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Supporting Information for ChemPhysChem:

**The Axial and Equatorial Hydrogen Bonds in the Tetrahydropyran...HF  
Complex**

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Table S1. Observed and calculated transition frequencies (MHz) for the axial conformer of tetrahydropyran...HF complex.

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $I'$ | $F'$ | $I''$ | $F''$ | <i>obs.</i> | <i>obs. - cal.</i> | $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $I'$ | $F'$ | $I''$ | $F''$ | <i>obs.</i> | <i>obs. - cal.</i> |
|------|-----------|-----------|-------|------------|------------|------|------|-------|-------|-------------|--------------------|------|-----------|-----------|-------|------------|------------|------|------|-------|-------|-------------|--------------------|
| 2    | 0         | 2         | 1     | 0          | 1          | 1    | 3    | 1     | 2     | 6836.573    | -0.001             | 4    | 0         | 4         | 3     | 0          | 3          | 1    | 5    | 1     | 4     | 13561.524   | 0.001              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 6836.573    | -0.001             |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13561.524   | 0.001              |
|      |           |           |       |            |            | 0    | 2    | 0     | 1     | 6836.573    | -0.001             |      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13561.524   | 0.001              |
|      |           |           |       |            |            | 1    | 1    | 1     | 0     | 6836.550    | -0.003             |      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13561.524   | 0.001              |
| 2    | 1         | 2         | 1     | 1          | 1          | 1    | 3    | 1     | 2     | 6685.964    | -0.002             | 4    | 1         | 4         | 3     | 1          | 3          | 1    | 5    | 1     | 4     | 13344.018   | 0.000              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 6685.944    | 0.003              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13344.018   | 0.000              |
|      |           |           |       |            |            | 0    | 2    | 0     | 1     | 6685.958    | -0.003             |      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13344.018   | 0.000              |
|      |           |           |       |            |            | 1    | 1    | 1     | 0     | 6685.991    | -0.001             |      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13344.018   | 0.000              |
| 2    | 1         | 1         | 1     | 1          | 0          | 1    | 3    | 1     | 2     | 7016.590    | 0.002              | 4    | 1         | 3         | 3     | 1          | 2          | 1    | 5    | 1     | 4     | 14000.537   | 0.002              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 7016.563    | 0.001              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 14000.537   | 0.002              |
|      |           |           |       |            |            | 0    | 2    | 0     | 1     | 7016.578    | -0.004             |      |           |           |       |            |            | 0    | 4    | 0     | 3     | 14000.537   | 0.002              |
| 2    | 1         | 1         | 1     | 0          | 1          | 1    | 3    | 1     | 2     | 8494.063    | 0.002              |      |           |           |       |            |            | 1    | 3    | 1     | 2     | 14000.537   | 0.002              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 8494.066    | -0.005             | 4    | 2         | 3         | 3     | 2          | 2          | 1    | 5    | 1     | 4     | 13690.577   | 0.002              |
|      |           |           |       |            |            | 0    | 2    | 0     | 1     | 8494.063    | 0.001              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13690.562   | -0.002             |
| 2    | 2         | 1         | 1     | 1          | 1          | 1    | 3    | 1     | 2     | 11118.344   | -0.004             |      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13690.577   | 0.002              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 11118.365   | 0.003              |      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13690.577   | 0.002              |
|      |           |           |       |            |            | 0    | 2    | 0     | 1     | 11118.351   | -0.001             | 4    | 2         | 2         | 3     | 2          | 1          | 1    | 5    | 1     | 4     | 13830.660   | -0.003             |
|      |           |           |       |            |            | 1    | 1    | 1     | 0     | 11118.351   | -0.001             |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13830.653   | 0.001              |
| 3    | 0         | 3         | 2     | 0          | 2          | 1    | 4    | 1     | 3     | 10218.715   | 0.000              |      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13830.660   | -0.003             |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 10218.715   | 0.000              |      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13830.660   | -0.003             |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 10218.715   | 0.000              | 4    | 3         | 2         | 3     | 3          | 1          | 1    | 5    | 1     | 4     | 13729.459   | -0.002             |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 10218.715   | 0.000              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13729.439   | 0.003              |
