

Table S4 QCISD/6-311++G(2df,2p) geometries for nitrogen dioxide and nitrous acid isomers; distances in Å, angles in degrees

NO ₂	R(N-O)	1.189 (1.195 ^a)
	∠ O-N-O	134.9 (133.9 ^a)
<i>trans</i> -HONO	R(H-O)	0.964
	R(HO-N)	1.409
	R(ON-O)	1.168
	∠ H-O-N	102.7
	∠ O-N-O	110.9
<i>cis</i> -HONO	R(H-O)	0.973
	R(HO-N)	1.379
	R(ON-O)	1.180
	∠ H-O-N	105.3
	∠ O-N-O	113.5
HNO ₂	R(H-N)	1.033
	R(N-O)	1.211
	∠ H-N-O	115.8
	∠ O-N-O	128.3

Note:

^a A. Cabana, M. Laurin, W. J. Lafferty and R. L. Sams, *Can. J. Phys.*, 1975, **53**, 1902.