

Supplementary Material:

High-resolution spectroscopy of  $[\text{H,C,N}]^+$ : I.  
Rotationally resolved vibrational bands of  
 $\text{HCN}^+$  and  $\text{HNC}^+$

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# Renner-Teller splitting for $\text{HCN}^+$

In section 4.3 of the main article, the Renner-Teller splitting of  $\text{HCN}^+$  is discussed. In particular, Tarroni et al.<sup>1</sup> calculated the fundamental excitation of the  $\nu_2$  bending vibration to be at  $294.1 \text{ cm}^{-1}$  and  $821.5 \text{ cm}^{-1}$ . Using these values we were able to estimate the bending frequency  $\omega_2$  and the Renner-Teller parameter  $\epsilon$ .

For one quanta in the  $\nu_2$  bending vibration,  $\omega_2$  and  $\epsilon$  were calculated, ignoring the spin-orbit coupling in  $\text{HCN}^+$ , using the vibronic energy  $G(\nu_2, K)$ , as given in Herzberg et al.,<sup>2</sup> with  $\nu_2 = 1$  and  $K = 0$ :

$$G^\pm(\nu_2, 0) = \omega_2 \sqrt{1 \pm \epsilon} \cdot (\nu_2 + 1) \quad (1)$$

Thereby  $G^+(\nu_2, K)$  denotes the upper Renner-Teller component while  $G^-(\nu_2, K)$  the lower Renner-Teller component.

Here the zero point energy contribution in the vibronic energy was taken into account using the following expression<sup>2</sup> and taking  $\nu_2 = 0$  and  $K = 1$ :

$$G(\nu_2, K) = \omega_2 [(\nu_2 + 1) - \frac{1}{8} \epsilon^2 K(K + 1)] \quad (2)$$

## Line list for $\text{HCN}^+$

### $\nu_1$ fundamental stretching band

Truncated fit file from PGOPHER. Transitions are given in units of  $\text{cm}^{-1}$ . L denotes the  $\Lambda$  component, while F indicates the  $\Omega$  state.

| Observed  | Calculated | Obs-Calc | J'L' F' | J" L" F" |
|-----------|------------|----------|---------|----------|
| 3030.8664 | 3030.8668  | -0.0004  | 8.5 f 1 | 9.5 f 1  |
| 3030.8787 | 3030.8791  | -0.0005  | 8.5 e 1 | 9.5 e 1  |
| 3033.6739 | 3033.6739  | 0.0000   | 7.5 f 1 | 8.5 f 1  |
| 3033.6859 | 3033.6857  | 0.0002   | 7.5 e 1 | 8.5 e 1  |
| 3036.4608 | 3036.4604  | 0.0003   | 6.5 f 1 | 7.5 f 1  |
| 3036.4714 | 3036.4711  | 0.0003   | 6.5 e 1 | 7.5 e 1  |
| 3037.6093 | 3037.6087  | 0.0006   | 5.5 e 2 | 6.5 e 2  |

