level of theory corrected by CV-effects (see text).
Table 2. Equilibrium rotational constants (in MHz) obtained at different coupled cluster levels of theory for the OCS-HCCCH and N₂O-HCCCH isomers experimentally observed in the present work.

|       | OCS-HCCCH | N₂O-HCCCH |
|-------|-----------|-----------|
|       | Isomer I  | Isomer I  |
| A     | 2856      | 2897      |
| B     | 1205      | 1274      |
| C     | 847       | 885       |

|       | CCSD(T)\(^a\) | CCSD(T\(^\ast\))\(-\)F12\(^c\)\(^b\) | CCSD(T)\(^a\) | CCSD(T\(^\ast\))\(-\)F12\(^c\)\(^b\) |
|-------|---------------|-----------------|---------------|-----------------|
| A     | 2856          | 2897            | 4487          | 4540            |
| B     | 1205          | 1274            | 1395          | 1446            |
| C     | 847           | 885             | 1064          | 1097            |

\(^a\) Optimized geometries obtained at CCSD(T, fc) level of theory in conjunction with cc-pVTZ basis set.

\(^b\) Optimized geometries obtained at CCSD(T\(^\ast\))\(-\)F12c level of theory in conjunction with VTZ-F12 basis set.
2. **Observed spectra**

The spectra were recorded as described previously [57-59], using a pulsed supersonic slit jet apparatus, a diode laser for OCS-HCCCH and a Daylight Solutions quantum cascade laser for N$_2$O-HCCCH. The expansion gas was a mixture of N$_2$O (0.1%) and C$_4$H$_2$ or C$_4$D$_2$ (0.3%) in helium as a carrier gas with a jet backing pressure of 8 atmospheres. The lower concentration of N$_2$O relative to HCCCH was needed to minimize the formation of N$_2$O clusters, which are known to absorb in the 2220 cm$^{-1}$ spectral region [3]. Similar conditions were used for OCS-HCCCH and its deuterated isotopologue.
The diacetylene was synthesized by the procedure described in Ref. [60]. DCCCCD was obtained by mixing HCCCCH with a 1 N solution of NaOD in D₂O as described by Etoh et al. [61]. The sample of diacetylene and diacetylene-d₂ thus prepared were purified by repeated distillation under vacuum and then stored at LN₂ temperature. The purity of the sample was checked using low resolution infrared spectroscopy. Spectral assignment and simulation were made using PGOPHER [62].

2.1. OCS-HCCCCH results

For all the minima of OCS-HCCCCH (listed in Table 1), the analysis of their structures (optimized at B2PLYP-D3/maug-cc-pVTZ level of theory) shows that there is an almost negligible variation in the intramolecular geometric parameters due to the complexation. Both the counterpoise corrected binding energies computed at DFT level of theory and those obtained from CCSD(T) extrapolated energies to the CBS limit identify isomer I (see Fig. 1) as the most stable form of OCS-HCCCCH (-2.22 kcal mol⁻¹ at B2PLYP level of theory, -1.95 kcal mol⁻¹ at CCSD(T) CBS limit). The inclusion of CV-effects is almost negligible, while the zero-point vibrational contributions reduce the binding energy (computed from extrapolated energies to the CBS limit at CCSD(T) level of theory) of isomer I to -1.37 kcal mol⁻¹. This isomer has a planar structure with nearly parallel side-by-side monomer units and the OCS S-atom on the inside (S-in). Furthermore, the calculated angle between the OCS monomer and the a inertial axis is 72°. Therefore the intramolecular fundamental in the region of the OCS monomer ν₁ fundamental is an a/b-hybrid band, with a b-type transition moment which is larger than that for a-type transitions by a factor of ~3. Isomer II is also planar with a similar structure to isomer I, but with the OCS monomer unit in reverse orientation (O-in). Here, the calculated angle between the OCS monomer and the a inertial axis is 42°. This implies an a/b-hybrid band for the intramolecular
fundamental in the $\nu_1$ region of the OCS with almost equal transition moments for the a- and b-type transitions. The expected rotational structure for isomer III is a nearly pure a-type band, as the calculated angle between the OCS monomer and the a inertial axis is only 12°. Finally, isomer IV is non-planar and would give rise to a mostly c-type band.

A segment of the experimental spectrum for OCS-HCCCCH, including the sharp Q-branch marked by an asterisk and a part of the R-branch, is shown in the second trace in Fig. 3. The corresponding segment for OCS-DCCCD is illustrated in the bottom trace. With a 1:3 mixture of OCS and diacetylene we observe a relatively strong a/b-hybrid band, which could be simulated with a b-type transition moment about three times that of the a-type transition moment. This implies that the band observed is due to the most stable form. Further evidence for this assignment is given in section 3.

A total of 245 transitions involving rotational levels up to $J = 12$ and $k_a = 11$ were assigned for OCS-HCCCCH. Preliminary analysis of the spectrum confirmed that the upper state rotational levels with $k_{a}^{\prime} > 6$ are perturbed. The assigned transitions were then used to obtain 90 ground state combination differences (GSCD). These were used in a frequency analysis to obtain five ground state parameters. The upper state parameters were subsequently obtained from a frequency analysis of the assigned transitions with $k_{a}^{\prime} \leq 6$ while keeping the ground state parameters fixed. The frequency analysis for GSCD gave a weighted standard deviation of 0.00015 cm$^{-1}$ and that for the upper vibrational state was 0.00018 cm$^{-1}$. The parameters thus obtained are listed in the second column of Table 3. The top two traces in Figure 3 show a comparison of observed and simulated spectra based on these parameters.

Analysis of the band for OCS-DCCCD was more straightforward, partly because the spectral region observed was more limited, to conserve the DCCCD sample, and partly because
the upper state rotational levels don’t seem to be affected by perturbations. A total of 159 transitions involving levels up to $J = 12$ and $k_a = 8$ were assigned and analysed to obtain the parameters listed in column 3 of Table 3. The third and fourth traces in Fig. 3 show a comparison of simulated and observed spectra using these parameters. The assigned transitions are listed along with their corresponding residuals in Table A-1 for OCS-HCCCCH, including the perturbed transitions with $k'_a > 6$ which were given zero weight, and Table A-2 for OCS-DCCCD.

Figure 3: Observed and simulated spectra of OCS-HCCCCH and OCS-DCCCD. The simulation is based on the fitted parameters of Table 3, an effective rotational temperature of 2.5 K, and an assumed Gaussian line width of 0.0018 cm$^{-1}$. Blank regions in the observed spectra are obscured by absorptions due to OCS monomer.
Table 3. Molecular parameters for OCS – HCCCCH.\(^a\)

|                      | This work | CCSD(T\(^*\))-F12c |
|----------------------|-----------|---------------------|
|                      | OCS – HCCCCCH | OCS – DCCCCCD | OCS – HCCCCCH | OCS – DCCCCCD |
| \(\nu_0\)/ cm\(^{-1}\) | 2056.16809(3) | 2055.98241(5) |        |                |
| \(A'/\text{MHz}\)    | 2891.907(68)  | 2692.82(28)      |        |                |
| \(B'/\text{MHz}\)    | 1242.930(34)  | 1205.53(12)      |        |                |
| \(C'/\text{MHz}\)    | 867.841(16)   | 831.664(79)      |        |                |
| \(D_K'/\text{kHz}\)  | 6.3(22)\(^c\) | 15.6(24)         |        |                |
| \(A''/\text{MHz}\)   | 2892.78(15)\(^b\) | 2693.92(28) | 2882.07\(^e\) | 2684.26\(^e\) |
| \(B''/\text{MHz}\)   | 1244.416(74)\(^b\) | 1206.46(12) | 1261.10\(^e\) | 1223.09\(^e\) |
| \(C''/\text{MHz}\)   | 869.008(55)\(^b\) | 832.221(83) | 876.38\(^e\) | 839.43\(^e\) |
| \(D_K''/\text{kHz}\) | 6.3(22)\(^b\) | 12.8(24)         |        |                |
| \(D_{JK''}/\text{kHz}\) | 5.7(19)\(^b\) | 12.8(24)         |        |                |
| \(\Delta / \text{a.m.u.A}^2\) | 0.78\(^d\) | 0.77\(^d\)       |        |                |

\(^a\) Uncertainties (1\(\sigma\)) in parentheses are in units of the last quoted digit.

\(^b\) Ground state parameters were obtained from the lower state combination differences. These were held fixed during the frequency analysis of the upper state rotational levels.

\(^c\) Excited state quartic parameters were held fixed at their ground state values.

\(^d\) Inertial defect, \(\Delta = I_c - I_a - I_b\).

\(^e\) Equilibrium rotational constants at CCSD(T\(^*\))-F12c/VTZ-F12 level of theory augmented by vibrational corrections computed at B3LYP-D3 level (see text).

2.2. \(\text{N}_2\text{O-HCCCCH}\) results

Figure 2 illustrates the three possible forms of \(\text{N}_2\text{O-HCCCCH}\) identified in the present work. For all the structures (obtained at B2PLYP-D3/maug-cc-pVTZ level of theory) the
complexation leads to negligible modifications in the intramolecular geometric parameters, as found for the isomers of OCS-HCCCCH. All the calculations carried out in the present work (see Table 1) identify isomer I (N-in) as the most stable form. Its binding energy, computed from extrapolated energies to the CBS limit at CCSD(T) level of theory corrected by CV-effects and taking into account zero-point vibrational contributions, is -1.35 kcal mol$^{-1}$. This isomer has a planar structure with two nearly parallel monomer units. Here, the calculated angle between the N$_2$O monomer and the a principal axis is 56°, implying that the intramolecular fundamental in the region of the N$_2$O monomer $v_1$ fundamental is an a/b-hybrid band with a b-type transition moment about 1.5 times that for the a-type transitions. The higher energy isomer (O-in) has a very similar structure with the N$_2$O monomer making an angle of 53° with the a axis, only 3° less than isomer I; thus the expected intramolecular bands for the two isomers have very similar rotational structure. Isomer III is non-planar with the N$_2$O monomer axis perpendicular to the ab plane, resulting in a purely c-type band.

A segment of the experimental spectrum for N$_2$O-HCCCCH is shown in the second trace of Fig. 4. Unlike OCS-HCCCCH, the Q-branch, marked by an asterisk, shows much more structure. The corresponding segment for N$_2$O-DCCCD is illustrated in the bottom trace. Again, we observe a relatively strong a/b-hybrid band which is simulated with the b-type transition moment ~1.5 times that of the a-type transition moment. Although the simulated spectrum with this ratio of the transition moments (1.5) gives better overall intensity agreement with the experimental spectrum than b-type/a-type = 1.3 as calculated for isomer II, this alone is insufficient to conclusively assign the observed band to isomer I. Further evidence in support of assignment of the observed band to isomer I is given in section 3.
Analysis of the bands for N₂O-HCCCH and N₂O-DCCCD was straightforward. A total of 166 transitions involving levels up to \( J = 11 \) and \( k_a = 8 \) for N₂O-HCCCH and 121 transitions involving levels up to \( J = 10 \) and \( k_a = 5 \) were assigned and analysed to obtain the parameters listed in columns 3 and 4 of Table 4. The weighted standard deviation of the fit for N₂O-HCCCH was 0.00023 cm\(^{-1}\) and that for N₂O-DCCCD was 0.00024 cm\(^{-1}\). The first and third traces in Fig. 4 show the simulated spectra using these parameters. The assigned transitions along with their corresponding residuals are listed in Table A-3 for N₂O-HCCCH and Table A-4 for N₂O-DCCCD.

Figure 4: Observed and simulated spectra of N₂O-HCCCH and N₂O-DCCCD. The simulation is based on the fitted parameters of Table 4, an effective rotational temperature of 2.5 K, and an assumed Gaussian line width of 0.0022 cm\(^{-1}\). Blank regions in the observed spectra are obscured by absorptions due to N₂O monomer.
Table 4. Molecular parameters for N₂O – HCCCCH.¹

|                      | This work       | CCSD(T*)-F12c       |
|----------------------|-----------------|---------------------|
| v₀ / cm⁻¹            | N₂O – HCCCCH 2226.05079(5) | N₂O – DCCCCCD 2226.07274(5) |
|                      | A' / MHz 4479.78(35) | 4117.27(20)         |
|                      | B' / MHz 1409.16(12) | 1358.51(12)         |
|                      | C' / MHz 1069.838(81) | 1019.606(90)        |
| Dₖ' / kHz            | 82.9(77)        |                     |
| Dⱼₖ' / kHz           | -12.2(25)       |                     |
| A'' / MHz            | 4498.57(28)     | 4134.60(52)         |
|                      | 4485.29³        | 4117.35³            |
| B'' / MHz            | 1409.03(12)     | 1358.33(12)         |
|                      | 1434.99³        | 1384.70³            |
| C'' / MHz            | 1070.783(76)    | 1020.552(99)        |
|                      | 1085.21³        | 1034.36³            |
| Dₖ'' / kHz           | 91.8(51)        | 93(28)              |
| Δ / a.m.u Å²         | 0.96b           | 0.91b               |

¹ Uncertainties (1σ) in parentheses are in units of the last quoted digit.

³ Equilibrium rotational constants at CCSD(T*)-F12c/VTZ-F12 level of theory augmented by vibrational corrections computed at B3LYP-D3 level (see text).

3. Discussion and conclusions

Comparison of the theoretical rotational constants for OCS-HCCCCH at all levels of theory, columns 2-5 in Table 1 and columns 2-3 in Table 2, with the experimental rotational constants, column 2 in Table 3, clearly indicates that the observed dimer corresponds to the
lowest energy isomer identified in the present work. Moreover, the best agreement for both the dimers is obtained at the highest level of theory, CCSD(T*)-F12c/VTZ-F12. The results for the deuterated isotopologue, columns 3 and 4 in Table 3, provide further support for this assignment. This, together with the expectation that the jet conditions employed in this work favor the formation of the lowest energy structure, leaves very little doubt that isomer I in Fig. 1 corresponds to the species observed.

Small and positive values for the inertial defects (Table 3) indicate that observed dimer is indeed planar. Positive contributions to the inertial defect result from Coriolis interactions associated with in-plane bending motions; in isomer I of OCS-HCCCCH these are larger than negative contributions from out-of-plane vibrations [63].

All of the arguments made above in support of isomer I of OCS-HCCCCH being the carrier of the observed band in the region of the \( \nu_1 \) fundamental of OCS can similarly be made for the most stable isomer of N\(_2\)O-HCCCCH. Therefore, the carrier of the intramolecular band in the region of the \( \nu_1 \) fundamental of N\(_2\)O is isomer I in Fig. 2. Again, the small and positive values for the inertial defects (Table 4) indicate that the observed dimer is planar. The slight increase in the magnitude of inertial defect, from 0.78 a.m.u. \( \hat{\text{Å}}^2 \) for OCS-HCCCCH to 0.96 a.m.u. \( \hat{\text{Å}}^2 \), is consistent with the fact that N\(_2\)O-HCCCCH is a lighter dimer.

