Supplementary Information

Bifunctional Hydrogen Bonding of Imidazole with Water

Explored by Rotational Spectroscopy and DFT Calculations

Eva Gougoula, Daniel J. Cole and Nicholas R. Walker

Chemistry- School of Natural and Environmental Sciences, Newcastle University, Bedson Building, Newcastle upon Tyne, NE1 7RU, UK
Table S1. Calculated atomic coordinates for imid·H$_2$O and H$_2$O·imid at the B3LYP(D3BJ)/aug-cc-pVTZ and ωB97XD/aug-cc-pVQZ levels of theory.

<table>
<thead>
<tr>
<th>B3LYP(D3BJ)/aug-cc-pVTZ</th>
<th>imid·H$_2$O</th>
<th>ωB97XD/aug-cc-pVQZ</th>
<th>imid·H$_2$O</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>$a$/Å</td>
<td>$b$/Å</td>
<td>$c$/Å</td>
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<tr>
<td>N1</td>
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<td>H1</td>
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<tr>
<td>C2</td>
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<tr>
<td>C5</td>
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<td>-0.545453</td>
<td>-0.039670</td>
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<tr>
<td>H5</td>
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<tr>
<td>H$_b$</td>
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<tr>
<td>O</td>
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<tr>
<td>H$_{ab}$</td>
<td>3.591841</td>
<td>-0.338637</td>
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<p>|                         | $a$/Å       | $b$/Å               | $c$/Å       |
| N1                      | -1.622908   | -0.800110           | -0.013285   |
| H1                      | -2.301568   | -1.537156           | -0.038116   |
| C2                      | -0.280639   | -0.952715           | 0.041072    |
| H2                      | 0.201260    | -1.915388           | 0.064178    |
| N3                      | 0.327091    | 0.203692            | 0.057305    |
| C4                      | -0.664420   | 1.147949            | 0.010111    |
| H4                      | -0.443213   | 2.200765            | 0.008406    |
| C5                      | -1.883636   | 0.545509            | -0.033524   |
| H5                      | -2.881975   | 0.939680            | -0.078315   |
| H$<em>b$                   | 2.253901    | 0.141020            | -0.054538   |
| O                       | 3.203723    | -0.048453           | -0.124829   |
| H$</em>{ab}$                | 3.584692    | 0.289172            | 0.682930    |</p>
<table>
<thead>
<tr>
<th></th>
<th>B3LYP(D3BJ)/aug-cc-pVTZ</th>
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<th>ωB97XD/aug-cc-pVQZ</th>
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<td>a/Å</td>
<td>b/Å</td>
<td>c/Å</td>
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<td>O</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>H2O⁻·imid</td>
<td></td>
<td>H2O⁻·imid</td>
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<tr>
<td>N1</td>
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<td>H</td>
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<td>-0.200038</td>
<td>0.763686</td>
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Table S2. Spectroscopic parameters determined for isotopologues of imid⋅H₂O.