|           |           |         |       |   |       |   |
|-----------|-----------|---------|-------|---|-------|---|
| 3037.6190 | 3037.6186 | 0.0005  | 5.5 f | 2 | 6.5 f | 2 |
| 3039.2266 | 3039.2263 | 0.0003  | 5.5 f | 1 | 6.5 f | 1 |
| 3039.2359 | 3039.2354 | 0.0004  | 5.5 e | 1 | 6.5 e | 1 |
| 3040.4811 | 3040.4809 | 0.0002  | 4.5 e | 2 | 5.5 e | 2 |
| 3040.4854 | 3040.4854 | -0.0000 | 4.5 f | 2 | 5.5 f | 2 |
| 3041.9716 | 3041.9714 | 0.0002  | 4.5 f | 1 | 5.5 f | 1 |
| 3041.9790 | 3041.9788 | 0.0002  | 4.5 e | 1 | 5.5 e | 1 |
| 3043.3372 | 3043.3375 | -0.0003 | 3.5 e | 2 | 4.5 e | 2 |
| 3043.3372 | 3043.3367 | 0.0006  | 3.5 f | 2 | 4.5 f | 2 |
| 3044.6956 | 3044.6958 | -0.0002 | 3.5 f | 1 | 4.5 f | 1 |
| 3044.7010 | 3044.7013 | -0.0003 | 3.5 e | 1 | 4.5 e | 1 |
| 3046.1715 | 3046.1718 | -0.0004 | 2.5 f | 2 | 3.5 f | 2 |
| 3046.1778 | 3046.1781 | -0.0003 | 2.5 e | 2 | 3.5 e | 2 |
| 3047.3999 | 3047.3996 | 0.0003  | 2.5 f | 1 | 3.5 f | 1 |
| 3047.4035 | 3047.4032 | 0.0003  | 2.5 e | 1 | 3.5 e | 1 |
| 3048.9904 | 3048.9906 | -0.0002 | 1.5 f | 2 | 2.5 f | 2 |
| 3049.0013 | 3049.0020 | -0.0007 | 1.5 e | 2 | 2.5 e | 2 |
| 3050.0833 | 3050.0830 | 0.0002  | 1.5 f | 1 | 2.5 f | 1 |
| 3050.0845 | 3050.0850 | -0.0005 | 1.5 e | 1 | 2.5 e | 1 |
| 3051.7914 | 3051.7924 | -0.0009 | 0.5 f | 2 | 1.5 f | 2 |
| 3051.8077 | 3051.8085 | -0.0008 | 0.5 e | 2 | 1.5 e | 2 |
| 3055.7438 | 3055.7441 | -0.0004 | 3.5 e | 2 | 3.5 f | 2 |
| 3055.8276 | 3055.8275 | 0.0000  | 2.5 e | 2 | 2.5 f | 2 |
| 3055.8706 | 3055.8707 | -0.0001 | 8.5 e | 1 | 8.5 f | 1 |
| 3055.8940 | 3055.8944 | -0.0004 | 1.5 e | 2 | 1.5 f | 2 |
| 3055.9064 | 3055.9063 | 0.0001  | 3.5 f | 2 | 3.5 e | 2 |
| 3055.9445 | 3055.9440 | 0.0005  | 0.5 e | 2 | 0.5 f | 2 |
| 3055.9542 | 3055.9544 | -0.0002 | 2.5 f | 2 | 2.5 e | 2 |
| 3055.9871 | 3055.9883 | -0.0012 | 0.5 f | 2 | 0.5 e | 2 |
| 3056.0369 | 3056.0374 | -0.0005 | 8.5 f | 1 | 8.5 e | 1 |
| 3056.0513 | 3056.0518 | -0.0005 | 7.5 e | 1 | 7.5 f | 1 |
| 3056.1709 | 3056.1710 | -0.0001 | 7.5 f | 1 | 7.5 e | 1 |
| 3056.2099 | 3056.2100 | -0.0001 | 6.5 e | 1 | 6.5 f | 1 |
| 3056.2908 | 3056.2910 | -0.0002 | 6.5 f | 1 | 6.5 e | 1 |
| 3056.3456 | 3056.3456 | -0.0000 | 5.5 e | 1 | 5.5 f | 1 |
| 3056.3973 | 3056.3971 | 0.0002  | 5.5 f | 1 | 5.5 e | 1 |
| 3056.4589 | 3056.4587 | 0.0002  | 4.5 e | 1 | 4.5 f | 1 |
| 3056.4888 | 3056.4886 | 0.0002  | 4.5 f | 1 | 4.5 e | 1 |
| 3056.5499 | 3056.5500 | -0.0000 | 3.5 e | 1 | 3.5 f | 1 |
| 3056.5651 | 3056.5651 | 0.0000  | 3.5 f | 1 | 3.5 e | 1 |
| 3056.6196 | 3056.6198 | -0.0002 | 2.5 e | 1 | 2.5 f | 1 |