The theoretical intermolecular distances for OCS-HCCCCH (S-in) and N\(_2\)O-HCCCCH (N-in) with the experimental vibrational shifts are listed in Table 5. In the case of OCS-HCCCCH, these are compared with the corresponding values for the two observed isomers of OCS-HCCH [3]. As can be seen, the intermolecular distance of \( R = 3.69 \) \( \hat{\text{Å}} \) for OCS-HCCCCH (S-in) is comparable to that for the near-parallel isomer of OCS-HCCH (S-in, \( R = 3.61 \) \( \hat{\text{Å}} \)) and expectedly much shorter than that for the T-shaped structure (\( R = 4.62 \)). In the case of N\(_2\)O-
HCCCCH (N-in), the calculated intermolecular distance is for 3.43 Å, somewhat larger than R = 3.30 Å for N₂O-HCCH (O-in). The larger R for N₂O-HCCCCH (N-in) may be explained by the combination of the Van der Waals radii, 1.55 Å for the oxygen atom and 1.50 Å for nitrogen [64], and the fact that the center of mass is shifted by 0.07 Å from the central nitrogen atom toward the oxygen atom in the N₂O monomer unit.

As always, the vibrational shifts are difficult to interpret. However, we note that the shifts for both diacetylene- and acetylene-containing species, as shown in Table 5, are consistently to lower frequency for dimers containing OCS and to higher frequency for dimers containing N₂O.

Table 5. Comparison of intermolecular distance and vibrational shift between acetylene and diacetylene containing dimers

|                     | OCS-HCCCCH Near-parallel (S-in) | OCS-HCCH Near-parallel (S-in) | OCS-HCCH T-shaped \(^a\) | N₂O-HCCCCH Near-parallel (N-in) \(^b\) | N₂O-HCCH Near-parallel (O-in) |
|---------------------|---------------------------------|-------------------------------|--------------------------|---------------------------------|---------------------------------|
| Intermolecular distance R (Å) | 3.69                            | 3.61                         | 4.62                     | 3.43                            | 3.30                            |
| Vibrational Shift (cm\(^{-1}\)) | -6.085                          | -0.286                       | -5.688                   | +2.219                          | +5.346                          |

\(^a\) The calculated intermolecular distance for T-shaped OCS-HCCCCH is 4.52 Å.
\(^b\) For comparison the calculated intermolecular distance for N₂O-HCCCCH (O-in) is 3.60 Å.

In summary, we have observed and analyzed spectra of the most stable isomers of OCS-HCCCCH and N₂O-HCCCCH using the vibrational fundamentals of OCS and N₂O monomers in the 4 micron region as IR chromophores. Both dimers were found to have planar structure with nearly parallel monomer units. A combination of experimental evidence and theoretical calculations, at several different levels of theory, was used to identify the carriers of the infrared bands. Theoretical calculations predicted four isomers for OCS-HCCCCH and three for N₂O-HCCCCH, and the observed structures were assigned to the lowest energy structures on the potential energy surfaces. The observed spectra for OCS-DCCCCD and N₂O-DCCCCD are
entirely consistent with the normal isotopologues. Given the similarities between the most stable structures for OCS-HCCCCH with OCS-HCCH and for N₂O-HCCCCH with N₂O-HCCH, we conclude that diacetylene closely parallels acetylene upon complexation with OCS or N₂O.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found in the online version of the manuscript.
References

[1] H. Takeuchi, Global minimum geometries of acetylene clusters (HCCH)\textsubscript{n} with \( n \leq 55 \) obtained by a heuristic method combined with geometrical perturbations. J. Comput. Chem. 31 (2010) 1699.

[2] S.R. Gadre, S. D. Yeole, and N. Sahu, Quantum chemical investigations on molecular clusters. Chem. Rev. 114 (2014) 12132.

[3] N. Moazzen-Ahmadi, A.R.W. McKellar, Spectroscopy of dimers, trimers and larger clusters of linear molecules. Int. Rev. Phys. Chem. 32 (2013) 611.

[4] M. Herman, T. Földes, K. Didriche, C. Lauzin, T. Vanfleteren, Overtone spectroscopy of molecular complexes containing small polyatomic molecules. Int. Rev. Phys. Chem. 35 (2016) 243.

[5] H.O. Leung, The microwave spectrum and nuclear quadrupole hyperfine structure of HCCH-N\textsubscript{2}O. J. Chem. Phys. 107 (1997) 2232.

[6] R.A. Peebles, S.A. Peebles, R.L. Kuczkowski, H.O. Leung, Isotopic Studies, Structure and Modeling of the Nitrous Oxide– Acetylene Complex. J. Phys. Chem. A 103, (1999) 10813.

[7] S.A. Peebles and R.L. Kuczkowski, Microwave Spectrum and Structure of the Acetylene–OCS Dimer. J. Phys. Chem. A 103 (1999) 3884.

[8] S.A. Peebles and R.L. Kuczkowski, Rotational spectrum, structure and modeling of an isomer of the HCCH–OCS dimer. Chem. Phys. Lett. 312 (1999) 357.

[9] A.M. ElSohly , B.W. Hopkins , K.L. Copeland, G.S. Tschumper, Anchoring the potential energy surface of the diacetylene dimer. Mol. Phys. 107 (2009) 923.

[10] K. Matsumura, F.H. Lovas, R.D. Suenram, Structures of the NH\textsubscript{3}-HCCCCH and H\textsubscript{2}O-HCCCCH complexes by Fourier-transform microwave spectroscopy. J. Mol. Spectrosc. 144 (1990) 123.
[11] X. Yang, R.Z. Pearson, K.K. Lehmann, G. Scoles, Molecular beam infrared spectroscopy of the HCCCN–HCCH and HCN–HCCCCH van der Waals complexes. J. Chem. Phys. 105 (1996) 10725.

[12] J.P. Perdew, Density-functional approximation for the correlation energy of the inhomogeneous electron gas. Phys. Rev. B, 33 (1986) 8822.

[13] J.P. Perdew, Y. Wang, Accurate and simple analytic representation of the electron-gas correlation energy. Phys. Rev. B 45 (1992) 13244.

[14] S. Grimme, Semiempirical hybrid density functional with perturbative second-order correlation. J. Chem. Phys. 124 (2006) 034108.

[15] S. Grimme, J. Anthony, S. Ehrlich, H. Krieg, A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. J. Chem. Phys. 132 (2010) 154104.

[16] E. Papajak, H.R. Leverentz, J. Zheng, D.G. Truhlar, Efficient Diffuse Basis Sets: cc-pVxZ+ and maug-cc-pVxZ. J. Chem. Theor. Comput. 5 (2009) 1197.

[17] C. Puzzarini, M. Biczysko, V. Barone, Accurate Harmonic/Anharmonic Vibrational Frequencies for Open-Shell Systems: Performances of the B3LYP/N07D Model for Semirigid Free Radicals Benchmarked by CCSD(T) Computations. J. Chem. Theory Comput. 6 (2010) 828.

[18] A. Pietropolli Charmet, G. Quartarone, L. Ronchin, C. Tortato, A. Vavasori, Quantum chemical investigation on indole: vibrational force field and theoretical determination of its aqueous pK (a) value. J. Phys. Chem. A 117 (2013) 6846.

[19] M. Piccardo, E. Penocchio, C. Puzzarini, M. Biczysko, V. Barone, Semi-experimental equilibrium structure determinations by employing B3LYP/SNSD anharmonic force fields: validation and application to semirigid organic molecules. J. Phys. Chem. A 119 (2015) 2058.

[20] A. Pietropolli Charmet, P. Stoppa, N. Tasinato, S. Giorgianni, Computing sextic centrifugal distortion constants by DFT: A benchmark analysis on halogenated compounds. J. Mol. Spectrosc. 335 (2017) 117.
[21] A. Pietropolli Charmet, Y. Cornaton, Benchmarking fully analytic DFT force fields for vibrational spectroscopy: A study on halogenated compounds. J. Mol. Struct. 160 (2018) 455.

[22] T. Fornaro, D. Burini, M. Biczysko, V. Barone, Hydrogen-bonding effects on infrared spectra from anharmonic computations: uracil–water complexes and uracil dimers. J. Phys. Chem. A 119 (2015) 4224.

[23] J. Scaranto, A. Pietropolli Charmet, P. Stoppa, S. Giorgianni, Vinyl halides adsorbed on TiO₂ surface: FTIR spectroscopy studies and ab initio calculations. J. Mol. Struct. 741 (2005) 213.

[24] J. Scaranto, A. Pietropolli Charmet, S. Giorgianni, IR Spectroscopy and Quantum-Mechanical Studies of the Adsorption of CH₂CCIF on TiO₂. J. Phys. Chem. C 112 (2008) 9443.

[25] J. Scaranto, P. Stoppa, A. Pietropolli Charmet, S. Giorgianni, IR spectroscopy of CH₂CBrF adsorbed on TiO₂ and quantum-mechanical studies. Mol. Phys. 107 (2009) 237.

[26] S. Grimme, Supramolecular binding thermodynamics by dispersion-corrected density functional theory. Chem. Eur. J. 18 (2012) 9955.

[27] R. Sure, S. Grimme, Comprehensive benchmark of association (free) energies of realistic host–guest complexes. J. Chem. Theor. Comput. 11 (2015) 3785.

[28] N. Tasinato, A. Turchetto, P. Stoppa, A. Pietropolli Charmet, and S. Giorgianni, J. Chem. Phys. 142 (2015) 134310.

[29] S.F. Boys, F. Bernardi, The calculation of small molecular interactions by the differences of separate total energies. Some procedures with reduced errors. Mol. Phys. 19 (1970) 553.

[30] G.D. Purvis, R.J. Bartlett, A full coupled-cluster singles and doubles model: The inclusion of disconnected triples. J. Chem. Phys. 76 (1982) 1910.

[31] K. Raghavachari, G.W. Trucks, J.A. Pople, M. Head-Gordon, A fifth-order perturbation comparison of electron correlation theories. Chem. Phys. Lett. 157 (1989) 479.
[32] C. Hampel, K.A. Peterson, H.-J. Werner, A comparison of the efficiency and accuracy of the quadratic configuration interaction (QCISD), coupled cluster (CCSD), and Brueckner coupled cluster (BCCD) methods. Chem. Phys. Lett. 190 (1992) 1.

[33] R.A. Kendall, T.H. Jr Dunning, R.J. Harrison, Electron affinities of the first-row atoms revisited. Systematic basis sets and wave functions. J. Chem. Phys. 96 (1992) 6796.

[34] D.E. Woon, T.H. Jr Dunning, Gaussian basis sets for use in correlated molecular calculations. III. The atoms aluminum through argon. J. Chem. Phys. 98 (1993) 1358.

[35] K.A. Peterson, D.E. Woon, T.H. Jr Dunning, Benchmark calculations with correlated molecular wave functions. IV. The classical barrier height of the H+H$_2$→H$_2$+H reaction. J. Chem. Phys. 100 (1994) 7410.

[36] D. Feller, The use of systematic sequences of wave functions for estimating the complete basis set, full configuration interaction limit in water. J. Chem. Phys. 98 (1993) 7059.

[37] H. Helgaker, W. Klopper, H. Koch, J. Noga, Basis-set convergence of correlated calculations on water. J. Chem. Phys. 106 (1997) 9639.

[38] K.A. Peterson, T.H. Jr Dunning, Accurate correlation consistent basis sets for molecular core–valence correlation effects: The second row atoms Al–Ar, and the first row atoms B–Ne revisited. J. Chem. Phys. 117 (2002) 10548.

[39] C. Hättig, D.P. Tew, A. Köhn, Accurate and efficient approximations to explicitly correlated coupled-cluster singles and doubles, CCSD-F12. J. Chem. Phys. 132 (2010) 231102.

[40] K.A. Peterson, T.B. Adler, H.-J. Werner, Systematically convergent basis sets for explicitly correlated wavefunctions: The atoms H, He, B–Ne, and Al–ArJ. Chem. Phys. 128 (2008) 084102.

[41] K.E. Yousaf, K.A. Peterson, Optimized auxiliary basis sets for explicitly correlated methods. J. Chem. Phys. 129 (2008) 184108.

[42] K.E. Yousaf, K.A. Peterson, Optimized complementary auxiliary basis sets for explicitly correlated methods: aug-cc-pVnZ orbital basis sets. Chem. Phys. Lett. 476 (2009) 303.
[43] H.H. Nielsen, The vibration-rotation energies of molecules. Rev. Mod. Phys. 23 (1951) 90.

[44] G. Amat, H.H. Nielsen, G. Tarrago, Rotation-vibration of Polyatomic Molecules, New York: Marcel Decker, Amsterdam, 1971.

[45] I. Carnimeo, C. Puzzarini, N. Tasinato, P. Stoppa, A. Pietropolli Charmet, M. Biczysko, C. Cappelli, V. Barone, Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds. J. Chem. Phys. 139 (2013) 074310.

[46] A. Pietropolli Charmet, P. Stoppa, N. Tasinato, S. Giorgianni, V. Barone, M. Biczysko, J. Bloino, C. Cappelli, I. Carnimeo, C. Puzzarini, An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. J. Chem. Phys. 139 (2013) 164302.

[47] A. Pietropolli Charmet, P. Stoppa, N. Tasinato, S. Giorgianni, and A. Gambi, Study of the Vibrational Spectra and Absorption Cross Sections of 1-Chloro-1-fluoroethene by a Joint Experimental and Ab Initio Approach. J. Phys. Chem. A 120 (2016) 8369.

[48] M. J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery, Jr., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, O. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, and D.J. Fox, Gaussian 09, Revision E.01; Gaussian, Inc., Wallingford CT, 2013.

[49] A. Pietropolli Charmet, P. Stoppa, S. Giorgianni, J. Bloino, N. Tasinato, I. Carnimeo, M. Biczysko, C. Puzzarini, Accurate vibrational–rotational parameters and infrared intensities of 1-
Bromo-1-fluoroethene: a joint experimental analysis and ab initio study. J. Phys. Chem. A 121 (2017) 3305.

[50] H.-J. Werner, P. J. Knowles, G. Knizia, F. R. Manby and M. Schütz, WIREs Comput Mol Sci 2 (2012) 242.

[51] MOLPRO, version 2015.1, a package of ab initio programs, H.-J. Werner, P.J. Knowles, G. Knizia, F.R. Manby, M. Schütz, P. Celani, W. Gyorffy, D. Kats, T. Korona, R. Lindh, A. Mitrushenkov, G. Rauhut, K.R. Shamasundar, T.B. Adler, R.D. Amos, A. Bernhardsson, A. Berning, D.L. Cooper, M.J. O. Deegan, A.J. Dobbyn, F. Eckert, E. Goll, C. Hampel, A. Hesselmann, G. Hetzer, T. Hrenar, G. Jansen, C. Köppl, Y. Liu, A.W. Lloyd, R.A. Mata, A.J. May, S.J. McNicholas, W. Meyer, M.E. Mura, A. Nicklass, D.P. O'Neill, P. Palmieri, D. Peng, K. Pflüger, R. Pitzer, M. Reiher, T. Shiozaki, H. Stoll, A.J. Stone, R. Tarroni, T. Thorsteinsson, and M. Wang, , see http://www.molpro.net.