<table>
<thead>
<tr>
<th></th>
<th>imid⋅D₁OH_{ab}</th>
<th>imid⋅H^{18}O</th>
<th>imid⋅H₂OD_{ab}</th>
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<tbody>
<tr>
<td>$A_0$ (MHz)</td>
<td>9481.55(46)$^a$</td>
<td>9499.20(45)</td>
<td>9422.95(34)</td>
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<tr>
<td>$B_0$ (MHz)</td>
<td>1793.3641(15)</td>
<td>1707.6406(23)</td>
<td>1742.7498(29)</td>
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<tr>
<td>$C_0$ (MHz)</td>
<td>1508.1838(10)</td>
<td>1447.3811(20)</td>
<td>1472.3732(15)</td>
</tr>
<tr>
<td>$D_f$ (kHz)</td>
<td>1.320(26)</td>
<td>1.427(22)</td>
<td>1.088(21)</td>
</tr>
<tr>
<td>$D_J$ (kHz)</td>
<td>60.97(25)</td>
<td>57.83(12)</td>
<td>57.29(19)</td>
</tr>
<tr>
<td>$d_1$ (kHz)</td>
<td>-</td>
<td>-0.276(23)</td>
<td>-0.139(24)</td>
</tr>
<tr>
<td>$\chi_{ab}(N1)$ (MHz)</td>
<td>[1.143(19)]</td>
<td>[1.143(19)]</td>
<td>[1.143(19)]</td>
</tr>
<tr>
<td>$\delta(N1)$</td>
<td>[-2.889(21)]</td>
<td>[-2.889(21)]</td>
<td>[-2.889(21)]</td>
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<tr>
<td>$\delta(N3)$</td>
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<td>[-1.07(11)]</td>
<td>[-1.07(11)]</td>
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<td>$\kappa$</td>
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<tr>
<td>$P_{aa}$ (u Å²)</td>
<td>281.797(21)</td>
<td>295.959(22)</td>
<td>289.799(16)</td>
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<tr>
<td>$P_{bb}$ (u Å²)</td>
<td>53.294(21)</td>
<td>53.209(22)</td>
<td>53.442(16)</td>
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<tr>
<td>$P_{cc}$ (u Å²)</td>
<td>0.008(21)</td>
<td>-0.007(22)</td>
<td>0.191(16)</td>
</tr>
<tr>
<td>$\Delta$ (u Å²)</td>
<td>-0.015(42)</td>
<td>0.014(44)</td>
<td>-0.381(32)</td>
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<tr>
<td>$N^b$</td>
<td>19</td>
<td>41</td>
<td>25</td>
</tr>
<tr>
<td>$\sigma_{RMS}$ (kHz)$^b$</td>
<td>9.2</td>
<td>13.3</td>
<td>10.3</td>
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$^a$ Numbers in parentheses are one standard deviation in units of the last significant figure.

$^b$ $N$ and $\sigma_{RMS}$ are respectively the number of measured transitions and the standard deviation of the fit.
Table S3. Spectroscopic parameters determined for isotopologues of H_2O–imid.

<table>
<thead>
<tr>
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<th>HDO–imid</th>
<th>H_2^{18}O–imid</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0^-</td>
<td>0^+</td>
</tr>
<tr>
<td>( A_0 ) (MHz)</td>
<td>9384.56(67)^a</td>
<td>9430.41(50)</td>
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<tr>
<td>( B_0 ) (MHz)</td>
<td>1586.6402(18)</td>
<td>1586.7041(26)</td>
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<tr>
<td>( C_0 ) (MHz)</td>
<td>1366.8028(15)</td>
<td>1366.6089(20)</td>
</tr>
<tr>
<td>( D_J ) (kHz)</td>
<td>0.633(23)</td>
<td>1.138(17)</td>
</tr>
<tr>
<td>( D_{JK} ) (kHz)</td>
<td>37.59(35)</td>
<td>34.62(29)</td>
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<tr>
<td>( d_1 ) (kHz)</td>
<td>-</td>
<td>-0.613(18)</td>
</tr>
<tr>
<td>( \chi_{aa}(N1) ) (MHz)</td>
<td>[0.923]</td>
<td>[0.916]</td>
</tr>
<tr>
<td>( [\chi_{bd}(N1) - \chi_{cc}(N1)] ) (MHz)</td>
<td>[3.80]</td>
<td>[4.07]</td>
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<tr>
<td>( \chi_{aa}(N3) ) (MHz)</td>
<td>[−1.932]</td>
<td>[−1.859]</td>
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<tr>
<td>( [\chi_{bd}(N3) - \chi_{cc}(N3)] ) (MHz)</td>
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<td>[−2.47]</td>
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<tr>
<td>( \kappa )</td>
<td>−0.945163(4)</td>
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<td>( P_{aa} ) (u Å^2)</td>
<td>317.2037(18)</td>
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<td>( P_{bb} ) (u Å^2)</td>
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<td>( P_{cc} ) (u Å^2)</td>
<td>1.3104(18)</td>
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<td>( \Delta ) (u Å^2)</td>
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<td>( N^b )</td>
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<td>15</td>
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<tr>
<td>( \sigma_{RMS} )</td>
<td>12.7</td>
<td>8.4</td>
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</table>

^a Numbers in parentheses are one standard deviation in units of the last significant figure.