|           |           |         |        |   |        |   |
|-----------|-----------|---------|--------|---|--------|---|
| 3056.6258 | 3056.6259 | -0.0000 | 2.5 f  | 1 | 2.5 e  | 1 |
| 3056.6685 | 3056.6687 | -0.0002 | 1.5 e  | 1 | 1.5 f  | 1 |
| 3056.6700 | 3056.6703 | -0.0002 | 1.5 f  | 1 | 1.5 e  | 1 |
| 3060.0909 | 3060.0903 | 0.0006  | 1.5 e  | 2 | 0.5 e  | 2 |
| 3060.1167 | 3060.1169 | -0.0002 | 1.5 f  | 2 | 0.5 f  | 2 |
| 3062.8186 | 3062.8184 | 0.0001  | 2.5 e  | 2 | 1.5 e  | 2 |
| 3062.8465 | 3062.8468 | -0.0003 | 2.5 f  | 2 | 1.5 f  | 2 |
| 3063.2077 | 3063.2070 | 0.0007  | 2.5 e  | 1 | 1.5 e  | 1 |
| 3063.2099 | 3063.2096 | 0.0003  | 2.5 f  | 1 | 1.5 f  | 1 |
| 3065.5279 | 3065.5267 | 0.0012  | 3.5 e  | 2 | 2.5 e  | 2 |
| 3065.5564 | 3065.5557 | 0.0006  | 3.5 f  | 2 | 2.5 f  | 2 |
| 3065.7764 | 3065.7762 | 0.0001  | 3.5 e  | 1 | 2.5 e  | 1 |
| 3065.7817 | 3065.7816 | 0.0001  | 3.5 f  | 1 | 2.5 f  | 1 |
| 3068.2154 | 3068.2145 | 0.0010  | 4.5 e  | 2 | 3.5 e  | 2 |
| 3068.2435 | 3068.2432 | 0.0003  | 4.5 f  | 2 | 3.5 f  | 2 |
| 3068.3278 | 3068.3280 | -0.0002 | 4.5 e  | 1 | 3.5 e  | 1 |
| 3068.3372 | 3068.3373 | -0.0001 | 4.5 f  | 1 | 3.5 f  | 1 |
| 3070.8631 | 3070.8628 | 0.0003  | 5.5 e  | 1 | 4.5 e  | 1 |
| 3070.8774 | 3070.8770 | 0.0003  | 5.5 f  | 1 | 4.5 f  | 1 |
| 3070.8819 | 3070.8814 | 0.0005  | 5.5 e  | 2 | 4.5 e  | 2 |
| 3070.9088 | 3070.9086 | 0.0002  | 5.5 f  | 2 | 4.5 f  | 2 |
| 3073.3807 | 3073.3808 | -0.0001 | 6.5 e  | 1 | 5.5 e  | 1 |
| 3073.4009 | 3073.4012 | -0.0002 | 6.5 f  | 1 | 5.5 f  | 1 |
| 3073.5274 | 3073.5269 | 0.0005  | 6.5 e  | 2 | 5.5 e  | 2 |
| 3073.5524 | 3073.5516 | 0.0008  | 6.5 f  | 2 | 5.5 f  | 2 |
| 3075.8820 | 3075.8824 | -0.0005 | 7.5 e  | 1 | 6.5 e  | 1 |
| 3075.9095 | 3075.9100 | -0.0005 | 7.5 f  | 1 | 6.5 f  | 1 |
| 3076.1511 | 3076.1509 | 0.0001  | 7.5 e  | 2 | 6.5 e  | 2 |
| 3076.1717 | 3076.1719 | -0.0002 | 7.5 f  | 2 | 6.5 f  | 2 |
| 3078.3673 | 3078.3678 | -0.0005 | 8.5 e  | 1 | 7.5 e  | 1 |
| 3078.4029 | 3078.4036 | -0.0006 | 8.5 f  | 1 | 7.5 f  | 1 |
| 3078.7528 | 3078.7531 | -0.0002 | 8.5 e  | 2 | 7.5 e  | 2 |
| 3078.7694 | 3078.7693 | 0.0001  | 8.5 f  | 2 | 7.5 f  | 2 |
| 3080.8369 | 3080.8370 | -0.0001 | 9.5 e  | 1 | 8.5 e  | 1 |
| 3080.8820 | 3080.8822 | -0.0002 | 9.5 f  | 1 | 8.5 f  | 1 |
| 3081.3321 | 3081.3332 | -0.0011 | 9.5 e  | 2 | 8.5 e  | 2 |
| 3081.3430 | 3081.3437 | -0.0006 | 9.5 f  | 2 | 8.5 f  | 2 |
| 3083.2907 | 3083.2902 | 0.0005  | 10.5 e | 1 | 9.5 e  | 1 |
| 3083.3458 | 3083.3457 | 0.0001  | 10.5 f | 1 | 9.5 f  | 1 |
| 3085.7277 | 3085.7274 | 0.0003  | 11.5 e | 1 | 10.5 e | 1 |
| 3085.7953 | 3085.7942 | 0.0011  | 11.5 f | 1 | 10.5 f | 1 |