[52] R. Lindh, The reduced multiplication scheme of the Rys-Gauss quadrature for 1st order integral derivatives. Theor. Chim. Acta 85 (1993) 423.

[53] T. Hrenar, G. Rauhut, H.-J. Werner, Impact of local and density fitting approximations on harmonic vibrational frequencies. J. Phys. Chem. A 110 (2006) 2060.

[54] M.J.O. Deegan and P.J. Knowles, Perturbative corrections to account for triple excitations in closed and open shell coupled cluster theories. Chem. Phys. Lett. 227 (1994) 321.

[55] T.B. Adler, G. Knizia, and H.-J. Werner, A simple and efficient CCSD (T)-F12 approximation. J. Chem. Phys. 127 (2007) 221106.

[56] H.-J. Werner, G. Knizia, and F.R. Manby, Explicitly correlated coupled cluster methods with pair-specific geminals. Mol. Phys. 109 (2011) 407.

[57] M. Dehghany, M. Afshari, Z. Abusara, C. Van Eck, N. Moazzen-Ahmadi, Isotope effects in the infrared spectra of the polar and nonpolar isomers of N2O dimer. J. Mol. Spectrosc. 247 (2008) 123.
[58] M. Rezaei, K.H. Michaelian, N. Moazzen-Ahmadi, Nonpolar nitrous oxide dimer: Observation of combination bands of \((^{14}\text{N}_2\text{O})_2\) and \((^{15}\text{N}_2\text{O})_2\) involving the torsion and antigeared bending modes. J. Chem. Phys. 136 (2012) 124308.

[59] M. Rezaei, S. Sheybani-Deloui, N. Moazzen-Ahmadi, K.H. Michaelian, A.R.W. McKellar, CO dimer: The infrared spectrum revisited. J. Phys. Chem. A 117 (2013) 9612.

[60] H.D. Verkuijssse, L. Brandsma, A detailed procedure for the preparation of butadiyne. Synth. Commun. 21 (1991) 657.

[61] T. Etoh, K. Matsumura, T. Tanaka, Microwave spectrum of monodeuterated diacetylene due to vibrationally induced dipole moment. J. Mol. Spectrosc. 89, 511 (1981).

[62] C.M. Western, PGOPHER, a program for simulating rotational structure version 8.0, 2014, University of Bristol Research Data Repository, doi:10.5523/bris.huflggvpuc1zvliqed497r2

[63] W. Gordy and R. L. Cook, Microwave Molecular Spectra (Wiley, New York, 1984).

[64] S. Batsanov, Van der Waals radii of elements. Inorg. Mater. (Transl. of Neorg. Mater.), 37 (2001) 871–885.
Table A-1. Observed and calculated transitions for OCS-HCCCCH in the region of the \( v_1 \) fundamental band of OCS (units of cm\(^{-1}\)).