^b \( N \) and \( \sigma_{RMS} \) are respectively the number of measured transitions and the standard deviation of the fit.
Table S4. Calculated rotational constants of imid·H$_2$O and H$_2$O···imid and their percentage deviations from the experimentally determined ground state rotational constants.

<table>
<thead>
<tr>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>imid·H$_2$O</td>
<td>H$_2$O···imid</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$A_e$ (MHz)</td>
<td>9522.83</td>
<td>9516.67</td>
</tr>
<tr>
<td></td>
<td>$B_e$ (MHz)</td>
<td>1788.40</td>
<td>1677.86</td>
</tr>
<tr>
<td></td>
<td>$C_e$ (MHz)</td>
<td>1512.19</td>
<td>1436.02</td>
</tr>
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<td>$\chi_{aa}(N1)$ (MHz)</td>
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</tr>
<tr>
<td></td>
<td>[\chi_{bb}(N1) − \chi_{cc}(N1)] (MHz)</td>
<td>3.858</td>
<td>3.451</td>
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<td></td>
<td>$\chi_{aa}(N3)$ (MHz)</td>
<td>−3.783</td>
<td>−2.267</td>
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<tr>
<td></td>
<td>[\chi_{bb}(N3) − \chi_{cc}(N3)] (MHz)</td>
<td>−0.49</td>
<td>−2.680</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>\mu_a</td>
<td>,</td>
</tr>
<tr>
<td>$\Delta E$ (cm$^{-1}$, kJ mol$^{-1}$)</td>
<td>0</td>
<td>263, 3.15</td>
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</table>

|                  | oB97XD/aug-cc-pVQZ |                   |                   |
|                  | imid·H$_2$O             | H$_2$O···imid     |
|                  | $A_e$ (MHz)             | 9608              | 9570.98           |
|                  | $B_e$ (MHz)             | 1778.24           | 1695.37           |
|                  | $C_e$ (MHz)             | 1507.59           | 1449.96           |
|                  | $\chi_{aa}(N1)$ (MHz)  | 1.145             | 0.839             |
|                  | [\chi_{bb}(N1) − \chi_{cc}(N1)] (MHz) | 3.792           | 3.296             |
|                  | $\chi_{aa}(N3)$ (MHz)  | −3.869            | −2.003            |
|                  | [\chi_{bb}(N3) − \chi_{cc}(N3)] (MHz) | −0.730           | −3.224            |
|                  | $|\mu_a|, |\mu_b|, |\mu_c|$ (D) | [5.3], [1.1], [1.2] | [6.2], [0.6], [0] |
| $\Delta E$ (cm$^{-1}$, kJ mol$^{-1}$) | 0                     | 606, 7.3          |

*Percentage deviation calculated as $\frac{A_{\text{calc}}-A_{\text{exp}}}{A_{\text{exp}}} \times 100$ where the comparison is between results for the parent isotopologues of imid·H$_2$O and H$_2$O···imid.

*Imid·H$_2$O is calculated to be the global minimum by both methods. The energy of the H$_2$O···imid isomer is given relative to the energy of imid·H$_2$O.
Table S5- Diagonalization of nuclear quadrupole coupling tensors to determine $\chi_{xx}$, $\chi_{yy}$ and $\chi_{zz}$.

$\chi_{xx}$, $\chi_{yy}$ and $\chi_{zz}$ represent projections of the nuclear quadrupole coupling tensor onto principal axes located on each individual nucleus. Determination of $\chi_{xx}$, $\chi_{yy}$ and $\chi_{zz}$ from the experimentally-determined values of $\chi_{aa}$, $\chi_{bb}$ and $\chi_{cc}$ (summarised in table 2) respectively was performed using Kisiel’s QDIAG available from the PROSPE$^1$ website. The off-diagonal term, $\chi_{ab}$, was calculated for each of imid$\cdots$H$_2$O and H$_2$O$\cdots$imid at the B3LYP-D3BJ/aug-cc-pVTZ level. The values of $\chi_{ab}$ used to diagonalize the tensors are $-0.094$ and $1.15$ for N1 and N3 of imid$\cdots$H$_2$O and $-0.076$ and $-2.96$ for N1 and N3 of H$_2$O$\cdots$imid, respectively. A 25% uncertainty was given to the off-diagonal terms when performing the diagonalizations.