## $\nu_1 + \nu_2$ stretching band

Truncated fit file from PGOPHER. Transitions are given in units of  $cm^{-1}$ . L denotes the  $\Lambda$  component, while F indicates the  $\Omega$  state.

| Observed  | Calculated | Obs-Calc | J'L'  | F'      | J" L" F"  |
|-----------|------------|----------|-------|---------|-----------|
| 3318.8392 | 3318.8393  | -0.0001  | 3.5 e | 1 2.5 e | 2         |
| 3318.8552 | 3318.8553  | -0.0001  |       | 2.5 f   | 2 2.5 e 2 |
| 3320.0880 | 3320.0879  | 0.0001   |       | 4.5 e   | 1 3.5 e 2 |
| 3320.1084 | 3320.1085  | -0.0001  |       | 3.5 f   | 2 3.5 e 2 |
| 3321.3023 | 3321.3023  | 0.0000   |       | 5.5 e   | 1 4.5 e 2 |
| 3321.3273 | 3321.3274  | -0.0001  |       | 4.5 f   | 2 4.5 e 2 |
| 3321.7010 | 3321.7016  | -0.0006  |       | 1.5 f   | 2 0.5 f 2 |
| 3322.4848 | 3322.4845  | 0.0003   |       | 6.5 e   | 1 5.5 e 2 |
| 3322.5142 | 3322.5142  | -0.0001  |       | 5.5 f   | 2 5.5 e 2 |
| 3323.6369 | 3323.6371  | -0.0002  |       | 7.5 e   | 1 6.5 e 2 |
| 3323.6715 | 3323.6714  | 0.0001   |       | 6.5 f   | 2 6.5 e 2 |
| 3324.7640 | 3324.7629  | 0.0011   |       | 8.5 e   | 1 7.5 e 2 |
| 3324.8018 | 3324.8018  | 0.0000   |       | 7.5 f   | 2 7.5 e 2 |
| 3325.7481 | 3325.7477  | 0.0003   |       | 2.5 f   | 2 1.5 f 2 |
| 3325.8640 | 3325.8649  | -0.0009  |       | 9.5 e   | 1 8.5 e 2 |
| 3325.9086 | 3325.9084  | 0.0002   |       | 8.5 f   | 2 8.5 e 2 |
| 3343.3510 | 3343.3507  | 0.0003   |       | 5.5 e   | 1 6.5 e 1 |
| 3346.7886 | 3346.7887  | -0.0001  |       | 4.5 e   | 1 5.5 e 1 |
| 3350.3259 | 3350.3259  | 0.0000   |       | 3.5 e   | 1 4.5 e 1 |
| 3353.9644 | 3353.9645  | -0.0001  |       | 2.5 e   | 1 3.5 e 1 |
| 3357.7066 | 3357.7064  | 0.0001   |       | 1.5 e   | 1 2.5 e 1 |
| 3359.7478 | 3359.7481  | -0.0003  |       | 6.5 e   | 1 6.5 f 1 |
| 3359.7785 | 3359.7778  | 0.0007   |       | 5.5 f   | 2 6.5 f 1 |
| 3360.4607 | 3360.4608  | -0.0001  |       | 5.5 e   | 1 5.5 f 1 |
| 3360.4855 | 3360.4860  | -0.0005  |       | 4.5 f   | 2 5.5 f 1 |
| 3361.2689 | 3361.2687  | 0.0003   |       | 4.5 e   | 1 4.5 f 1 |
| 3361.2887 | 3361.2893  | -0.0006  |       | 3.5 f   | 2 4.5 f 1 |
| 3361.5537 | 3361.5533  | 0.0005   |       | 0.5 e   | 1 1.5 e 1 |
| 3362.1745 | 3362.1746  | -0.0000  |       | 3.5 e   | 1 3.5 f 1 |
| 3362.1901 | 3362.1906  | -0.0005  |       | 2.5 f   | 2 3.5 f 1 |
| 3363.1820 | 3363.1810  | 0.0009   |       | 2.5 e   | 1 2.5 f 1 |
| 3363.1927 | 3363.1924  | 0.0002   |       | 1.5 f   | 2 2.5 f 1 |
| 3364.2904 | 3364.2902  | 0.0003   |       | 1.5 e   | 1 1.5 f 1 |
| 3364.2969 | 3364.2970  | -0.0001  |       | 0.5 f   | 2 1.5 f 1 |
| 3369.7684 | 3369.7682  | 0.0002   |       | 2.5 e   | 1 1.5 e 1 |
| 3369.7792 | 3369.7797  | -0.0004  |       | 1.5 f   | 2 1.5 e 1 |