| J' | Ka' | Kc' | J'' | Ka'' | Kc'' | Observed       | Calculated      | Obs-Calc | Weight |
|----|-----|-----|-----|------|------|----------------|----------------|----------|--------|
| 9  | 5   | 5   | 10  | 6    | 4    | 2054.78574     | 2054.78454     | 0.00119  | 0.25   |
| 9  | 5   | 4   | 10  | 6    | 5    | 2054.78574     | 2054.78566     | 0.00007  | 0.25   |
| 7  | 6   | 1   | 8   | 7    | 2    | 2054.80586     | 2054.80560     | 0.00025  | 0.25   |
| 7  | 6   | 2   | 8   | 7    | 1    | 2054.80586     | 2054.80560     | 0.00025  | 0.25   |
| 9  | 4   | 6   | 10  | 5    | 5    | 2054.90163     | 2054.90135     | 0.00027  | 0.25   |
| 7  | 5   | 3   | 8   | 6    | 2    | 2054.92716     | 2054.92732     | -0.00015 | 0.25   |
| 7  | 5   | 2   | 8   | 6    | 3    | 2054.92716     | 2054.92740     | -0.00023 | 0.25   |
| 8  | 4   | 4   | 9   | 5    | 5    | 2054.98389     | 2054.98370     | 0.00018  | 1.00   |
| 6  | 5   | 2   | 7   | 6    | 1    | 2054.99872     | 2054.99886     | -0.00014 | 0.25   |
| 6  | 5   | 1   | 7   | 6    | 2    | 2054.99872     | 2054.99887     | -0.00015 | 0.25   |
| 6  | 5   | 1   | 7   | 6    | 2    | 2054.99872     | 2054.99887     | -0.00015 | 0.25   |
| 6  | 5   | 2   | 7   | 6    | 1    | 2054.99872     | 2054.99886     | -0.00014 | 0.25   |
| 7  | 4   | 4   | 8   | 5    | 3    | 2055.04882     | 2055.04872     | 0.00010  | 1.00   |
| 7  | 4   | 3   | 8   | 5    | 4    | 2055.05140     | 2055.05131     | 0.00009  | 1.00   |
| 5  | 5   | 1   | 6   | 6    | 0    | 2055.07068     | 2055.07044     | 0.00023  | 0.25   |
| 5  | 5   | 0   | 6   | 6    | 1    | 2055.07068     | 2055.07044     | 0.00023  | 0.25   |
| 6  | 4   | 2   | 7   | 5    | 3    | 2055.12095     | 2055.12124     | -0.00028 | 0.25   |
| 6  | 4   | 3   | 7   | 5    | 2    | 2055.12095     | 2055.12052     | 0.00042  | 0.25   |
| 8  | 3   | 5   | 9   | 4    | 6    | 2055.14721     | 2055.14712     | 0.00008  | 1.00   |
| 7  | 3   | 5   | 8   | 4    | 4    | 2055.15611     | 2055.15621     | -0.00009 | 1.00   |
| 5  | 4   | 1   | 6   | 5    | 2    | 2055.19192     | 2055.19223     | -0.00031 | 0.25   |
| 5  | 4   | 2   | 6   | 5    | 1    | 2055.19192     | 2055.19209     | -0.00017 | 0.25   |
| 7  | 3   | 4   | 8   | 4    | 5    | 2055.19521     | 2055.19534     | -0.00013 | 1.00   |
| 6  | 3   | 4   | 7   | 4    | 3    | 2055.23641     | 2055.23653     | -0.00011 | 1.00   |
| 6  | 3   | 3   | 7   | 4    | 4    | 2055.25275     | 2055.25291     | -0.00015 | 1.00   |
| 4  | 4   | 0   | 5   | 5    | 1    | 2055.26320     | 2055.26362     | -0.00042 | 0.25   |
| 4 | 4 | 1 | 5 | 5 | 0 | 2055.26320 | 2055.26361 | -0.00040 | 0.25 |
|---|---|---|---|---|---|------------|------------|----------|------|
| 6 | 2 | 5 | 7 | 3 | 4 | 2055.29749 | 2055.29772 | -0.00022 | 1.00 |
| 5 | 3 | 3 | 6 | 4 | 2 | 2055.31161 | 2055.31191 | -0.00029 | 1.00 |
| 5 | 3 | 2 | 6 | 4 | 3 | 2055.31750 | 2055.31748 | 0.00001 | 1.00 |
| 8 | 2 | 6 | 9 | 3 | 7 | 2055.36010 | 2055.36014 | -0.00003 | 1.00 |
| 11 | 3 | 9 | 12 | 4 | 8 | 2055.36796 | 2055.36715 | 0.00080 | 1.00 |
| 5 | 1 | 5 | 6 | 2 | 4 | 2055.37112 | 2055.37133 | -0.00020 | 1.00 |
| 11 | 3 | 8 | 12 | 2 | 11 | 2055.37506 | 2055.37462 | 0.00043 | 1.00 |
| 7 | 2 | 5 | 8 | 3 | 6 | 2055.39129 | 2055.39159 | -0.00029 | 1.00 |
| 5 | 2 | 4 | 6 | 3 | 3 | 2055.40216 | 2055.40241 | -0.00025 | 1.00 |
| 11 | 0 | 11 | 12 | 1 | 12 | 2055.43818 | 2055.43790 | 0.00027 | 0.25 |
| 11 | 1 | 11 | 12 | 0 | 12 | 2055.43818 | 2055.43814 | 0.00003 | 0.25 |
| 10 | 2 | 9 | 11 | 3 | 8 | 2055.44544 | 2055.44539 | 0.00004 | 1.00 |
| 3 | 3 | 0 | 4 | 4 | 1 | 2055.45660 | 2055.45688 | -0.00028 | 0.25 |
| 3 | 3 | 1 | 4 | 4 | 0 | 2055.45660 | 2055.45668 | -0.00008 | 0.25 |
| 5 | 2 | 3 | 6 | 3 | 3 | 2055.47156 | 2055.47185 | -0.00029 | 1.00 |
| 9 | 1 | 8 | 10 | 2 | 9 | 2055.48121 | 2055.48133 | -0.00011 | 1.00 |
| 4 | 2 | 3 | 5 | 3 | 2 | 2055.49264 | 2055.49289 | -0.00025 | 1.00 |
| 10 | 1 | 10 | 11 | 0 | 11 | 2055.49706 | 2055.49710 | -0.00004 | 0.25 |
| 10 | 0 | 10 | 11 | 1 | 11 | 2055.49706 | 2055.49658 | 0.00048 | 0.25 |
| 9 | 2 | 8 | 10 | 1 | 9 | 2055.51063 | 2055.51052 | 0.00011 | 1.00 |
| 4 | 2 | 2 | 5 | 3 | 3 | 2055.52359 | 2055.52391 | -0.00031 | 1.00 |
| 8 | 1 | 7 | 9 | 2 | 8 | 2055.52909 | 2055.52920 | -0.00010 | 1.00 |
| 8 | 2 | 7 | 9 | 1 | 8 | 2055.57994 | 2055.57996 | -0.00002 | 1.00 |
| 3 | 2 | 1 | 4 | 3 | 2 | 2055.58407 | 2055.58425 | -0.00017 | 1.00 |
| 8 | 1 | 8 | 9 | 0 | 9 | 2055.61533 | 2055.61541 | -0.00007 | 1.00 |
| 8 | 1 | 8 | 9 | 0 | 9 | 2055.61541 | 2055.61541 | 0.00000 | 1.00 |
| 3 | 1 | 3 | 4 | 2 | 2 | 2055.63864 | 2055.63860 | 0.00004 | 1.00 |
| 2 | 2 | 1 | 3 | 3 | 0 | 2055.64887 | 2055.64891 | -0.00003 | 1.00 |
| 7 | 2 | 6 | 8 | 1 | 7 | 2055.65504 | 2055.65542 | -0.00037 | 1.00 |
| 7 | 0 | 7 | 8 | 1 | 8 | 2055.67033 | 2055.67035 | -0.00002 | 1.00 |
| 7 | 1 | 7 | 8 | 0 | 8 | 2055.67517 | 2055.67520 | -0.00003 | 1.00 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10| 2 | 9|   | 10| 3 | 8|   | 2055.70243| 2055.70254| -0.00011| 1.00|
| 10| 3 | 8|   | 10| 4 | 7|   | 2055.70452| 2055.70451| 0.00000| 1.00|
| 9 | 3 | 7|   | 9 | 4 | 6|   | 2055.72130| 2055.72148| -0.00017| 1.00|
| 6 | 0 | 6|   | 7 | 1 | 7|   | 2055.72639| 2055.72645| -0.00006| 1.00|
| 7 | 3 | 4|   | 7 | 4 | 3|   | 2055.76826| 2055.76864| -0.00038| 1.00|
| 8 | 0 | 8|   | 8 | 1 | 7|   | 2055.77681| 2055.77681| 0.00000| 1.00|
| 5 | 0 | 5|   | 6 | 1 | 6|   | 2055.78047| 2055.78064| -0.00017| 1.00|
| 10| 1 | 9|   | 10| 2 | 8|   | 2055.78362| 2055.78354| 0.00008| 1.00|
| 2 | 1 | 1|   | 3 | 2 | 2|   | 2055.79137| 2055.79139| -0.00002| 1.00|
| 5 | 1 | 5|   | 6 | 0 | 6|   | 2055.79864| 2055.79879| -0.00014| 1.00|
| 7 | 2 | 6|   | 7 | 3 | 5|   | 2055.80888| 2055.80889| -0.00000| 1.00|
| 5 | 2 | 4|   | 6 | 1 | 5|   | 2055.82692| 2055.82657| 0.00035| 1.00|
| 1 | 1 | 0|   | 2 | 2 | 1|   | 2055.84992| 2055.84955| 0.00036| 1.00|
| 4 | 1 | 4|   | 5 | 0 | 5|   | 2055.86473| 2055.86454| 0.00018| 1.00|
| 4 | 2 | 2|   | 4 | 3 | 1|   | 2055.88015| 2055.87996| 0.00019| 1.00|
| 5 | 2 | 3|   | 5 | 3 | 2|   | 2055.89600| 2055.89603| -0.00003| 1.00|
| 2 | 0 | 2|   | 3 | 1 | 3|   | 2055.93210| 2055.93187| 0.00023| 1.00|
| 3 | 1 | 3|   | 3 | 2 | 2|   | 2055.94540| 2055.94520| 0.00019| 1.00|
| 7 | 1 | 6|   | 7 | 2 | 5|   | 2055.96164| 2055.96176| -0.00011| 1.00|
| 5 | 0 | 5|   | 5 | 1 | 4|   | 2055.97204| 2055.97218| -0.00014| 1.00|
| 1 | 0 | 1|   | 2 | 1 | 2|   | 2055.98462| 2055.98455| 0.00007| 1.00|
| 6 | 1 | 5|   | 6 | 2 | 4|   | 2055.99379| 2055.99393| -0.00014| 1.00|
| 2 | 1 | 1|   | 2 | 2 | 0|   | 2056.00104| 2056.00097| 0.00006| 1.00|
| 2 | 1 | 2|   | 3 | 0 | 3|   | 2056.00820| 2056.00808| 0.00012| 1.00|
| 4 | 1 | 3|   | 4 | 2 | 2|   | 2056.01557| 2056.01574| -0.00017| 1.00|
| 4 | 0 | 4|   | 4 | 1 | 3|   | 2056.02294| 2056.02297| -0.00003| 1.00|
| 0 | 0 | 0|   | 1 | 1 | 1|   | 2056.04269| 2056.04261| 0.00008| 1.00|
| 3 | 0 | 3|   | 3 | 1 | 2|   | 2056.06072| 2056.06081| -0.00009| 1.00|
| 1 | 0 | 1|   | 1 | 1 | 0|   | 2056.10038| 2056.10049| -0.00011| 1.00|
| 1 | 1 | 0|   | 1 | 0 | 1|   | 2056.23532| 2056.23551| -0.00019| 1.00|
| 2 | 1 | 1|   | 2 | 0 | 2|   | 2056.24956| 2056.24975| -0.00019| 1.00|
| 3 | 1 | 2|   | 3 | 0 | 3|   | 2056.27402| 2056.27431| -0.00029| 1.00|
1 1 1 0 0 0 2056.29430 2056.29350 0.00079 1.00
1 1 1 0 0 0 2056.29430 2056.29350 0.00079 1.00
1 1 1 0 0 0 2056.29430 2056.29350 0.00079 1.00
4 1 3 4 0 4 2056.31152 2056.31146 0.00005 1.00
4 2 2 4 1 3 2056.31873 2056.31866 0.00006 1.00
3 2 1 3 1 2 2056.32431 2056.32431 0.00000 1.00
3 0 3 2 1 2 2056.32748 2056.32735 0.00013 1.00
2 2 0 2 1 1 2056.33499 2056.33473 0.00026 1.00
6 2 4 6 1 5 2056.33845 2056.33845 -0.00000 1.00
2 1 2 1 0 1 2056.35146 2056.35131 0.00015 1.00
5 1 4 5 0 5 2056.36143 2056.36140 0.00003 1.00
7 2 5 7 1 6 2056.36954 2056.36939 0.00015 1.00
3 2 2 3 1 3 2056.39009 2056.39002 0.00007 1.00
8 3 5 8 2 6 2056.39469 2056.39451 0.00018 1.00
4 0 4 3 0 3 2056.43246 2056.43235 0.00010 1.00
5 3 2 5 2 3 2056.43745 2056.43758 -0.00012 1.00
5 2 4 5 1 5 2056.44988 2056.44984 0.00004 1.00
5 0 5 4 1 4 2056.46968 2056.46959 0.00009 1.00
5 1 5 4 0 4 2056.50167 2056.50172 -0.00005 1.00
6 1 5 5 2 4 2056.50626 2056.50648 -0.00021 1.00
7 3 5 7 2 6 2056.52256 2056.52255 0.00000 1.00
6 0 6 5 1 5 2056.53447 2056.53447 0.00000 1.00
8 4 4 8 3 5 2056.54053 2056.54061 -0.00007 1.00
8 4 4 8 3 5 2056.54053 2056.54061 -0.00007 1.00
8 4 4 8 3 5 2056.54053 2056.54061 -0.00007 1.00
