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Supplementary Table 1. Pernitric Acid Optimized Geometries.

	HF 6-31G**	B3LYP 6-31G**	MP2 6-31G**
O <sub>2</sub> -N	1.175	1.199	1.206
O <sub>3</sub> --N	1.173	1.199	1.210
O <sub>4</sub> -N	1.370	1.510	1.533
O-O	1.367	1.405	1.418
H-O	0.95	0.975	0.972
∠O <sub>2</sub> NO <sub>3</sub>	130.5	133.3	134.5
∠O <sub>2</sub> NO <sub>4</sub>	117.8	116.5	116.2
∠O <sub>3</sub> NO <sub>4</sub>	111.7	110.2	109.3
∠NO <sub>4</sub> O <sub>5</sub>	111.2	109.1	107.6
∠OOH	104.5	102.8	101.7
D(OONO <sub>3</sub> )	-194.0	170.7	171.5
D(HOON)	79.56	84.46	86.15