|           |           |         |       |         |   |
|-----------|-----------|---------|-------|---------|---|
| 3371.4010 | 3371.4008 | 0.0001  | 3.5 e | 1 2.5 e | 1 |
| 3371.4166 | 3371.4168 | -0.0002 | 2.5 f | 2 2.5 e | 1 |
| 3373.1381 | 3373.1380 | 0.0001  | 4.5 e | 1 3.5 e | 1 |
| 3373.1583 | 3373.1586 | -0.0002 | 3.5 f | 2 3.5 e | 1 |
| 3374.9778 | 3374.9780 | -0.0002 | 5.5 e | 1 4.5 e | 1 |
| 3375.0032 | 3375.0032 | 0.0000  | 4.5 f | 2 4.5 e | 1 |
| 3376.9487 | 3376.9486 | 0.0001  | 5.5 f | 2 5.5 e | 1 |
| 3378.0003 | 3378.0005 | -0.0003 | 2.5 f | 2 1.5 f | 1 |
| 3378.9574 | 3378.9581 | -0.0007 | 7.5 e | 1 6.5 e | 1 |
| 3378.9932 | 3378.9924 | 0.0007  | 6.5 f | 2 6.5 e | 1 |
| 3382.3749 | 3382.3751 | -0.0002 | 3.5 f | 2 2.5 f | 1 |
| 3386.8518 | 3386.8519 | -0.0001 | 4.5 f | 2 3.5 f | 1 |

## Line list for HNC<sup>+</sup>

### $\nu_1$ fundamental stretching band

Truncated fit file from PGOPHER. Transitions are given in units of  $cm^{-1}$ . S denotes the spin-doublet, while F indicates the  $\Omega$  state.