3 2 2 2 1 1 2056.54412 2056.54405 0.00007 1.00
3 2 2 2 1 1 2056.54412 2056.54405 0.00007 1.00
3 2 2 2 1 1 2056.54412 2056.54405 0.00007 1.00
8 3 6 8 2 7 2056.54984 2056.54983 0.00000 1.00
8 3 6 8 2 7 2056.54984 2056.54983 0.00000 1.00
8 3 6 8 2 7 2056.54984 2056.54983 0.00000 1.00
6 1 6 5 0 5 2056.55276 2056.55260 0.00015 1.00
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 7 | 4 | 3 | 7 | 3 | 4 | 2056.56282 | 2056.56280 | 0.00002 | 1.00 |
| 8 | 2 | 6 | 7 | 3 | 5 | 2056.56882 | 2056.569097 | -0.00026 | 1.00 |
| 6 | 4 | 2 | 6 | 3 | 3 | 2056.57806 | 2056.57818 | -0.00011 | 1.00 |
| 5 | 4 | 1 | 5 | 3 | 2 | 2056.58687 | 2056.58725 | -0.00038 | 1.00 |
| 7 | 1 | 7 | 6 | 0 | 6 | 2056.60589 | 2056.60576 | 0.00012 | 1.00 |
| 9 | 2 | 8 | 9 | 1 | 9 | 2056.63641 | 2056.63631 | 0.00009 | 1.00 |
| 5 | 2 | 4 | 4 | 1 | 3 | 2056.64049 | 2056.64040 | 0.00008 | 1.00 |
| 8 | 0 | 8 | 7 | 1 | 7 | 2056.65586 | 2056.65583 | 0.00002 | 1.00 |
| 8 | 1 | 8 | 7 | 0 | 7 | 2056.66063 | 2056.66067 | -0.00004 | 1.00 |
| 6 | 2 | 5 | 5 | 1 | 4 | 2056.68088 | 2056.68096 | -0.00008 | 1.00 |
| 3 | 3 | 1 | 2 | 2 | 0 | 2056.68476 | 2056.68458 | 0.00017 | 1.00 |
| 3 | 3 | 1 | 2 | 2 | 0 | 2056.68476 | 2056.68458 | 0.00017 | 1.00 |
| 3 | 3 | 0 | 2 | 2 | 1 | 2056.68655 | 2056.68667 | -0.00012 | 1.00 |
| 3 | 3 | 0 | 2 | 2 | 1 | 2056.68655 | 2056.68667 | -0.00012 | 1.00 |
| 4 | 2 | 2 | 3 | 1 | 3 | 2056.69637 | 2056.69623 | 0.00013 | 1.00 |
| 8 | 5 | 3 | 8 | 4 | 4 | 2056.70012 | 2056.70008 | 0.00003 | 1.00 |
| 9 | 0 | 9 | 8 | 1 | 8 | 2056.71423 | 2056.71428 | -0.00005 | 1.00 |
| 9 | 1 | 9 | 8 | 0 | 8 | 2056.71641 | 2056.71665 | -0.00023 | 1.00 |
| 7 | 2 | 6 | 6 | 1 | 5 | 2056.71895 | 2056.71918 | -0.00023 | 1.00 |
| 8 | 2 | 7 | 7 | 1 | 6 | 2056.75793 | 2056.75804 | -0.00010 | 1.00 |
| 4 | 3 | 1 | 3 | 2 | 2 | 2056.76120 | 2056.76120 | 0.00000 | 1.00 |
| 10 | 0 | 10 | 9 | 1 | 9 | 2056.77257 | 2056.77205 | 0.00052 | 0.25 |
| 10 | 1 | 10 | 9 | 0 | 9 | 2056.77257 | 2056.77317 | -0.00060 | 0.25 |
| 9 | 2 | 8 | 8 | 1 | 7 | 2056.80010 | 2056.80009 | 0.00000 | 1.00 |
| 5 | 3 | 3 | 4 | 2 | 2 | 2056.81014 | 2056.81019 | -0.00005 | 1.00 |
| 10 | 1 | 9 | 9 | 2 | 8 | 2056.81691 | 2056.81725 | -0.00034 | 1.00 |
| 11 | 1 | 11 | 10 | 0 | 10 | 2056.82965 | 2056.82996 | -0.00030 | 0.25 |
| 11 | 0 | 11 | 10 | 1 | 10 | 2056.82965 | 2056.82943 | 0.00021 | 0.25 |
| 10 | 2 | 9 | 9 | 1 | 8 | 2056.84647 | 2056.84642 | 0.00004 | 1.00 |
| 6 | 3 | 4 | 5 | 2 | 3 | 2056.86120 | 2056.86123 | -0.00003 | 1.00 |
| 12 | 1 | 12 | 11 | 0 | 11 | 2056.88645 | 2056.88682 | -0.00037 | 0.25 |
| 12 | 0 | 12 | 11 | 1 | 11 | 2056.88645 | 2056.88658 | -0.00013 | 0.25 |
11 2 10 10 1 9 2056.89657 2056.89662 -0.00004 1.00
7 3 5 6 2 4 2056.90371 2056.90373 -0.00002 1.00
6 3 3 5 2 4 2056.93080 2056.93073 0.00007 1.00
8 3 6 7 2 5 2056.93892 2056.93894 -0.00002 1.00
12 3 9 11 2 10 2056.94087 2056.94120 -0.00033 1.00
9 3 7 8 2 6 2056.96887 2056.96887 -0.00000 1.00
10 3 8 9 2 7 2056.99650 2056.99621 0.00029 1.00
14 0 14 13 1 13 2057.00025 2057.00048 -0.00022 0.25
14 1 14 13 0 13 2057.00025 2057.00053 -0.00027 0.25
13 2 12 12 3 9 2057.00415 2057.00426 -0.00011 1.00
6 4 3 5 3 2 2057.01575 2057.01584 -0.00008 1.00
6 4 2 5 3 3 2057.02139 2057.02142 -0.00003 1.00
11 3 9 10 2 8 2057.02495 2057.02417 0.00077 1.00
5 5 0 4 4 1 2057.07104 2057.07097 0.00006 0.25
5 5 1 4 4 0 2057.07104 2057.07096 0.00008 0.25
7 4 4 6 3 3 2057.07910 2057.07921 -0.00010 1.00
7 4 3 6 3 4 2057.09541 2057.09562 -0.00020 1.00
16 2 14 15 1 15 2057.11431 2057.11399 0.00031 0.25
16 1 16 15 2 13 2057.11431 2057.11400 0.00030 0.25
8 4 5 7 3 4 2057.13517 2057.13538 -0.00020 1.00
6 5 2 5 4 1 2057.14135 2057.14136 -0.00000 0.25
6 5 1 5 4 2 2057.14135 2057.14150 -0.00015 0.25
8 3 5 7 2 6 2057.15555 2057.15565 -0.00010 1.00
9 4 6 8 3 5 2057.18222 2057.18201 0.00021 0.25
7 5 2 6 4 3 2057.21133 2057.21189 -0.00056 0.25
7 5 3 6 4 2 2057.21133 2057.21118 0.00015 0.25
6 6 0 5 5 1 2057.26372 2057.26347 0.00025 0.25
6 6 1 5 5 0 2057.26372 2057.26346 0.00025 0.25
8 5 4 7 4 3 2057.27946 2057.27974 -0.00027 1.00
8 5 3 7 4 4 2057.28250 2057.28233 0.00016 1.00
7 6 2 6 5 1 2057.33372 2057.33386 -0.00014 0.25
7 6 1 6 5 2 2057.33372 2057.33388 -0.00015 0.25
| 9 5 5 8 4 | 4 2057.34601 2057.34578 0.00023 0.25 |
| 9 5 4 8 4 | 5 2057.35372 2057.35342 0.00029 0.25 |
| 8 6 2 7 5 | 3 2057.40446 2057.40406 0.00039 0.25 |
| 8 6 3 7 5 | 2 2057.40446 2057.40396 0.00047 0.25 |
| 13 6 8 12 | 5 7 2057.73328 2057.73461 -0.00133 0.00 |
| 10 7 3 11 | 8 4 2054.46520 2054.46885 -0.00365 0.00 |
| 10 7 4 11 | 8 3 2054.46520 2054.46884 -0.00364 0.00 |
| 11 7 4 12 | 8 5 2054.39494 2054.39724 -0.00230 0.00 |
| 11 7 5 12 | 8 4 2054.39494 2054.39722 -0.00228 0.00 |
| 12 7 5 13 | 8 6 2054.32388 2054.32583 -0.00195 0.00 |
| 12 7 6 13 | 8 5 2054.32388 2054.32578 -0.00190 0.00 |
| 12 7 5 11 | 6 6 2057.80230 2057.80476 -0.00245 0.00 |
| 12 7 6 11 | 6 5 2057.80230 2057.80429 -0.00199 0.00 |
| 13 7 6 14 | 8 7 2054.25311 2054.25477 -0.00166 0.00 |
| 13 7 7 14 | 8 6 2054.25311 2054.25459 -0.00148 0.00 |
| 9 8 1 8 7 | 2 2057.71409 2057.71834 -0.00424 0.00 |
| 9 8 2 8 7 | 1 2057.71409 2057.71834 -0.00424 0.00 |
| 9 8 1 10 | 9 2 2054.41467 2054.41912 -0.00445 0.00 |
| 9 8 2 10 | 9 1 2054.41467 2054.41912 -0.00445 0.00 |
| 10 8 2 9 | 7 3 2057.78517 2057.78840 -0.00323 0.00 |
| 10 8 3 9 | 7 2 2057.78517 2057.78840 -0.00323 0.00 |
| 10 8 2 11 | 9 3 2054.34389 2054.34725 -0.00336 0.00 |
| 10 8 3 11 | 9 2 2054.34389 2054.34725 -0.00336 0.00 |
| 11 8 3 10 | 7 4 2057.85517 2057.85823 -0.00305 0.00 |
| 11 8 4 10 | 7 3 2057.85517 2057.85823 -0.00305 0.00 |
| 11 8 3 12 | 9 4 2054.27241 2054.27539 -0.00298 0.00 |
| 11 8 4 12 | 9 3 2054.27241 2054.27539 -0.00298 0.00 |
| 12 8 4 11 | 7 5 2057.92511 2057.92777 -0.00265 0.00 |
| 12 8 5 11 | 7 4 2057.92511 2057.92776 -0.00264 0.00 |
| 12 8 4 13 | 9 5 2054.20064 2054.20360 -0.00296 0.00 |
| 12 8 5 13 | 9 4 2054.20064 2054.20359 -0.00295 0.00 |
| 13 8 5 12 | 7 6 2057.99424 2057.99694 -0.00270 0.00 |
|     |     |     |     |     |     |     | 13 | 8 | 6 | 12 | 7 | 5 | 2057.99424 | 2057.99689 | -0.00264 | 0.00 |
|-----|-----|-----|-----|-----|-----|-----|-----|---|---|----|---|---|-----------------|-----------------|----------|-----|
| 9   | 9   | 0   | 8   | 8   | 1   | 2057.83664 | 2057.84024 | -0.00359 | 0.00 |
| 9   | 9   | 1   | 8   | 8   | 0   | 2057.83664 | 2057.84024 | -0.00359 | 0.00 |
| 9   | 9   | 0   | 10  | 10  | 1   | 2054.29437 | 2054.29783 | -0.00346 | 0.00 |
| 9   | 9   | 1   | 10  | 10  | 0   | 2054.29437 | 2054.29783 | -0.00346 | 0.00 |
| 10  | 9   | 1   | 9   | 8   | 2   | 2057.90713 | 2057.91037 | -0.00323 | 0.00 |
| 10  | 9   | 2   | 9   | 8   | 1   | 2057.90713 | 2057.91037 | -0.00323 | 0.00 |
| 10  | 9   | 1   | 11  | 10  | 2   | 2054.22240 | 2054.22592 | -0.00352 | 0.00 |
| 10  | 9   | 2   | 11  | 10  | 1   | 2054.22240 | 2054.22592 | -0.00352 | 0.00 |
| 11  | 9   | 2   | 10  | 8   | 3   | 2057.97724 | 2057.98034 | -0.00310 | 0.00 |
| 11  | 9   | 3   | 10  | 8   | 2   | 2057.97724 | 2057.98034 | -0.00310 | 0.00 |
| 13  | 9   | 4   | 14  | 10  | 5   | 2054.00690 | 2054.01007 | -0.00317 | 0.00 |
| 13  | 9   | 5   | 14  | 10  | 4   | 2054.00690 | 2054.01007 | -0.00317 | 0.00 |
| 11  | 10  | 1   | 10  | 9   | 2   | 2058.09945 | 2058.10225 | -0.00279 | 0.00 |
| 11  | 10  | 2   | 10  | 9   | 1   | 2058.09945 | 2058.10225 | -0.00279 | 0.00 |
| 11  | 10  | 1   | 12  | 11  | 2   | 2054.03009 | 2054.03277 | -0.00268 | 0.00 |
| 11  | 10  | 2   | 12  | 11  | 1   | 2054.03009 | 2054.03277 | -0.00268 | 0.00 |
| 12  | 10  | 2   | 11  | 9   | 3   | 2058.16962 | 2058.17213 | -0.00250 | 0.00 |
| 12  | 10  | 3   | 11  | 9   | 2   | 2058.16962 | 2058.17213 | -0.00250 | 0.00 |
| 13  | 10  | 3   | 12  | 9   | 4   | 2058.23988 | 2058.24184 | -0.00196 | 0.00 |
| 13  | 10  | 4   | 12  | 9   | 3   | 2058.23988 | 2058.24184 | -0.00196 | 0.00 |
| 14  | 10  | 4   | 13  | 9   | 5   | 2058.30437 | 2058.31134 | -0.00697 | 0.00 |
| 14  | 10  | 5   | 13  | 9   | 4   | 2058.30437 | 2058.31134 | -0.00697 | 0.00 |
| 11  | 11  | 0   | 10  | 10  | 1   | 2058.22057 | 2058.22406 | -0.00348 | 0.00 |
| 11  | 11  | 1   | 10  | 10  | 0   | 2058.22057 | 2058.22406 | -0.00348 | 0.00 |
| 12  | 11  | 1   | 11  | 10  | 2   | 2058.29059 | 2058.29397 | -0.00337 | 0.00 |
| 12  | 11  | 2   | 11  | 10  | 1   | 2058.29059 | 2058.29397 | -0.00337 | 0.00 |
Table A-2. Observed and calculated transitions for OCS-DCCCD in the region of the $v_1$ fundamental band of OCS (units of cm$^{-1}$).

