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MW $\text{H}_3\text{NO}_4$ **Nitric acid – water (1/1)**  
(weakly bound complex) $\text{C}_s$   
(effective symmetry class)  
(large-amplitude motion)  
 $\text{HNO}_3 \cdot \text{H}_2\text{O}$ 

$r_0$	$\text{\AA}$	$\theta_0$	deg
O(1)...H(3)	1.779(33)	O(3)...H(1)–O(1)	119.3(5) <sup>a)</sup>
O(3)...H(1)	2.30(2) <sup>a)</sup>	$\alpha$ <sup>b)</sup>	174.5(41)
		$\beta$ <sup>c)</sup>	92(8)
		$\gamma$ <sup>d)</sup>	30(10)

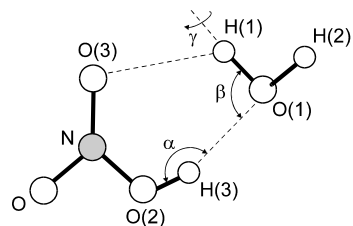
The observed spectra are consistent with a structure in which the nitric acid forms a near-linear, 1.78 Å hydrogen bond to the oxygen of the water. A second, presumably weaker hydrogen bond is formed between a water hydrogen and one of the  $\text{HNO}_3$  oxygen. The resulting cyclic structure adopts a planar configuration except for the non-hydrogen bonded proton of the  $\text{H}_2\text{O}$ . In complexes containing DOH, only the isomer with the deuterium in the plane is observed, confirming the contribution of the secondary O...H interaction to the overall stabilization of the system. The *a*- and *b*-type transitions of the  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$  containing species exhibit a doubling which disappears in the DOH complex, providing evidence for the existence of a proton interchange motion in the system. Moreover, *c*-type rotational transitions do not appear at their predicted rigid rotor positions, even for the DOH species, providing indirect evidence for a second motion which is interpreted as a large-amplitude wagging of the non-hydrogen bonded proton of the water.

<sup>a)</sup> Uncertainty was not estimated in the original paper.

<sup>b)</sup> O(1)...H(3)–O(2) angle, see figure for the definition.

<sup>c)</sup> H(1)–O(1)...H(3) angle, see figure for the definition.

<sup>d)</sup> Azimuthal angle of the O(1)–H(2) bond about the O(1)–H(1) axis, see figure for the definition.



Canagaratna, M., Phillips, J.A., Ott, M.E., Leopold, K.R.: J. Phys. Chem. A **102** (1998) 1489.