| Observed  | Calculated | Obs-Cal | J'S' F' | J" S" F"          |
|-----------|------------|---------|---------|-------------------|
| 3372.0542 | 3372.0527  | 0.0015  |         | 10.5 e 1 11.5 e 1 |
| 3372.0542 | 3372.0573  | -0.0031 |         | 9.5 f 1 10.5 f 1  |
| Blend     | 3372.0549  | -0.0007 |         |                   |
| 3375.4298 | 3375.4278  | 0.0020  |         | 9.5 e 1 10.5 e 1  |
| 3375.4298 | 3375.4322  | -0.0024 |         | 8.5 f 1 9.5 f 1   |
| Blend     | 3375.4299  | -0.0001 |         |                   |
| 3378.7818 | 3378.7801  | 0.0016  |         | 8.5 e 1 9.5 e 1   |
| 3378.7846 | 3378.7844  | 0.0002  |         | 7.5 f 1 8.5 f 1   |
| 3382.1115 | 3382.1097  | 0.0019  |         | 7.5 e 1 8.5 e 1   |
| 3382.1115 | 3382.1138  | -0.0022 |         | 6.5 f 1 7.5 f 1   |
| Blend     | 3382.1116  | -0.0000 |         |                   |
| 3385.4185 | 3385.4162  | 0.0023  |         | 6.5 e 1 7.5 e 1   |
| 3385.4185 | 3385.4202  | -0.0017 |         | 5.5 f 1 6.5 f 1   |
| Blend     | 3385.4181  | 0.0004  |         |                   |
| 3388.7012 | 3388.6998  | 0.0014  |         | 5.5 e 1 6.5 e 1   |
| 3388.7012 | 3388.7036  | -0.0024 |         | 4.5 f 1 5.5 f 1   |
| Blend     | 3388.7015  | -0.0004 |         |                   |
| 3388.7174 | 3388.7186  | -0.0012 |         | 5.5 e 1 5.5 f 1   |
| 3391.9620 | 3391.9602  | 0.0018  |         | 4.5 e 1 5.5 e 1   |

