TABLE 1: Structures of Nitrous Acid, Protonated Nitrous Acid and of their Dissociation Products[a]

		HONO and H_2ONO^+						Dissociation Fragments			
Method & Basis Set	**Molecule**	**HO**	**O–N**	**N=O**	**HOH**	**HON**	**ONO**	**NO**	**HO**	**HO**	**HOH**
B3LYP/6-311++G(2df,2p)	*E*-HONO	0.968	1.429	1.164		102.9	111.0	1.057	0.965		
	Z-HONO	0.978	1.389	1.177		106.4	113.9				
	H_2ONO^+	0.970	2.173	1.073	106.0	113.4	104.5			0.961	105.2
MPW1PW91/6-311++G(2df,2p)	*E*-HONO	0.964	1.398	1.162		103.2	111.3	1.053	0.961		
	Z-HONO	0.975	1.365	1.174		106.4	113.9				
	H_2ONO^+	0.966	2.122	1.067	106.0	113.4	104.6			0.957	105.0
MP2(full)/6-311++G(2df,2p)	*E*-HONO	0.967	1.415	1.176		101.9	111.0	1.079	0.963		
	Z-HONO	0.977	1.379	1.189		104.9	113.5				
	H_2ONO^+	0.963	2.278	1.083	104.9	122.5	98.5			0.958	104.3
QCISD(full)/6-311++G(2df,2p)	*E*-HONO	0.962	1.405	1.167		102.8	111.0	1.061	0.961		
	Z-HONO	0.971	1.375	1.179		105.4	113.5				
	H_2ONO^+	0.960	2.317	1.064	104.9	124.2	98.4			0.956	104.6
QCISD(fc,T)/6-311++G(2df,2p)	*E*-HONO	0.966	1.428	1.172		102.1	110.8	1.068	0.963		
	Z-HONO	0.975	1.392	1.185		104.8	113.4				
	H_2ONO^+	0.963	2.271	1.072	104.9	122.6	99.4			0.958	104.3
CCSD(fc)/6-311++G(2df,2p)	*E*-HONO	0.963	1.401	1.167		102.9	110.9	1.060	0.961		
	Z-HONO	0.972	1.373	1.178		105.5	113.5				
	H_2ONO^+	0.961	2.324	1.062	104.9	124.5	98.3			0.957	104.5
CCSD(fc,T)/6-311++G(2df,2p)	*E*-HONO	0.967	1.425	1.174		102.1	110.8	1.068	0.964		
	Z-HONO	0.976	1.390	1.186		104.8	113.4				
	H_2ONO^+	0.964	2.277	1.072	104.8	122.8	99.3			0.959	104.3
MP2(full)/6-31G(d)[b]	*E*-HONO	0.980	1.423	1.197		101.9	110.3	1.103	0.980		

	Z-HONO	0.991	1.385	1.209		104.5	112.8				
	H_2ONO^+	0.977	2.193	1.109	104.8	119.4	100.3			0.969	104.0
MP2(full)/6-31G(d')[c]	*E*-HONO	0.972	1.416	1.185		102.8	110.7	1.090	0.979		
	Z-HONO	0.984	1.376	1.198		106.0	113.2				
	H_2ONO^+ (np)	0.968	2.203	1.094	106.6	121.8	99.8			0.962	105.9
	H_2ONO^+ (p)	0.967	2.160	1.094	107.5	135.1 /117.4	107.8				

[a] Distances in Ångstroms and angles in degrees.
[b] Optimizied geometry employed at G1, G2, and G3.
[c] Optimizied geometry employed in CBS-Q level.