| J'  | Ka' | Kc' | J"  | Ka" | Kc" | Observed   | Calculated  | Obs-Calc | Weight |
|-----|-----|-----|-----|-----|-----|------------|-------------|----------|--------|
| 11  | 5   | 6   | 12  | 6   | 7   | 2054.55716 | 2054.55717  | -0.00001 | 1.00   |
| 9   | 6   | 3   | 10  | 7   | 4   | 2054.57229 | 2054.57229  | -0.00000 | 0.25   |
| 9   | 6   | 4   | 10  | 7   | 3   | 2054.57229 | 2054.57224  | 0.00005  | 0.25   |
| 7   | 7   | 0   | 8   | 8   | 1   | 2054.59903 | 2054.59874  | 0.00028  | 0.25   |
| 7   | 7   | 1   | 8   | 8   | 0   | 2054.59903 | 2054.59874  | 0.00028  | 0.25   |
| 10  | 5   | 6   | 11  | 6   | 5   | 2054.61494 | 2054.61503  | -0.00009 | 1.00   |
| 8   | 6   | 2   | 9   | 7   | 3   | 2054.64101 | 2054.64100  | 0.00001  | 0.25   |
| 8   | 6   | 3   | 9   | 7   | 2   | 2054.64101 | 2054.64099  | 0.00002  | 0.25   |
| 7   | 6   | 1   | 8   | 7   | 2   | 2054.70992 | 2054.70987  | 0.00004  | 0.25   |
| 7   | 6   | 2   | 8   | 7   | 1   | 2054.70992 | 2054.70987  | 0.00005  | 0.25   |
| 8   | 5   | 3   | 9   | 6   | 4   | 2054.75274 | 2054.75293  | -0.00018 | 0.25   |
| 8   | 5   | 4   | 9   | 6   | 3   | 2054.75274 | 2054.75247  | 0.00027  | 0.25   |
| 10  | 4   | 6   | 11  | 5   | 7   | 2054.76227 | 2054.76242  | -0.00014 | 1.00   |
| 6   | 6   | 0   | 7   | 7   | 1   | 2054.77895 | 2054.77881  | 0.00013  | 0.25   |
| 6   | 6   | 1   | 7   | 7   | 0   | 2054.77895 | 2054.77881  | 0.00013  | 0.25   |
| 7   | 5   | 2   | 8   | 6   | 3   | 2054.82113 | 2054.82124  | -0.00011 | 0.25   |
| 7   | 5   | 3   | 8   | 6   | 2   | 2054.82113 | 2054.82114  | -0.00000 | 0.25   |
| 9   | 4   | 6   | 10  | 5   | 5   | 2054.78812 | 2054.78808  | 0.00004  | 1.00   |
| 6   | 5   | 1   | 7   | 6   | 2   | 2054.89003 | 2054.88996  | 0.00007  | 0.25   |
| 6   | 5   | 2   | 7   | 6   | 1   | 2054.89003 | 2054.88994  | 0.00009  | 0.25   |
| 7   | 4   | 4   | 8   | 5   | 3   | 2054.93185 | 2054.93173  | 0.00012  | 1.00   |
| 5   | 5   | 0   | 6   | 6   | 1   | 2054.95901 | 2054.95883  | 0.00018  | 0.25   |
| 5   | 5   | 1   | 6   | 6   | 0   | 2054.95901 | 2054.95883  | 0.00018  | 0.25   |
| 5   | 4   | 1   | 6   | 5   | 2   | 2055.07020 | 2055.07010  | 0.00009  | 0.25   |
| 5   | 4   | 2   | 6   | 5   | 1   | 2055.07020 | 2055.06992  | 0.00027  | 0.25   |
| 12 | 4 | 8 | 13 | 3 | 11 | 2055.09382 | 2055.09400 | -0.00018 | 1.00 |
| 6 | 3 | 3 | 7 | 4 | 4 | 2055.12487 | 2055.12454 | 0.00032 | 1.00 |
| 4 | 4 | 0 | 5 | 5 | 1 | 2055.13889 | 2055.13882 | 0.00009 | 0.25 |
| 4 | 4 | 1 | 5 | 5 | 0 | 2055.13889 | 2055.13880 | 0.00016 | 0.25 |
| 5 | 3 | 3 | 6 | 4 | 2 | 2055.17885 | 2055.17868 | 0.00002 | 0.25 |
| 5 | 3 | 2 | 6 | 4 | 3 | 2055.18534 | 2055.18533 | 0.00000 | 0.25 |
| 9 | 2 | 7 | 10 | 3 | 8 | 2055.19955 | 2055.19957 | -0.00002 | 1.00 |
| 10 | 1 | 9 | 11 | 2 | 10 | 2055.28005 | 2055.27936 | 0.00068 | 1.00 |
| 11 | 0 | 11 | 12 | 1 | 12 | 2055.28591 | 2055.28556 | 0.00034 | 0.25 |
| 11 | 1 | 11 | 12 | 0 | 12 | 2055.28591 | 2055.28570 | 0.00020 | 0.25 |
| 3 | 3 | 0 | 4 | 4 | 1 | 2055.31860 | 2055.31887 | -0.00027 | 0.25 |
| 3 | 3 | 1 | 4 | 4 | 0 | 2055.31860 | 2055.31863 | -0.00003 | 0.25 |
| 10 | 0 | 10 | 11 | 1 | 11 | 2055.34159 | 2055.34140 | 0.00018 | 0.25 |
| 10 | 1 | 10 | 11 | 0 | 11 | 2055.34159 | 2055.34173 | -0.00014 | 0.25 |
| 4 | 2 | 3 | 5 | 3 | 2 | 2055.34514 | 2055.34527 | -0.00013 | 1.00 |
| 9 | 0 | 9 | 10 | 1 | 10 | 2055.39754 | 2055.39709 | 0.00044 | 0.25 |
| 9 | 1 | 9 | 10 | 0 | 10 | 2055.39754 | 2055.39782 | -0.00028 | 0.25 |
| 8 | 2 | 7 | 9 | 1 | 8 | 2055.41435 | 2055.41467 | -0.00032 | 1.00 |
| 3 | 2 | 2 | 4 | 3 | 1 | 2055.42416 | 2055.42453 | -0.00037 | 1.00 |
| 3 | 2 | 1 | 4 | 3 | 2 | 2055.43607 | 2055.43604 | 0.00002 | 1.00 |
| 6 | 1 | 5 | 7 | 2 | 6 | 2055.45954 | 2055.45964 | -0.00010 | 1.00 |
| 7 | 0 | 7 | 8 | 1 | 8 | 2055.50741 | 2055.50738 | 0.00002 | 0.25 |
| 7 | 1 | 7 | 8 | 0 | 8 | 2055.51002 | 2055.51079 | -0.00077 | 0.25 |
| 6 | 0 | 6 | 7 | 1 | 7 | 2055.56121 | 2055.56129 | -0.00008 | 0.25 |
| 6 | 2 | 5 | 7 | 1 | 6 | 2055.56121 | 2055.56063 | 0.00057 | 0.25 |
| 1 | 1 | 0 | 1 | 0 | 1 | 2056.04460 | 2056.04444 | 0.00016 | 1.00 |
| 2 | 1 | 1 | 2 | 0 | 2 | 2056.05888 | 2056.05888 | -0.00000 | 1.00 |
| 2 | 0 | 2 | 1 | 1 | 1 | 2056.06663 | 2056.06658 | 0.00004 | 1.00 |
| 1 | 1 | 1 | 0 | 0 | 0 | 2056.09997 | 2056.09997 | -0.00000 | 1.00 |
| 4 | 1 | 3 | 5 | 2 | 4 | 2055.53668 | 2055.53666 | 0.00001 | 1.00 |
| 11 | 3 | 8 | 11 | 2 | 9 | 2055.53325 | 2055.53289 | 0.00035 | 1.00 |
| 6 | 1 | 6 | 7 | 0 | 7 | 2055.56817 | 2055.56836 | -0.00019 | 1.00 |
| 9 | 3 | 7 | 9 | 4 | 6 | 2055.57106 | 2055.57128 | -0.00022 | 1.00  |
|---|---|---|---|---|---|----------|----------|----------|------|
| 4 | 2 | 2 | 4 | 1 | 3 | 2056.11979 | 2056.11961 | 0.00018  | 1.00  |
| 3 | 0 | 3 | 2 | 1 | 2 | 2056.13946 | 2056.13899 | 0.00046  | 1.00  |
| 2 | 2 | 0 | 2 | 1 | 1 | 2056.13315 | 2056.13312 | 0.00003  | 1.00  |
| 6 | 2 | 4 | 6 | 1 | 5 | 2056.14468 | 2056.14491 | -0.00022 | 1.00  |
| 2 | 1 | 2 | 1 | 0 | 1 | 2056.15536 | 2056.15540 | -0.00004 | 1.00  |
| 2 | 2 | 1 | 2 | 1 | 2 | 2056.16830 | 2056.16850 | -0.00020 | 1.00  |
| 5 | 1 | 4 | 5 | 0 | 5 | 2056.17220 | 2056.17223 | -0.00003 | 1.00  |
| 7 | 2 | 5 | 7 | 1 | 6 | 2056.17954 | 2056.17930 | 0.00024  | 1.00  |
| 8 | 3 | 5 | 8 | 2 | 6 | 2056.18999 | 2056.19003 | -0.00003 | 1.00  |
| 7 | 3 | 4 | 7 | 2 | 5 | 2056.19231 | 2056.19265 | -0.00034 | 1.00  |
| 5 | 3 | 2 | 5 | 4 | 1 | 2055.59985 | 2055.59995 | -0.00010 | 1.00  |
| 5 | 0 | 5 | 6 | 1 | 6 | 2055.61391 | 2055.61357 | 0.00033  | 1.00  |
| 5 | 2 | 4 | 6 | 1 | 5 | 2055.64359 | 2055.64386 | -0.00027 | 1.00  |
| 4 | 0 | 4 | 5 | 1 | 5 | 2055.66344 | 2055.66358 | -0.00014 | 1.00  |
| 7 | 0 | 7 | 7 | 1 | 6 | 2055.66677 | 2055.66698 | -0.00021 | 1.00  |
| 6 | 1 | 6 | 6 | 2 | 5 | 2055.67429 | 2055.67481 | -0.00052 | 1.00  |
| 5 | 1 | 5 | 5 | 2 | 4 | 2055.71450 | 2055.71495 | -0.00045 | 1.00  |
| 4 | 2 | 2 | 4 | 3 | 1 | 2055.72270 | 2055.72267 | 0.00002  | 1.00  |
| 5 | 2 | 3 | 5 | 3 | 2 | 2055.73871 | 2055.73906 | -0.00035 | 1.00  |
| 4 | 1 | 4 | 4 | 2 | 3 | 2055.74874 | 2055.74885 | -0.00011 | 1.00  |
| 5 | 0 | 5 | 5 | 1 | 4 | 2055.79150 | 2055.79111 | 0.00038  | 1.00  |
| 2 | 1 | 2 | 2 | 2 | 1 | 2055.79590 | 2055.79598 | -0.00008 | 1.00  |
| 1 | 0 | 1 | 2 | 1 | 2 | 2055.80963 | 2055.80922 | 0.00040  | 1.00  |
| 6 | 1 | 5 | 6 | 2 | 4 | 2055.81790 | 2055.81758 | 0.00032  | 1.00  |
| 3 | 2 | 2 | 4 | 1 | 3 | 2055.82091 | 2055.82148 | -0.00056 | 1.00  |
| 2 | 1 | 2 | 3 | 0 | 3 | 2055.82577 | 2055.82540 | 0.00037  | 1.00  |
| 3 | 1 | 5 | 4 | 5 | 2 | 2055.83071 | 2055.83003 | 0.00054  | 1.00  |
| 0 | 0 | 0 | 1 | 1 | 1 | 2055.86479 | 2055.86479 | -0.00000 | 1.00  |
| 4 | 1 | 3 | 3 | 2 | 0 | 2056.64492 | 2056.64482 | 0.00009  | 0.25  |
| 4 | 4 | 0 | 3 | 3 | 1 | 2056.64492 | 2056.64506 | -0.00014 | 0.25  |
| 7 | 4 | 3 | 6 | 3 | 4 | 2056.85729 | 2056.85681 | 0.00047  | 1.00  |
|    |     |     |     |   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|----|-----|-----|-----|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|    |     |     |     |   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|  6 |  4  |  3  |  5  |  3 |  2  | 2056.77731 | 2056.77727 | 0.00003 | 1.00 |
|  9 |  6  |  3  |  8  |  5 |  4  | 2057.20685 | 2057.20707 | -0.00022 | 0.25 |
|  9 |  6  |  4  |  8  |  5 |  3  | 2057.20685 | 2057.20661 | 0.00023 | 0.25 |
|  7 |  7  |  0  |  6  |  6 |  1  | 2057.18208 | 2057.18218 | -0.00010 | 0.25 |
|  7 |  7  |  1  |  6  |  6 |  0  | 2057.18208 | 2057.18218 | -0.00010 | 0.25 |
| 10 |  5  |  6  |  9  |  4 |  5  | 2057.14631 | 2057.14616 | 0.00014 | 0.25 |
| 10 |  4  |  6  |  9  |  3 |  7  | 2057.12740 | 2057.12777 | 0.00037 | 0.25 |
|  9 |  5  |  4  |  8  |  4 |  5  | 2057.09857 | 2057.09859 | -0.00002 | 1.00 |
|  7 |  6  |  1  |  6  |  5 |  2  | 2057.07136 | 2057.07142 | -0.00006 | 0.25 |
|  7 |  6  |  2  |  6  |  5 |  1  | 2057.07136 | 2057.07140 | -0.00004 | 0.25 |
| 10 |  8  |  2  |  9  |  7 |  3  | 2057.49658 | 2057.49662 | 0.00004 | 0.25 |
| 10 |  8  |  3  |  9  |  7 |  2  | 2057.49658 | 2057.49662 | -0.00004 | 0.25 |
|  9 |  8  |  1  |  8  |  7 |  2  | 2057.42877 | 2057.42883 | -0.00006 | 0.25 |
|  9 |  8  |  2  |  8  |  7 |  1  | 2057.42877 | 2057.42883 | -0.00006 | 0.25 |
| 10 |  7  |  3  |  9  |  6 |  4  | 2057.38581 | 2057.38574 | 0.00006 | 0.25 |
| 10 |  7  |  4  |  9  |  6 |  3  | 2057.38581 | 2057.38568 | 0.00012 | 0.25 |
|  8 |  8  |  0  |  7  |  7 |  1  | 2057.36076 | 2057.36088 | -0.00012 | 0.25 |
|  8 |  8  |  1  |  7  |  7 |  0  | 2057.36076 | 2057.36088 | -0.00012 | 0.25 |
| 11 |  6  |  5  | 10  |  5 |  6  | 2057.34179 | 2057.34220 | -0.00041 | 1.00 |
|  9 |  7  |  2  |  8  |  6 |  3  | 2057.31803 | 2057.31811 | -0.00008 | 0.25 |
|  9 |  7  |  3  |  8  |  6 |  2  | 2057.31803 | 2057.31810 | -0.00007 | 0.25 |
| 13 |  5  |  9  | 12  |  2 |  10 | 2057.25971 | 2057.25985 | -0.00014 | 1.00 |
| 11 |  5  |  7  | 10  |  4 |  6  | 2057.19538 | 2057.19515 | 0.00022 | 1.00 |
|  8 |  5  |  3  |  7  |  4 |  4  | 2057.02941 | 2057.02911 | 0.00029 | 1.00 |
| 14 |  4  | 11  | 13  |  1 |  12 | 2057.04275 | 2057.04245 | 0.00029 | 1.00 |
|  8 |  6  |  2  |  7  |  5 |  3  | 2057.13926 | 2057.13937 | -0.00011 | 0.25 |
|  8 |  6  |  3  |  7  |  5 |  2  | 2057.13926 | 2057.13926 | -0.00000 | 0.25 |
| 11 |  4  |  8  | 10  |  3 |  7  | 2056.98823 | 2056.98815 | 0.00007 | 1.00 |
|  6 |  6  |  0  |  5  |  5 |  1  | 2057.00303 | 2057.00327 | -0.00024 | 0.25 |
|  6 |  6  |  1  |  5  |  5 |  0  | 2057.00303 | 2057.00327 | -0.00024 | 0.25 |
|  7 |  5  |  3  |  6  |  4 |  2  | 2056.96040 | 2056.95975 | 0.00064 | 0.25 |
|  7 |  5  |  2  |  6  |  4 |  3  | 2056.96040 | 2056.96068 | -0.00028 | 0.25 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 8 | 4 | 4 | 7 | 3 | 5 | 2056.93556 | 2056.93548 | 0.00007 |   | 0.25 |
| 8 | 3 | 5 | 7 | 2 | 6 | 2056.93556 | 2056.93502 | 0.00053 |   | 0.25 |
| 9 | 4 | 6 | 8 | 3 | 5 | 2056.93181 | 2056.93174 | 0.00006 |   | 1.00 |
| 6 | 5 | 2 | 5 | 4 | 1 | 2056.89257 | 2056.89228 | 0.00028 |   | 0.25 |
| 6 | 5 | 1 | 5 | 4 | 2 | 2056.89257 | 2056.89247 | 0.00009 |   | 0.25 |
| 8 | 4 | 5 | 7 | 3 | 4 | 2056.88966 | 2056.88950 | 0.00015 |   | 1.00 |
| 10 | 3 | 8 | 9 | 2 | 7 | 2056.76016 | 2056.75982 | 0.00033 |   | 1.00 |
| 13 | 1 | 13 | 12 | 0 | 12 | 2056.72816 | 2056.72838 | -0.00022 |   | 0.25 |
| 13 | 0 | 13 | 12 | 1 | 12 | 2056.72816 | 2056.72832 | -0.00016 |   | 0.25 |
| 11 | 2 | 10 | 10 | 1 | 9 | 2056.67985 | 2056.67972 | 0.00012 |   | 1.00 |
| 11 | 3 | 8 | 10 | 2 | 9 | 2056.66947 | 2056.66913 | 0.00033 |   | 1.00 |
| 11 | 1 | 11 | 10 | 0 | 10 | 2056.61810 | 2056.61849 | -0.00039 |   | 0.25 |
| 11 | 0 | 11 | 10 | 1 | 10 | 2056.61810 | 2056.61817 | -0.00007 |   | 0.25 |
| 10 | 1 | 9 | 9 | 2 | 8 | 2056.60957 | 2056.60950 | 0.00006 |   | 1.00 |
| 10 | 1 | 10 | 9 | 0 | 9 | 2056.56307 | 2056.56363 | -0.00056 |   | 0.25 |
| 10 | 0 | 10 | 9 | 1 | 1 | 2056.56307 | 2056.56291 | 0.00015 |   | 0.25 |
| 4 | 3 | 2 | 3 | 2 | 1 | 2056.52788 | 2056.52779 | 0.00008 |   | 1.00 |
| 8 | 1 | 7 | 7 | 2 | 6 | 2056.47694 | 2056.47739 | -0.00045 |   | 1.00 |
| 9 | 1 | 8 | 8 | 2 | 7 | 2056.54552 | 2056.54619 | -0.00067 |   | 1.00 |
| 8 | 1 | 8 | 7 | 0 | 7 | 2056.45488 | 2056.45477 | 0.00010 |   | 1.00 |
| 8 | 0 | 8 | 7 | 1 | 7 | 2056.45132 | 2056.45136 | -0.00004 |   | 1.00 |
| 9 | 4 | 6 | 9 | 3 | 7 | 2056.38848 | 2056.38849 | -0.00001 |   | 1.00 |
| 7 | 1 | 7 | 6 | 0 | 6 | 2056.40113 | 2056.40146 | -0.00033 |   | 0.25 |
| 7 | 1 | 6 | 6 | 2 | 5 | 2056.40113 | 2056.40167 | -0.00054 |   | 0.25 |
| 6 | 4 | 2 | 6 | 3 | 3 | 2056.35278 | 2056.35309 | -0.00031 |   | 1.00 |
| 6 | 1 | 6 | 5 | 0 | 5 | 2056.34946 | 2056.34970 | -0.00024 |   | 1.00 |
| 5 | 0 | 5 | 4 | 1 | 4 | 2056.27446 | 2056.27422 | 0.00024 |   | 1.00 |
| 3 | 3 | 1 | 3 | 2 | 2 | 2056.26223 | 2056.26246 | -0.00023 |   | 1.00 |
| 5 | 2 | 4 | 5 | 1 | 5 | 2056.24839 | 2056.24843 | -0.00004 |   | 1.00 |
| 8 | 2 | 6 | 8 | 1 | 7 | 2056.22874 | 2056.22859 | 0.00015 |   | 1.00 |
| 4 | 2 | 3 | 4 | 1 | 4 | 2056.21514 | 2056.21498 | 0.00015 |   | 1.00 |
| 4 | 0 | 4 | 3 | 1 | 3 | 2056.20858 | 2056.20875 | -0.00016 |   | 1.00 |
Table A-3. Observed and calculated transitions for N₂O-HCCCH in the region of the ν₁ fundamental band of N₂O (in units of cm⁻¹).

