Table 1. Geometries[a] of the cis and trans isomers of the HOOO radical.

Species	R(O1-O2)	R(O2-O3)	R(O3-H)	θ (O1-O2-O3)	θ (O2-O3-H)	Method
cis ($^2A'$)	1.450	1.518	0.979	101.6	101.7	CASSCF(19,13)[b]/6-31+G(d,p)
	1.424	1.484	0.974	101.7	102.6	QCISD/6-31G(d,p)[c]
	1.347	1.504	0.953	103.8	103.3	MRCI[d]/6-31+G(d,p)
trans ($^2A'$)	1.454	1.513	0.976	98.6	96.1	CASSCF(19,13)[b]/6-31+G(d,p)
	1.426	1.478	0.970	99.4	96.8	QCISD/6-31G(d,p)[c]
	1.347	1.499	0.951	100.6	97.5	MRCI[d]/6-31+G(d,p)
cis-TS ($^2A'$)	1.365	1.698	0.982	101.8	99.3	CASSCF(19,13)[b]/6-31+G(d,p)
	1.294	1.678	0.955	103.4	100.3	MRCI[d]/6-31+G(d,p)
tran-TS ($^2A'$)	1.362	1.712	0.979	101.7	92.0	CASSCF(19,13)[b]/6-31+G(d,p)
	1.288	1.696	0.953	101.7	93.3	MRCI[d]/6-31+G(d,p)
trans($^2A''$)	1.225	1.688	0.972	111.0	90.0	Expt[e]

[a] Bond lengths are given in Å and angles in degree. [b] The CASSCF calculations are performed with all 19 valence electrons seeded in all the 13 valence orbitals. [c] From ref 11. [d] The active space of MRCI is generated by distributing 9 electrons into 8 valence orbitals. [e]From ref 27.