| 3    | 1         | 3         | 2     | 1          | 2          | 1    | 4    | 1     | 3     | 10019.880   | 0.000              |      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13729.459   | 0.004              |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 10019.880   | 0.000              |      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13729.476   | 0.006              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 10019.880   | 0.000              | 4    | 3         | 1         | 3     | 3          | 0          | 1    | 5    | 1     | 4     | 13734.336   | 0.003              |
|      |           |           |       |            |            | 1    | 1    | 1     | 0     | 10019.880   | 0.000              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13734.305   | -0.003             |
| 3    | 1         | 2         | 2     | 1          | 1          | 1    | 4    | 1     | 3     | 10515.044   | 0.001              |      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13734.326   | 0.000              |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 10515.033   | -0.002             |      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13734.343   | 0.001              |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 10515.044   | 0.002              | 5    | 0         | 5         | 4     | 0          | 4          | 1    | 6    | 1     | 5     | 16862.474   | 0.002              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 10515.044   | 0.002              |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 16862.474   | 0.002              |
| 3    | 1         | 2         | 2     | 0          | 2          | 1    | 4    | 1     | 3     | 12172.530   | 0.002              |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 16862.474   | 0.002              |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 12172.533   | 0.000              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 16862.474   | 0.002              |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 12172.530   | 0.001              | 5    | 1         | 5         | 4     | 1          | 4          | 1    | 6    | 1     | 5     | 16656.801   | -0.002             |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 12172.517   | -0.004             |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 16656.801   | -0.002             |
| 3    | 2         | 2         | 2     | 1          | 2          | 1    | 4    | 1     | 3     | 14709.239   | 0.001              |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 16656.801   | -0.002             |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 14709.253   | 0.002              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 16656.801   | -0.002             |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 14709.244   | 0.003              | 5    | 1         | 4         | 4     | 1          | 3          | 1    | 6    | 1     | 5     | 17466.813   | 0.003              |
| 3    | 2         | 1         | 2     | 1          | 1          | 1    | 4    | 1     | 3     | 14285.847   | 0.001              |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 17466.813   | 0.003              |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 14285.857   | -0.002             |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 17466.813   | 0.003              |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 14285.847   | -0.002             |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 17466.813   | 0.003              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 14285.837   | -0.001             | 5    | 2         | 4         | 4     | 2          | 3          | 1    | 6    | 1     | 5     | 17094.183   | 0.005              |
| 3    | 3         | 1         | 2     | 2          | 1          | 1    | 4    | 1     | 3     | 17259.389   | 0.002              |      |           |           |       |            |            | 1    | 5    | 0     | 4     | 17094.183   | 0.005              |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 17259.419   | -0.003             |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 17094.183   | 0.005              |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 17259.389   | -0.001             |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 17094.183   | 0.005              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 17259.389   | -0.001             | 5    | 2         | 3         | 4     | 2          | 2          | 1    | 6    | 1     | 5     | 17357.707   | -0.001             |
| 3    | 3         | 0         | 2     | 2          | 0          | 1    | 4    | 1     | 3     | 17245.550   | 0.001              |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 17357.707   | -0.001             |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 17245.553   | 0.001              |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 17357.707   | -0.001             |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 17245.553   | 0.001              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 17357.707   | -0.001             |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 17245.553   | 0.001              | 5    | 3         | 3         | 4     | 3          | 2          | 1    | 6    | 1     | 5     | 17169.655   | -0.004             |
|      |           |           |       |            |            |      |      |       |       |             |                    |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 17169.643   | -0.004             |
|      |           |           |       |            |            |      |      |       |       |             |                    |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 17169.655   | -0.004             |
|      |           |           |       |            |            |      |      |       |       |             |                    |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 17169.655   | -0.004             |