|           |           |         |       |   |       |   |
|-----------|-----------|---------|-------|---|-------|---|
| 3391.9620 | 3391.9638 | -0.0018 | 3.5 f | 1 | 4.5 f | 1 |
| Blend     | 3391.9618 | 0.0002  |       |   |       |   |
| 3391.9763 | 3391.9761 | 0.0002  | 4.5 e | 1 | 4.5 f | 1 |
| 3395.1981 | 3395.1974 | 0.0007  | 3.5 e | 1 | 4.5 e | 1 |
| 3395.1981 | 3395.2009 | -0.0028 | 2.5 f | 1 | 3.5 f | 1 |
| Blend     | 3395.1989 | -0.0008 |       |   |       |   |
| 3395.2097 | 3395.2104 | -0.0007 | 3.5 e | 1 | 3.5 f | 1 |
| 3398.4124 | 3398.4146 | -0.0021 | 1.5 f | 1 | 2.5 f | 1 |
| 3398.4124 | 3398.4113 | 0.0012  | 2.5 e | 1 | 3.5 e | 1 |
| Blend     | 3398.4126 | -0.0002 |       |   |       |   |
| 3398.4207 | 3398.4214 | -0.0007 | 2.5 e | 1 | 2.5 f | 1 |
| 3401.6023 | 3401.6017 | 0.0005  | 1.5 e | 1 | 2.5 e | 1 |
| 3401.6061 | 3401.6049 | 0.0013  | 0.5 f | 1 | 1.5 f | 1 |
| 3401.6092 | 3401.6090 | 0.0002  | 1.5 e | 1 | 1.5 f | 1 |
| 3404.7695 | 3404.7687 | 0.0008  | 0.5 e | 1 | 1.5 e | 1 |
| 3404.7742 | 3404.7731 | 0.0011  | 0.5 e | 1 | 0.5 f | 1 |
| 3411.0322 | 3411.0347 | -0.0024 | 1.5 e | 1 | 0.5 e | 1 |
| 3411.0322 | 3411.0306 | 0.0017  | 0.5 f | 1 | 0.5 e | 1 |
| Blend     | 3411.0333 | -0.0011 |       |   |       |   |
| 3414.1284 | 3414.1306 | -0.0022 | 2.5 e | 1 | 1.5 e | 1 |
| 3417.1929 | 3417.1932 | -0.0003 | 2.5 f | 1 | 2.5 e | 1 |
| 3417.2010 | 3417.2028 | -0.0018 | 3.5 e | 1 | 2.5 e | 1 |
| 3420.2405 | 3420.2388 | 0.0017  | 3.5 f | 1 | 3.5 e | 1 |
| 3420.2514 | 3420.2490 | 0.0024  | 3.5 f | 1 | 2.5 f | 1 |
| 3420.2528 | 3420.2511 | 0.0017  | 4.5 e | 1 | 3.5 e | 1 |
| 3423.2602 | 3423.2606 | -0.0003 | 4.5 f | 1 | 4.5 e | 1 |
| 3423.2746 | 3423.2756 | -0.0010 | 5.5 e | 1 | 4.5 e | 1 |
| 3423.2746 | 3423.2736 | 0.0010  | 4.5 f | 1 | 3.5 f | 1 |
| Blend     | 3423.2747 | -0.0001 |       |   |       |   |
| 3426.2577 | 3426.2583 | -0.0007 | 5.5 f | 1 | 5.5 e | 1 |
| 3426.2756 | 3426.2743 | 0.0014  | 5.5 f | 1 | 4.5 f | 1 |
| 3426.2756 | 3426.2761 | -0.0005 | 6.5 e | 1 | 5.5 e | 1 |
| Blend     | 3426.2753 | 0.0004  |       |   |       |   |
| 3429.2306 | 3429.2321 | -0.0015 | 6.5 f | 1 | 6.5 e | 1 |
| 3429.2522 | 3429.2510 | 0.0012  | 6.5 f | 1 | 5.5 f | 1 |
| 3429.2522 | 3429.2526 | -0.0005 | 7.5 e | 1 | 6.5 e | 1 |
| Blend     | 3429.2518 | 0.0003  |       |   |       |   |
| 3432.1815 | 3432.1818 | -0.0003 | 7.5 f | 1 | 7.5 e | 1 |
| 3432.2040 | 3432.2036 | 0.0004  | 7.5 f | 1 | 6.5 f | 1 |
| 3432.2040 | 3432.2051 | -0.0011 | 8.5 e | 1 | 7.5 e | 1 |
| Blend     | 3432.2044 | -0.0004 |       |   |       |   |

|           |           |         |        |   |       |   |
|-----------|-----------|---------|--------|---|-------|---|
| 3435.1330 | 3435.1321 | 0.0009  | 8.5 f  | 1 | 7.5 f | 1 |
| 3435.1330 | 3435.1334 | -0.0004 | 9.5 e  | 1 | 8.5 e | 1 |
| Blend     | 3435.1328 | 0.0002  |        |   |       |   |
| 3438.0376 | 3438.0376 | -0.0001 | 10.5 e | 1 | 9.5 e | 1 |
| 3438.0376 | 3438.0365 | 0.0011  | 9.5 f  | 1 | 8.5 f | 1 |
| Blend     | 3438.0371 | 0.0005  |        |   |       |   |

## References

- (1) Tarroni, R.; Mitrushenkov, A.; Palmieri, P.; Carter, S. Energy levels of  $\text{HCN}^+$  and  $\text{DCN}^+$  in the vibronically coupled  $X^2\Pi$  and  $A^2\Sigma^+$  states. *The Journal of Chemical Physics* **2001**, *115*, 11200–11212.
- (2) Herzberg, G. *Molecular Spectra and Molecular Structure. Vol.III: Electronic Spectra and Electronic Structure of Polyatomic Molecules*; 1950; Vol. 3.