| J' Ka' Kc' | J Ka" Kc" | Observed       | Calculated     | Obs-Calc | Weight |
|------------|------------|----------------|----------------|----------|--------|
| 8 7 1      | 9 8 2      | 2223.65138     | 2223.65179     | -0.00041 | 0.25   |
| 8 7 2      | 9 8 1      | 2223.65138     | 2223.65179     | -0.00041 | 0.25   |
| 7 7 1      | 8 8 0      | 2223.73462     | 2223.73466     | -0.00004 | 0.25   |
| 7 7 0      | 8 8 1      | 2223.73462     | 2223.73466     | -0.00004 | 0.25   |
| 10 5 6     | 11 6 5     | 2223.93132     | 2223.93177     | -0.00045 | 0.25   |
| 10 5 5     | 11 6 6     | 2223.93132     | 2223.93197     | -0.00065 | 0.25   |
| 7 6 2      | 8 7 1      | 2223.95739     | 2223.95735     | 0.00004  | 0.25   |
| 7 6 1      | 8 7 2      | 2223.95739     | 2223.95735     | 0.00004  | 0.25   |
| 9 5 4      | 10 6 5     | 2224.01392     | 2224.01420     | -0.00028 | 0.25   |
| 9 5 5      | 10 6 4     | 2224.01392     | 2224.01413     | -0.00021 | 0.25   |
| 8 5 4      | 9 6 3      | 2224.09656     | 2224.09675     | -0.00018 | 0.25   |
| 8 5 3      | 9 6 4      | 2224.09656     | 2224.09677     | -0.00020 | 0.25   |
| 7 5 2      | 8 6 3      | 2224.17925     | 2224.17956     | -0.00030 | 0.25   |
| 7 5 3      | 8 6 2      | 2224.17925     | 2224.17955     | -0.00030 | 0.25   |
| 6 5 1      | 7 6 2      | 2224.26267     | 2224.26248     | 0.00019  | 0.25   |
| 6 5 2      | 7 6 1      | 2224.26267     | 2224.26248     | 0.00019  | 0.25   |
| 8 | 4 | 4 | 9 | 5 | 5 | 2224.31880 | 2224.31958 | -0.00077 | 0.25 |
| 8 | 4 | 5 | 9 | 5 | 4 | 2224.31880 | 2224.31865 | 0.00014 | 0.25 |
| 5 | 5 | 0 | 6 | 6 | 1 | 2224.34583 | 2224.34548 | 0.00035 | 0.25 |
| 5 | 5 | 1 | 6 | 6 | 0 | 2224.34583 | 2224.34548 | 0.00035 | 0.25 |
| 6 | 4 | 2 | 7 | 5 | 3 | 2224.48427 | 2224.48417 | 0.00009 | 0.25 |
| 6 | 4 | 3 | 7 | 5 | 2 | 2224.48427 | 2224.48409 | 0.00018 | 0.25 |
| 8 | 3 | 6 | 9 | 4 | 5 | 2224.53313 | 2224.53329 | -0.00015 | 1.00 |
| 4 | 4 | 0 | 5 | 5 | 1 | 2224.65028 | 2224.65004 | 0.00024 | 0.25 |
| 4 | 4 | 1 | 5 | 5 | 0 | 2224.65028 | 2224.65004 | 0.00024 | 0.25 |
| 8 | 2 | 7 | 9 | 3 | 6 | 2224.67479 | 2224.67467 | 0.00011 | 1.00 |
| 6 | 3 | 4 | 7 | 4 | 3 | 2224.70375 | 2224.70388 | -0.00013 | 1.00 |
| 6 | 3 | 3 | 7 | 4 | 4 | 2224.70755 | 2224.70775 | -0.00019 | 1.00 |
| 5 | 3 | 2 | 6 | 4 | 3 | 2224.78805 | 2224.78875 | -0.00070 | 0.25 |
| 5 | 3 | 3 | 6 | 4 | 2 | 2224.78805 | 2224.78747 | 0.00058 | 0.25 |
| 9 | 2 | 7 | 10 | 3 | 8 | 2224.80968 | 2224.80981 | -0.00012 | 1.00 |
| 11 | 5 | 6 | 11 | 6 | 5 | 2224.85303 | 2224.85186 | 0.00116 | 1.00 |
| 4 | 3 | 1 | 5 | 4 | 2 | 2224.87090 | 2224.87101 | -0.00010 | 0.25 |
| 4 | 3 | 2 | 5 | 4 | 1 | 2224.87090 | 2224.87069 | 0.00021 | 0.25 |
| 6 | 2 | 5 | 7 | 3 | 4 | 2224.89668 | 2224.89693 | -0.00025 | 1.00 |
| 7 | 2 | 5 | 8 | 3 | 6 | 2224.90338 | 2224.90342 | -0.00004 | 1.00 |
| 3 | 3 | 1 | 4 | 4 | 0 | 2224.95399 | 2224.95380 | 0.00018 | 0.25 |
| 3 | 3 | 0 | 4 | 4 | 1 | 2224.95399 | 2224.95385 | 0.00014 | 0.25 |
| 6 | 2 | 4 | 7 | 3 | 5 | 2224.96127 | 2224.96114 | 0.00013 | 1.00 |
| 5 | 2 | 4 | 6 | 3 | 3 | 2224.99364 | 2224.99374 | -0.00010 | 1.00 |
| 10 | 0 | 13 | 14 | 1 | 14 | 2225.00922 | 2225.00769 | 0.00152 | 0.25 |
| 10 | 1 | 13 | 14 | 0 | 14 | 2225.00922 | 2225.00969 | -0.00047 | 0.25 |
| 4 | 2 | 2 | 5 | 3 | 3 | 2225.09870 | 2225.09873 | -0.00003 | 1.00 |
| 3 | 2 | 1 | 4 | 3 | 2 | 2225.17593 | 2225.17627 | -0.00034 | 1.00 |
| 10 | 0 | 10 | 11 | 1 | 11 | 2225.22035 | 2225.22048 | -0.00012 | 1.00 |
| 10 | 1 | 10 | 11 | 0 | 11 | 2225.22991 | 2225.22988 | 0.00002 | 1.00 |
| 2 | 2 | 0 | 3 | 3 | 1 | 2225.25661 | 2225.25718 | -0.00057 | 0.25 |
| 2 | 2 | 1 | 3 | 3 | 0 | 2225.25661 | 2225.25625 | 0.00035 | 0.25 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 6 | 1 | 5 | 7 | 2 | 6 | 2225.26118 | 2225.26150 | -0.00032 | 1.00 |
| 9 | 1 | 9 | 10 | 0 | 10 | 2225.30499 | 2225.30486 | 0.00013 | 1.00 |
| 5 | 1 | 4 | 6 | 2 | 5 | 2225.31179 | 2225.31202 | -0.00023 | 1.00 |
| 8 | 0 | 8 | 9 | 1 | 9 | 2225.35692 | 2225.35704 | -0.00011 | 1.00 |
| 8 | 1 | 8 | 9 | 1 | 9 | 2225.37214 | 2225.37180 | 0.00033 | 1.00 |
| 7 | 3 | 5 | 8 | 3 | 6 | 2225.37679 | 2225.37723 | -0.00043 | 1.00 |
| 8 | 1 | 8 | 9 | 0 | 9 | 2225.38138 | 2225.38138 | 0.00000 | 1.00 |
| 7 | 0 | 7 | 8 | 1 | 8 | 2225.42222 | 2225.42241 | -0.00019 | 1.00 |
| 3 | 1 | 2 | 4 | 2 | 3 | 2225.42703 | 2225.42715 | -0.00012 | 1.00 |
| 7 | 1 | 7 | 8 | 0 | 8 | 2225.46038 | 2225.46009 | 0.00028 | 1.00 |
| 6 | 0 | 6 | 7 | 1 | 7 | 2225.48526 | 2225.48536 | -0.00010 | 1.00 |
| 6 | 2 | 5 | 6 | 3 | 4 | 2225.48900 | 2225.48944 | -0.00043 | 1.00 |
| 2 | 1 | 1 | 3 | 2 | 2 | 2225.49287 | 2225.49287 | 0.00000 | 1.00 |
| 4 | 2 | 2 | 4 | 3 | 1 | 2225.51453 | 2225.51461 | -0.00008 | 1.00 |
| 6 | 1 | 6 | 7 | 1 | 7 | 2225.51875 | 2225.51868 | 0.00006 | 1.00 |
| 5 | 0 | 5 | 6 | 0 | 6 | 2225.57996 | 2225.57991 | 0.00004 | 1.00 |
| 8 | 2 | 6 | 8 | 3 | 5 | 2225.58605 | 2225.58583 | 0.00021 | 1.00 |
| 5 | 1 | 5 | 6 | 1 | 6 | 2225.59292 | 2225.59290 | 0.00002 | 1.00 |
| 6 | 1 | 6 | 6 | 2 | 5 | 2225.59977 | 2225.59967 | 0.00009 | 1.00 |
| 4 | 0 | 4 | 5 | 1 | 5 | 2225.60561 | 2225.60546 | 0.00014 | 1.00 |
| 4 | 1 | 3 | 5 | 1 | 4 | 2225.61265 | 2225.61256 | 0.00009 | 1.00 |
| 4 | 2 | 2 | 5 | 2 | 3 | 2225.62060 | 2225.62047 | 0.00013 | 1.00 |
| 8 | 0 | 8 | 8 | 1 | 7 | 2225.64611 | 2225.64571 | 0.00039 | 1.00 |
| 4 | 0 | 4 | 5 | 0 | 5 | 2225.65296 | 2225.65291 | 0.00005 | 1.00 |
| 10 | 1 | 9 | 10 | 2 | 8 | 2225.68326 | 2225.68259 | 0.00067 | 0.25 |
| 10 | 1 | 9 | 10 | 2 | 8 | 2225.68326 | 2225.68259 | 0.00067 | 0.25 |
| 3 | 1 | 3 | 3 | 2 | 2 | 2225.68968 | 2225.68947 | 0.00020 | 1.00 |
| 3 | 1 | 2 | 4 | 1 | 3 | 2225.69874 | 2225.69856 | 0.00018 | 1.00 |
| 2 | 1 | 1 | 2 | 2 | 0 | 2225.74070 | 2225.74014 | 0.00055 | 1.00 |
| 3 | 1 | 3 | 4 | 1 | 4 | 2225.74337 | 2225.74322 | 0.00015 | 1.00 |
| 3 | 1 | 2 | 3 | 2 | 1 | 2225.75381 | 2225.75299 | 0.00082 | 0.25 |
| 3 | 1 | 2 | 3 | 2 | 1 | 2225.75381 | 2225.75299 | 0.00082 | 0.25 |
| 8 | 1 | 7 | 8 | 2 | 6 | 2225.75635 | 2225.75599 | 0.00035 | 0.25 |
| 8 | 1 | 7 | 8 | 2 | 6 | 2225.75635 | 2225.75599 | 0.00035 | 0.25 |
| 4 | 1 | 3 | 4 | 2 | 2 | 2225.76614 | 2225.76583 | 0.00031 | 1.00 |
| 1 | 0 | 1 | 2 | 1 | 2 | 2225.79369 | 2225.79355 | 0.00014 | 1.00 |
| 2 | 1 | 2 | 3 | 1 | 3 | 2225.81918 | 2225.81933 | -0.00015 | 1.00 |
| 0 | 0 | 0 | 1 | 1 | 1 | 2225.86480 | 2225.86501 | -0.00021 | 1.00 |
| 4 | 0 | 4 | 4 | 1 | 3 | 2225.87445 | 2225.87490 | -0.00044 | 1.00 |
| 1 | 0 | 1 | 2 | 0 | 2 | 2225.88606 | 2225.88620 | -0.00013 | 1.00 |
| 3 | 0 | 3 | 3 | 1 | 2 | 2225.90388 | 2225.90424 | -0.00036 | 1.00 |
| 2 | 0 | 2 | 2 | 1 | 1 | 2225.92405 | 2225.92419 | -0.00014 | 1.00 |
| 1 | 0 | 1 | 1 | 0 | 0 | 2225.93642 | 2225.93642 | -0.00000 | 1.00 |
| 3 | 2 | 1 | 3 | 2 | 2 | 2226.05264 | 2226.05259 | 0.00004 | 0.25 |
| 7 | 3 | 4 | 7 | 3 | 5 | 2226.05264 | 2226.05364 | -0.00099 | 0.25 |
| 1 | 0 | 1 | 0 | 0 | 0 | 2226.13349 | 2226.13347 | 0.00001 | 1.00 |
| 1 | 1 | 0 | 1 | 0 | 1 | 2226.16425 | 2226.16450 | -0.00024 | 1.00 |
| 2 | 1 | 1 | 2 | 0 | 2 | 2226.17649 | 2226.17664 | -0.00015 | 1.00 |
| 3 | 1 | 2 | 3 | 0 | 3 | 2226.19634 | 2226.19643 | -0.00009 | 1.00 |
| 5 | 1 | 4 | 5 | 0 | 5 | 2226.26530 | 2226.26546 | -0.00015 | 1.00 |
| 3 | 1 | 3 | 2 | 1 | 2 | 2226.28063 | 2226.28060 | 0.00003 | 1.00 |
| 3 | 2 | 1 | 2 | 2 | 0 | 2226.29982 | 2226.29987 | -0.00005 | 1.00 |
| 2 | 1 | 2 | 1 | 0 | 1 | 2226.30713 | 2226.30724 | -0.00010 | 1.00 |
| 4 | 2 | 2 | 4 | 1 | 3 | 2226.33238 | 2226.33245 | -0.00006 | 1.00 |
| 8 | 2 | 6 | 8 | 1 | 7 | 2226.34160 | 2226.34159 | 0.00001 | 1.00 |
| 3 | 2 | 1 | 3 | 1 | 2 | 2226.34524 | 2226.34536 | -0.00011 | 1.00 |
| 2 | 2 | 1 | 2 | 1 | 2 | 2226.39118 | 2226.39123 | -0.00004 | 1.00 |
| 4 | 1 | 3 | 3 | 1 | 2 | 2226.40149 | 2226.40160 | -0.00010 | 1.00 |
| 3 | 2 | 2 | 3 | 1 | 3 | 2226.40890 | 2226.40861 | 0.00029 | 1.00 |
| 10 | 2 | 8 | 10 | 1 | 9 | 2226.41372 | 2226.41364 | 0.00007 | 1.00 |
| 4 | 1 | 4 | 3 | 0 | 3 | 2226.43526 | 2226.43504 | 0.00022 | 1.00 |
| 5 | 0 | 5 | 4 | 0 | 4 | 2226.44760 | 2226.44751 | 0.00009 | 1.00 |
| 8 | 1 | 7 | 8 | 0 | 8 | 2226.45220 | 2226.45202 | 0.00017 | 1.00 |
| 6 | 0 | 6 | 5 | 1 | 5 | 2226.47244 | 2226.47234 | 0.00010 | 1.00 |
| Row | Col1 | Col2 | Col3 | Col4 | Col5 | Col6 | Col7 | Col8 | Col9 | Col10 | Col11 | Col12 | Col13 |
|-----|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|
| 5   | 2    | 3    | 4    | 2    | 2    | 2226.47626 | 2226.47602 | 0.00024 | 1.00 |
| 6   | 0    | 6    | 5    | 0    | 5    | 2226.51996 | 2226.51978 | 0.00017 | 1.00 |
| 2   | 2    | 1    | 1    | 1    | 0    | 2226.53431 | 2226.53410 | 0.00020 | 1.00 |
| 6   | 1    | 6    | 5    | 0    | 5    | 2226.55302 | 2226.55311 | -0.00008 | 1.00 |
| 7   | 0    | 7    | 6    | 1    | 6    | 2226.55645 | 2226.55654 | -0.00009 | 1.00 |
| 6   | 1    | 5    | 5    | 1    | 4    | 2226.57185 | 2226.57171 | 0.00013 | 1.00 |
| 5   | 3    | 3    | 5    | 2    | 4    | 2226.59617 | 2226.59571 | 0.00046 | 1.00 |
| 7   | 2    | 6    | 6    | 2    | 5    | 2226.61935 | 2226.61978 | -0.00042 | 1.00 |
| 8   | 0    | 8    | 7    | 1    | 7    | 2226.63751 | 2226.63718 | 0.00032 | 1.00 |
| 3   | 2    | 1    | 2    | 1    | 2    | 2226.64379 | 2226.64371 | 0.00007 | 1.00 |
| 4   | 2    | 3    | 3    | 1    | 2    | 2226.67106 | 2226.67104 | 0.00001 | 1.00 |
| 8   | 1    | 8    | 7    | 0    | 7    | 2226.67504 | 2226.67497 | 0.00006 | 1.00 |
| 9   | 1    | 9    | 8    | 0    | 8    | 2226.73920 | 2226.73922 | -0.00002 | 1.00 |
| 6   | 2    | 5    | 5    | 1    | 4    | 2226.78573 | 2226.78568 | 0.00004 | 1.00 |
| 10  | 0    | 10   | 9    | 1    | 9    | 2226.78977 | 2226.79008 | -0.00030 | 1.00 |
| 10  | 1    | 10   | 9    | 0    | 9    | 2226.80526 | 2226.80544 | -0.00017 | 1.00 |
| 11  | 0    | 11   | 10   | 1    | 10   | 2226.86323 | 2226.86370 | -0.00046 | 1.00 |
| 4   | 3    | 1    | 3    | 2    | 2    | 2226.92169 | 2226.92174 | -0.00005 | 1.00 |
| 5   | 3    | 3    | 4    | 2    | 2    | 2226.99444 | 2226.99454 | -0.00009 | 1.00 |
| 6   | 3    | 4    | 5    | 2    | 3    | 2227.06689 | 2227.06671 | 0.00018 | 1.00 |
| 6   | 3    | 3    | 5    | 2    | 4    | 2227.09924 | 2227.09923 | 0.00000 | 1.00 |
| 4   | 4    | 1    | 3    | 3    | 0    | 2227.13235 | 2227.13224 | 0.00010 | 0.25 |
| 4   | 4    | 0    | 3    | 3    | 1    | 2227.13235 | 2227.13229 | 0.00005 | 0.25 |
| 5   | 4    | 1    | 4    | 3    | 2    | 2227.21530 | 2227.21529 | 0.00001 | 0.25 |
| 5   | 4    | 2    | 4    | 3    | 1    | 2227.21530 | 2227.21497 | 0.00032 | 0.25 |
| 6   | 4    | 3    | 5    | 3    | 2    | 2227.29774 | 2227.29712 | 0.00061 | 0.25 |
| 6   | 4    | 2    | 5    | 3    | 3    | 2227.29774 | 2227.29839 | -0.00065 | 0.25 |
| 7   | 4    | 4    | 6    | 3    | 3    | 2227.37801 | 2227.37803 | -0.00002 | 1.00 |
| 7   | 4    | 3    | 6    | 3    | 4    | 2227.38185 | 2227.38184 | 0.00001 | 1.00 |
| 5   | 5    | 0    | 4    | 4    | 1    | 2227.42659 | 2227.42642 | 0.00016 | 0.25 |
| 5   | 5    | 1    | 4    | 4    | 0    | 2227.42659 | 2227.42642 | 0.00016 | 0.25 |
| 8   | 4    | 5    | 7    | 3    | 4    | 2227.45644 | 2227.45667 | -0.00022 | 1.00 |
|   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 5 | 1 | 5 | 4 | 2 | 2227.50945 | 2227.50938 | 0.00007 | 0.25 |
| 6 | 5 | 2 | 5 | 4 | 1 | 2227.50945 | 2227.50936 | 0.00009 | 0.25 |
| 9 | 4 | 6 | 8 | 3 | 5 | 2227.53119 | 2227.53156 | -0.00037 | 1.00 |
| 7 | 5 | 2 | 6 | 4 | 3 | 2227.59209 | 2227.59224 | -0.00015 | 0.25 |
| 7 | 5 | 3 | 6 | 4 | 2 | 2227.59209 | 2227.59216 | -0.00007 | 0.25 |
| 11 | 4 | 8 | 10 | 3 | 7 | 2227.66293 | 2227.66304 | -0.00010 | 1.00 |
| 8 | 5 | 4 | 7 | 4 | 3 | 2227.67511 | 2227.67468 | 0.00042 | 0.25 |
| 8 | 5 | 3 | 7 | 4 | 4 | 2227.67511 | 2227.67498 | 0.00012 | 0.25 |
| 9 | 5 | 4 | 8 | 4 | 5 | 2227.75734 | 2227.75757 | -0.00023 | 0.25 |
| 9 | 5 | 5 | 8 | 4 | 4 | 2227.75734 | 2227.75667 | 0.00066 | 0.25 |
| 7 | 6 | 2 | 6 | 5 | 1 | 2227.80253 | 2227.80224 | 0.00028 | 0.25 |
| 7 | 6 | 1 | 6 | 5 | 2 | 2227.80253 | 2227.80224 | 0.00028 | 0.25 |
| 8 | 6 | 3 | 7 | 5 | 2 | 2227.88545 | 2227.88521 | 0.00024 | 0.25 |
| 8 | 6 | 2 | 7 | 5 | 3 | 2227.88545 | 2227.88521 | 0.00023 | 0.25 |
| 11 | 5 | 7 | 10 | 4 | 6 | 2227.91733 | 2227.91733 | -0.00000 | 1.00 |
| 11 | 5 | 6 | 10 | 4 | 7 | 2227.92221 | 2227.92276 | -0.00054 | 1.00 |
| 9 | 6 | 4 | 8 | 5 | 3 | 2227.96819 | 2227.96805 | 0.00013 | 0.25 |
| 9 | 6 | 3 | 8 | 5 | 4 | 2227.96819 | 2227.96807 | 0.00011 | 0.25 |
| 7 | 7 | 0 | 6 | 6 | 1 | 2228.01059 | 2228.01067 | -0.00007 | 0.25 |
| 7 | 7 | 1 | 6 | 6 | 0 | 2228.01059 | 2228.01067 | -0.00007 | 0.25 |
| 10 | 6 | 5 | 9 | 5 | 4 | 2228.05081 | 2228.05071 | 0.00010 | 0.25 |
| 10 | 6 | 4 | 9 | 5 | 5 | 2228.05081 | 2228.05078 | 0.00003 | 0.25 |