Table S2. Observed and calculated transition frequencies (MHz) for the axial conformer of  $^{13}\text{C}_\alpha$ -tetrahydropyran...HF species.

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $I'$ | $F'$ | $I''$ | $F''$ | <i>obs.</i> | <i>obs. - cal.</i> | $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $I'$ | $F'$ | $I''$ | $F''$ | <i>obs.</i> | <i>obs. - cal.</i> |
|------|-----------|-----------|-------|------------|------------|------|------|-------|-------|-------------|--------------------|------|-----------|-----------|-------|------------|------------|------|------|-------|-------|-------------|--------------------|
| 2    | 0         | 2         | 1     | 0          | 1          | 1    | 3    | 1     | 2     | 6811.142    | -0.001             | 4    | 2         | 3         | 3     | 2          | 2          | 1    | 5    | 1     | 4     | 13640.898   | 0.001              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 6811.142    | -0.001             |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13640.886   | 0.000              |
|      |           |           |       |            |            | 0    | 2    | 0     | 1     | 6811.142    | -0.001             |      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13640.890   | -0.004             |
|      |           |           |       |            |            | 1    | 1    | 1     | 0     | 6811.123    | 0.001              |      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13640.898   | -0.001             |
| 2    | 1         | 2         | 1     | 1          | 1          | 1    | 3    | 1     | 2     | 6658.138    | 0.001              | 4    | 2         | 2         | 3     | 2          | 1          | 1    | 5    | 1     | 4     | 13789.659   | 0.002              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 6658.114    | 0.003              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13789.649   | 0.003              |
|      |           |           |       |            |            | 0    | 2    | 0     | 1     | 6658.129    | -0.002             |      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13789.655   | 0.001              |
| 2    | 1         | 1         | 1     | 1          | 0          | 1    | 3    | 1     | 2     | 6995.488    | 0.000              |      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13789.659   | -0.001             |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 6995.465    | 0.001              | 5    | 0         | 5         | 4     | 0          | 4          | 1    | 6    | 1     | 5     | 16786.307   | -0.002             |
|      |           |           |       |            |            | 0    | 2    | 0     | 1     | 6995.483    | -0.001             |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 16786.307   | -0.002             |
| 3    | 0         | 3         | 2     | 0          | 2          | 1    | 4    | 1     | 3     | 10178.273   | 0.000              |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 16786.307   | -0.002             |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 10178.273   | 0.000              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 16786.307   | -0.002             |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 10178.273   | 0.000              | 5    | 1         | 5         | 4     | 1          | 4          | 1    | 6    | 1     | 5     | 16583.907   | 0.001              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 10178.273   | 0.000              |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 16583.907   | 0.001              |
| 3    | 1         | 3         | 2     | 1          | 2          | 1    | 4    | 1     | 3     | 9977.574    | -0.002             |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 16583.907   | 0.001              |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 9977.574    | -0.002             |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 16583.907   | 0.001              |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 9977.574    | -0.002             | 5    | 1         | 4         | 4     | 1          | 3          | 1    | 6    | 1     | 5     | 17408.840   | 0.003              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 9977.574    | -0.002             |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 17408.840   | 0.003              |
| 3    | 1         | 2         | 2     | 1          | 1          | 1    | 4    | 1     | 3     | 10482.743   | 0.000              |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 17408.840   | 0.003              |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 10482.735   | -0.001             |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 17408.840   | 0.003              |
|      |           |           |       |            |            | 0    | 3    | 0     | 2     | 10482.739   | -0.001             | 5    | 2         | 4         | 4     | 2          | 3          | 1    | 6    | 1     | 5     | 17030.893   | 0.000              |
|      |           |           |       |            |            | 1    | 2    | 1     | 1     | 10482.743   | 0.000              |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 17030.893   | 0.000              |
| 4    | 0         | 4         | 3     | 0          | 3          | 1    | 5    | 1     | 4     | 13503.937   | 0.001              |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 17030.893   | 0.000              |
|      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13503.937   | 0.001              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 17030.893   | 0.000              |
|      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13503.937   | 0.001              | 5    | 2         | 3         | 4     | 2          | 2          | 1    | 6    | 1     | 5     | 17309.418   | -0.001             |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13503.937   | 0.001              |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 17309.410   | -0.002             |
| 4    | 1         | 4         | 3     | 1          | 3          | 1    | 5    | 1     | 4     | 13286.692   | 0.001              |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 17309.418   | 0.000              |
|      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13286.692   | 0.001              |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 17309.418   | 0.000              |
|      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13286.692   | 0.001              | 5    | 3         | 3         | 4     | 3          | 2          | 1    | 6    | 1     | 5     | 17110.950   | 0.001              |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13286.692   | 0.001              |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 17110.938   | 0.002              |
| 4    | 1         | 3         | 3     | 1          | 2          | 1    | 5    | 1     | 4     | 13956.115   | -0.001             |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 17110.950   | 0.001              |
|      |           |           |       |            |            | 1    | 4    | 1     | 3     | 13956.115   | -0.001             |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 17110.950   | 0.001              |
|      |           |           |       |            |            | 0    | 4    | 0     | 3     | 13956.115   | -0.001             | 5    | 3         | 2         | 4     | 3          | 1          | 1    | 6    | 1     | 5     | 17129.714   | -0.001             |
|      |           |           |       |            |            | 1    | 3    | 1     | 2     | 13956.115   | -0.001             |      |           |           |       |            |            | 1    | 5    | 1     | 4     | 17129.702   | -0.001             |
|      |           |           |       |            |            |      |      |       |       |             |                    |      |           |           |       |            |            | 0    | 5    | 0     | 4     | 17129.714   | -0.001             |
|      |           |           |       |            |            |      |      |       |       |             |                    |      |           |           |       |            |            | 1    | 4    | 1     | 3     | 17129.714   | -0.001             |









