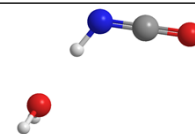
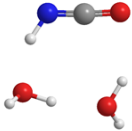
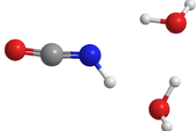


Supporting information

Table S1: Theoretical vibrational frequencies (cm^{-1}) calculated at the PW91PW91/6-311++G** level of theory from the most stable optimized structures for HNCO and its complexes with one or two molecules of water. The numbers in italics are the calculated relative intensities (in $\text{km}\cdot\text{mol}^{-1}$). The most intense modes, as predicted by the theory, are underlined in yellow.

HNCO			[HNCO][H ₂ O]			
Theoretical frequencies	Attribution	Observed at	Theoretical frequencies	Attribution	Observed at	
557.4621	69.2855	N-C-O bend	32.6310	<i>44.5060</i>	H ₂ O rocking	
607.7260	<i>0.6726</i>	Torsion	72.5876	<i>5.8117</i>		
756.3479	<i>191.2739</i>	H-N-C bend	183.8550	<i>14.1945</i>		
1297.0087	<i>0.5311</i>	N-C-O s. stretch	212.9379	<i>1.0266</i>	H ₂ O rocking	
2296.9036	648.3282	N-C-O as. stretch	244.1912	<i>231.8073</i>	H ₂ O wagging	
3618.3971	<i>143.7374</i>	N-H stretch	557.5174	<i>83.5091</i>	N-C-O bend	
			584.6701	<i>57.2660</i>	Torsion	
			617.2037	<i>4.0119</i>	Torsion	
			721.4542	<i>15.2488</i>	N-C-O bend	
			741.4083	<i>92.7038</i>	Torsion	
			856.6151	<i>268.9464</i>	H-N-C bend	
			1297.8463	<i>14.6785</i>	N-C-O s. stretch	
			1584.670	<i>57.27</i>	H ₂ O scissoring	
			2296.6287	662.7453	N-C-O as. stretch	
			3322.1058	1154.6192	N-H stretch	3295.2
			3721.454	<i>15.25</i>	H ₂ O s. stretch	
			3826.5784	<i>82.8601</i>	H ₂ O as. stretch	



$[\text{HNCO}][\text{H}_2\text{O}]_2$		$[\text{HNCO}][\text{H}_2\text{O}]_2$		Attribution
				
54.2287	1.8050	33.0475	0.4900	General mode
76.7321	4.5791	78.6143	7.3732	General mode
101.6025	1.7107	143.6310	3.6042	General mode
162.2371	58.0441	211.2534	34.5939	General mode
205.5332	11.9874	226.2066	30.6101	(H ₂ O) ₂
220.3488	19.6322	238.5750	125.2304	(H ₂ O) ₂
267.9919	144.2484	290.3879	111.2822	(H ₂ O) ₂
290.9538	62.8704	320.2608	6.4550	(H ₂ O) ₂
396.6723	97.4381	406.4250	84.0887	(H ₂ O) ₂
427.7764	107.0181	537.6535	136.9088	(H ₂ O) ₂
569.1027	80.2789	576.7485	102.8138	General mode
611.7326	19.0400	635.9199	55.4766	Torsion
710.4485	63.6318	744.9176	202.6887	General mode
777.2552	219.7629	791.5064	324.6472	General mode
988.9173	209.3427	1065.8670	235.5614	H-N-C bend
1289.1786	17.9448	1296.5465	13.6616	N-C-O s. stretch
1590.3173	60.9822	1583.9931	78.7067	H ₂ O scissoring
1606.8535	39.7540	1598.3801	14.1374	H ₂ O scissoring
2280.9678	621.9487	2293.7375	716.8038	N-C-O as. stretch
3155.8763	995.4931	3064.7568	1361.9389	N-H stretch
3456.6896	509.9097	3416.2237	515.0792	H ₂ O stretch
3674.4532	73.3352	3567.5646	357.9374	H ₂ O stretch
3792.4649	72.5683	3790.6507	80.6790	H ₂ O stretch
3800.2339	112.8632	3793.1489	90.7218	H ₂ O stretch