The $a$- and $b$-axes are rotated through an angle, $\phi(X)$, where X is the nucleus on which the axes are centred. The labelling system used for the nitrogen atoms was chosen to be consistent with that used by Christen et al. in their study of imidazole$^2$. For the pyrrolic nitrogen atom (N1), the $z$-axis is out of the molecular plane and $\phi$ is the angle between the $a$ and $y$-axes. For the pyridinic nitrogen (N3), the $y$-axis is perpendicular to the plane of the molecule, and $\phi$ is the angle between the $a$ and $x$-axes. The results allow direct comparisons with $\chi_{xx}$, $\chi_{yy}$ and $\chi_{zz}$ provided in other works. All values of $\chi_{xx}$, $\chi_{yy}$ and $\chi_{zz}$ are in agreement with those determined for the isolated imidazole molecule confirming the assignment of the fitted tensors to their corresponding N1 or N3 nuclei.

<table>
<thead>
<tr>
<th></th>
<th>Imid$\cdots$H$_2$O</th>
<th>H$_2$O$\cdots$Imid</th>
<th>Imidazole$^a$</th>
</tr>
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<tbody>
<tr>
<td>$\chi_{xx}$ (N1)</td>
<td>1.096(27)</td>
<td>0.912(74)</td>
<td>0.890(52)</td>
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<tr>
<td>$\chi_{yy}$ (N1)</td>
<td>1.332(54)</td>
<td>1.45(51)</td>
<td>1.633(58)</td>
</tr>
<tr>
<td>$\chi_{zz}$ (N1)</td>
<td>$-2.428(30)$</td>
<td>$-2.36(23)$</td>
<td>$-2.524(12)$</td>
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<td>$\eta^b$</td>
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<td>0.23(22)</td>
<td>0.1361(59)</td>
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<tr>
<td>$\chi_{xx}$ (N3)</td>
<td>1.23(19)</td>
<td>1.92(78)</td>
<td>1.835(23)</td>
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<tr>
<td>$\chi_{yy}$ (N3)</td>
<td>1.980(56)</td>
<td>2.30(22)</td>
<td>2.278(24)</td>
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<tr>
<td>$\chi_{zz}$ (N3)</td>
<td>$-3.21(15)$</td>
<td>$-4.21(74)$</td>
<td>$-4.113(34)$</td>
</tr>
<tr>
<td>$\eta^b$</td>
<td>0.234(63)</td>
<td>0.09(19)</td>
<td>0.060(20)</td>
</tr>
</tbody>
</table>

$^a$ Results from Christen et al.$^2$

$^b$ $\eta = (\chi_{xx} - \chi_{yy})/\chi_{zz}$
Table S6. Calculated atomic coordinates and residuals for the alternative, experimentally-determined, $r_0$ geometries of imid···H$_2$O described under “Molecular Geometry”. The geometry determined while assuming $\angle$(H$_{ab}$–O–H$_b$···N3) = 180°, $\angle$(O–H$_b$···N3–C2) =0° leads to the parameters and coordinates displayed in Tables 3 and 4. All c-coordinates are constrained to zero by the assumption that the molecule is planar.

### imid···H$_2$O (\(\angle$(H$_{ab}$–O–H$_b$···N3) = 180°, \(\angle$(O–H$_b$···N3–C2) =0°)

<table>
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<th>a/Å</th>
<th>da/Å</th>
<th>b/Å</th>
<th>db/Å</th>
<th>c/Å</th>
<th>dc/Å</th>
</tr>
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### imid···H$_2$O (\(\angle$(H$_{ab}$–O–H$_b$···N3) = 180°, \(\angle$(O–H$_b$···N3–C2) =180°)

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Supplementary References

S1 PROSPE, http://www.ifpan.edu.pl/~kisiel/prospe.htm, 04/03/2020