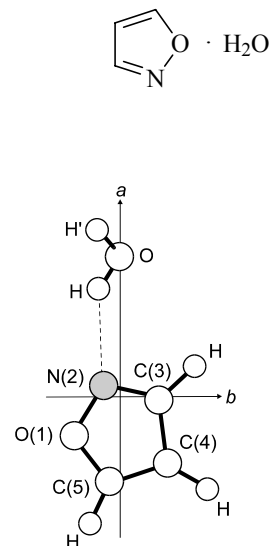


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MW $C_3H_5NO_2$ **Isoxazole – water (1/1)**
(weakly bound complex) **C_s**
(effective symmetry class)
(large-amplitude motion)

| r_0 | $\text{\AA}^a)$ | θ_0 | $\text{deg}^a)$ |
|-----------|-----------------|----------------|-----------------|
| O(1)–N(2) | 1.3988(50) | O(1)–N(2)–C(3) | 105.28(50) |
| N(2)–C(3) | 1.3084(50) | N(2)–C(3)–C(4) | 112.32(50) |
| C(3)–C(4) | 1.4257(50) | C(3)–C(4)–C(5) | 103.04(50) |
| C(4)–C(5) | 1.3566(50) | C(4)–C(5)–O(1) | 110.49(50) |
| C(5)–O(1) | 1.3437(50) | C(5)–O(1)–N(2) | 108.88(50) |
| C(3)–H | 1.0776(50) | H–C(3)–N(2) | 118.61(50) |
| C(4)–H | 1.0741(50) | H–C(4)–C(3) | 128.47(50) |
| C(5)–H | 1.0738(50) | H–C(5)–C(4) | 133.39(50) |
| O–H | 0.8837(50) | H–O–H' | 93.98(50) |
| O–H' | 0.8837(50) | N(2)...H–O | 141.12(50) |
| N(2)...H | 2.1467(50) | C(3)–N(2)...H | 108.75(50) |
| | | N(2)...H–O–H' | 150.96(50) |

| Atom | $ a_s [\text{\AA}]$ | $ b_s [\text{\AA}]$ |
|----------|----------------------|----------------------|
| H(bound) | 2.4391 | 0.4701 |
| N(2) | 0.2261 | 0.3616 |



Water is bound to nitrogen in the ring plane of isoxazole. Small splittings of the rotational transitions were interpreted as being the result of an internal rotation of water with respect to isoxazole.

^{a)} Uncertainties were not estimated in the original paper.

McGlone, S., Moreschini, P., Ha, T.-K., Bauder, A.: Mol. Phys. **99** (2001) 1353.