*****************************************************************************************************************************************************************
Table A-4. Observed and calculated transitions for N$_2$O-DCCCD in the region of the $v_1$

fundamental band of N$_2$O (units of cm$^{-1}$).

| $J'$ | $K_a'$ | $K_c'$ | $J''$ | $K_a''$ | $K_c''$ | Observed   | Calculated  | Obs-Calc | Weight |
|------|--------|--------|-------|--------|--------|------------|-------------|----------|--------|
| 4    | 4      | 1      | 5     | 5      | 0      | 2224.78432 | 2224.78432 | -0.000001| 0.25   |
| 4    | 4      | 0      | 5     | 5      | 1      | 2224.78432 | 2224.78432 | -0.000004| 0.25   |
| 6    | 3      | 4      | 7     | 4      | 3      | 2224.82286 | 2224.82278 | 0.000086 | 1.00   |
| 6    | 3      | 3      | 7     | 4      | 4      | 2224.82767 | 2224.82750 | 0.000168 | 1.00   |
| 4    | 3      | 2      | 5     | 4      | 1      | 2224.98345 | 2224.98323 | 0.000226 | 0.25   |
| 4    | 3      | 1      | 5     | 4      | 2      | 2224.98345 | 2224.98362 | -0.000165| 0.25   |
| 6    | 2      | 5      | 7     | 3      | 4      | 2224.99255 | 2224.99153 | 0.001019 | 1.00   |
| 7    | 2      | 5      | 8     | 3      | 6      | 2225.00849 | 2225.00895 | -0.000466| 1.00   |
| 5    | 2      | 4      | 6     | 3      | 3      | 2225.08651 | 2225.08668 | -0.000174| 1.00   |
| 4    | 2      | 3      | 5     | 3      | 2      | 2225.17501 | 2225.17514 | -0.000130| 1.00   |
| 4    | 2      | 2      | 5     | 3      | 3      | 2225.19063 | 2225.19080 | -0.000170| 1.00   |
| 8    | 1      | 7      | 9     | 2      | 8      | 2225.24995 | 2225.24986 | 0.000088 | 1.00   |
| 3    | 2      | 2      | 4     | 3      | 1      | 2225.25906 | 2225.25924 | -0.000176| 1.00   |
| 9    | 1      | 8      | 10    | 1      | 9      | 2225.27476 | 2225.27445 | 0.000311 | 1.00   |
| 8    | 2      | 6      | 9     | 2      | 7      | 2225.31020 | 2225.31024 | -0.000041| 1.00   |
| 8    | 3      | 5      | 9     | 3      | 6      | 2225.32742 | 2225.32718 | 0.000240 | 1.00   |
| 9    | 1      | 9      | 10    | 0      | 10     | 2225.35989 | 2225.35982 | 0.000076 | 1.00   |
| 7    | 0      | 7      | 8     | 1      | 8      | 2225.47724 | 2225.47739 | -0.000153| 1.00   |
| 6    | 2      | 4      | 7     | 2      | 5      | 2225.48253 | 2225.48282 | -0.000291| 1.00   |
| 7    | 0      | 7      | 8     | 0      | 8      | 2225.48845 | 2225.48860 | -0.000154| 1.00   |
| 2    | 1      | 2      | 3     | 2      | 1      | 2225.51752 | 2225.51763 | -0.000109| 1.00   |
| 8    | 2      | 7      | 8     | 3      | 6      | 2225.53152 | 2225.53176 | -0.000245| 1.00   |
| 6    | 0      | 6      | 7     | 1      | 7      | 2225.53851 | 2225.53832 | 0.000190 | 1.00   |
| 4    | 2      | 3      | 4     | 3      | 2      | 2225.57613 | 2225.57614 | -0.000015| 1.00   |
| 5    | 0      | 5      | 6     | 1      | 6      | 2225.59733 | 2225.59690 | 0.000436 | 1.00   |
| 5 | 2 | 3 | 5 | 3 | 2 | 2225.60158 | 2225.60148 | 0.000092 | 1.00 |
|---|---|---|---|---|---|-----------|-----------|--------|-----|
| 5 | 0 | 5 | 6 | 0 | 6 | 2225.62405 | 2225.62394 | 0.000107 | 1.00 |
| 5 | 1 | 5 | 6 | 1 | 6 | 2225.63543 | 2225.63554 | -0.000115 | 1.00 |
| 7 | 2 | 5 | 7 | 3 | 4 | 2225.63939 | 2225.63941 | -0.000019 | 1.00 |
| 4 | 2 | 2 | 5 | 2 | 3 | 2225.65825 | 2225.65833 | -0.000080 | 1.00 |
| 5 | 1 | 5 | 6 | 0 | 6 | 2225.66230 | 2225.66259 | -0.000289 | 1.00 |
| 4 | 3 | 2 | 5 | 3 | 3 | 2225.66735 | 2225.66811 | -0.000761 | 0.25 |
| 4 | 3 | 1 | 5 | 3 | 2 | 2225.66735 | 2225.66704 | 0.000309 | 0.25 |
| 9 | 2 | 7 | 9 | 3 | 6 | 2225.68135 | 2225.68167 | -0.000324 | 1.00 |
| 5 | 1 | 5 | 5 | 2 | 4 | 2225.68894 | 2225.68908 | -0.000135 | 1.00 |
| 4 | 0 | 4 | 5 | 0 | 5 | 2225.69320 | 2225.69307 | 0.000137 | 1.00 |
| 4 | 1 | 4 | 5 | 1 | 5 | 2225.70667 | 2225.70684 | -0.000166 | 1.00 |
| 3 | 0 | 3 | 4 | 1 | 4 | 2225.71065 | 2225.71080 | -0.000149 | 1.00 |
| 4 | 1 | 4 | 4 | 2 | 3 | 2225.71914 | 2225.71908 | 0.000062 | 1.00 |
| 3 | 1 | 2 | 4 | 1 | 3 | 2225.73427 | 2225.73429 | -0.000018 | 1.00 |
| 3 | 2 | 2 | 4 | 2 | 3 | 2225.75384 | 2225.75372 | 0.000119 | 1.00 |
| 2 | 0 | 2 | 3 | 1 | 3 | 2225.76973 | 2225.76977 | -0.000043 | 1.00 |
| 3 | 1 | 3 | 4 | 1 | 4 | 2225.77872 | 2225.77882 | -0.000098 | 1.00 |
| 5 | 2 | 4 | 6 | 1 | 5 | 2225.78407 | 2225.78423 | -0.000157 | 1.00 |
| 2 | 1 | 1 | 2 | 2 | 0 | 2225.79366 | 2225.79341 | 0.000249 | 1.00 |
| 3 | 1 | 2 | 3 | 2 | 1 | 2225.80589 | 2225.80583 | 0.000056 | 1.00 |
| 6 | 0 | 6 | 6 | 1 | 5 | 2225.81229 | 2225.81219 | 0.000097 | 1.00 |
| 2 | 1 | 2 | 3 | 1 | 3 | 2225.85140 | 2225.85147 | -0.000066 | 1.00 |
| 5 | 0 | 5 | 5 | 1 | 4 | 2225.86516 | 2225.86523 | -0.000071 | 1.00 |
| 4 | 2 | 3 | 5 | 1 | 4 | 2225.89018 | 2225.89045 | -0.000275 | 1.00 |
| 1 | 0 | 1 | 2 | 0 | 2 | 2225.91523 | 2225.91498 | 0.000253 | 1.00 |
| 2 | 1 | 2 | 3 | 0 | 3 | 2225.92010 | 2225.92011 | -0.000016 | 1.00 |
| 1 | 1 | 1 | 2 | 1 | 2 | 2225.92471 | 2225.92469 | 0.000017 | 1.00 |
| 3 | 0 | 3 | 3 | 1 | 2 | 2225.93630 | 2225.93633 | -0.000032 | 1.00 |
| 2 | 0 | 2 | 2 | 1 | 1 | 2225.95653 | 2225.95654 | -0.000016 | 1.00 |
| 3 | 2 | 1 | 3 | 2 | 2 | 2226.07532 | 2226.07522 | 0.000098 | 1.00 |
| 2 | 1 | 1 | 2 | 1 | 2 | 2226.10629 | 2226.10596 | 0.000330 | 1.00 |
|   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 0 | 2226.15194 | 2226.15206 | -0.000124 | 1.00 |
| 1 | 1 | 0 | 1 | 0 | 2226.17603 | 2226.17604 | -0.000003 | 1.00 |
| 2 | 1 | 1 | 2 | 0 | 2226.18823 | 2226.18826 | -0.000027 | 1.00 |
| 3 | 1 | 2 | 3 | 0 | 2226.20835 | 2226.20832 | 0.000028 | 1.00 |
| 4 | 1 | 3 | 4 | 0 | 2226.23804 | 2226.23797 | 0.000074 | 1.00 |
| 5 | 1 | 4 | 5 | 0 | 2226.27812 | 2226.27875 | -0.000629 | 1.00 |
| 6 | 1 | 5 | 6 | 0 | 2226.30724 | 2226.30676 | 0.000478 | 1.00 |
| 6 | 1 | 4 | 3 | 1 | 2226.33670 | 2226.33672 | -0.000021 | 1.00 |
| 8 | 2 | 6 | 8 | 1 | 7226.34560 | 2226.34523 | 0.000370 | 1.00 |
| 6 | 1 | 5 | 5 | 2 | 2226.35736 | 2226.35769 | -0.000338 | 1.00 |
| 4 | 1 | 4 | 3 | 1 | 2226.36475 | 2226.36479 | -0.000032 | 1.00 |
| 4 | 1 | 3 | 3 | 1 | 2226.40981 | 2226.40991 | -0.000098 | 1.00 |
| 8 | 3 | 5 | 8 | 2 | 6 | 2226.47608 | 2226.47642 | -0.000340 | 1.00 |
| 7 | 3 | 4 | 7 | 2 | 5 | 2226.49869 | 2226.49871 | -0.000018 | 1.00 |
| 6 | 1 | 6 | 5 | 1 | 2226.50694 | 2226.50701 | -0.000065 | 1.00 |
| 2 | 2 | 0 | 1 | 1 | 2226.53036 | 2226.53044 | -0.000072 | 1.00 |
| 5 | 3 | 2 | 5 | 2 | 2226.53684 | 2226.53658 | 0.000257 | 1.00 |
| 6 | 2 | 5 | 5 | 2 | 2226.54262 | 2226.54168 | 0.000944 | 1.00 |
| 3 | 3 | 0 | 3 | 2 | 1 | 2226.55491 | 2226.55460 | 0.000309 | 1.00 |
| 5 | 3 | 3 | 5 | 2 | 4 | 2226.56673 | 2226.56665 | 0.000074 | 1.00 |
| 7 | 1 | 7 | 6 | 1 | 6 | 2226.57657 | 2226.57692 | -0.000354 | 1.00 |
| 3 | 2 | 2 | 2 | 1 | 1 | 2226.58646 | 2226.58620 | 0.000258 | 0.25 |
| 7 | 0 | 7 | 6 | 0 | 6 | 2226.58646 | 2226.58658 | -0.000121 | 0.25 |
| 7 | 1 | 7 | 6 | 0 | 6 | 2226.60362 | 2226.60396 | -0.000343 | 1.00 |
| 7 | 2 | 6 | 6 | 2 | 5 | 2226.61777 | 2226.61767 | 0.000105 | 1.00 |
| 3 | 2 | 1 | 2 | 1 | 2 | 2226.62477 | 2226.62484 | -0.000070 | 1.00 |
| 8 | 0 | 8 | 7 | 1 | 7 | 2226.63516 | 2226.63520 | -0.000044 | 1.00 |
| 7 | 2 | 5 | 6 | 2 | 4 | 2226.65815 | 2226.65829 | -0.000134 | 1.00 |
| 8 | 1 | 8 | 7 | 0 | 7 | 2226.66395 | 2226.66390 | 0.000049 | 1.00 |
| 9 | 1 | 8 | 8 | 2 | 7 | 2226.67326 | 2226.67344 | -0.000181 | 1.00 |
| 8 2 7 7 2 6 | 2226.69252 2226.69257 -0.000043 1.00 |
|-------------|-----------------------------------------|
| 9 0 9 8 1 8 | 2226.70805 2226.70811 -0.000053 1.00 |
| 9 1 9 8 1 8 | 2226.71462 2226.71479 -0.000171 1.00 |
| 7 4 3 7 3 4 | 2226.73713 2226.73761 -0.000483 1.00 |
| 6 2 5 5 1 4 | 2226.75643 2226.75648 -0.000049 1.00 |
| 9 2 8 8 2 7 | 2226.76645 2226.76631 0.000138 1.00 |
| 10 0 10 9 1 9 | 2226.77921 2226.77900 0.000213 1.00 |
| 3 3 0 2 2 1 | 2226.79695 2226.79744 -0.000485 0.25 |
| 3 3 1 2 2 0 | 2226.79695 2226.79642 0.000534 0.25 |
| 7 2 6 6 1 5 | 2226.80360 2226.80356 0.000040 1.00 |
| 4 3 2 3 2 1 | 2226.87373 2226.87365 0.000080 1.00 |
| 4 3 1 3 2 2 | 2226.87874 2226.87881 -0.000070 1.00 |
| 5 3 2 4 2 3 | 2226.96279 2226.96273 0.000060 1.00 |
| 4 4 0 3 3 1 | 2227.06853 2227.06896 -0.000426 0.25 |
| 4 4 1 3 3 0 | 2227.06853 2227.06890 -0.000371 0.25 |
| 7 3 5 6 2 4 | 2227.07595 2227.07580 0.000152 1.00 |
| 5 4 2 4 3 1 | 2227.14806 2227.14820 -0.000140 0.25 |
| 5 4 1 4 3 2 | 2227.14806 2227.14858 -0.000525 0.25 |
| 6 4 2 5 3 3 | 2227.22764 2227.22836 -0.000718 0.25 |
| 6 4 3 5 3 2 | 2227.22764 2227.22681 0.000830 0.25 |
| 7 4 3 6 3 4 | 2227.30857 2227.30860 -0.000030 1.00 |
| 5 5 1 4 4 0 | 2227.34004 2227.34009 -0.000058 1.00 |
| 5 5 0 4 4 1 | 2227.34004 2227.34010 -0.000061 1.00 |
| 8 4 5 7 3 4 | 2227.37881 2227.37840 0.000410 1.00 |
| 8 4 4 7 3 5 | 2227.38984 2227.38995 -0.000111 1.00 |
| 6 5 2 5 4 1 | 2227.41948 2227.41958 -0.000104 0.25 |
| 6 5 1 5 4 2 | 2227.41948 2227.41960 -0.000126 0.25 |
| 9 4 6 8 3 5 | 2227.44869 2227.44848 0.000209 1.00 |
| 7 5 2 6 4 3 | 2227.49894 2227.49900 -0.000060 0.25 |
| 7 5 3 6 4 2 | 2227.49894 2227.49889 0.000050 0.25 |
| 8 5 3 7 4 4 | 2227.57826 2227.57826 -0.000004 0.25 |
| 8 5 4 7 4 3 | 2227.57826 2227.57786 0.000401 0.25 |
