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Table 5: Energies (hartree) of the HOMO and LUMO orbitals (ϵ_{HOMO} and ϵ_{LUMO} , respectively) and HOMO–LUMO gap (ϵ_{gap}) .

basis set	ϵ_{HOMO}	ϵ_{LUMO}	ϵ_{gap}
N₂O₃			
<i>3s2p</i>	-0.5297	0.1017	0.6314
<i>3s2p1d</i>	-0.4997	0.2091	0.7088
<i>4s3p2d</i>	-0.4961	0.1983	0.6944
<i>4s3p2d1f</i>	-0.4945	0.2020	0.6965
N₄O₆			
<i>3s2p</i>	-0.5308	0.1015	0.6323
<i>3s2p1d</i>	-0.5023	0.1905	0.6928
<i>4s3p2d</i>	-0.4934	0.1954	0.6888
<i>4s3p2d1f</i>	-0.4928	0.1986	0.6914
N₈O₁₂			
<i>3s2p</i>	-0.5104	0.0520	0.5624
<i>3s2p1d</i>	-0.4815	0.1414	0.6229

Table 6: Mulliken total charges on nitrogen and oxygen.

Method		atom	N ₂ O ₃	N ₄ O ₆	N ₈ O ₁₂
<i>3s2p</i>	SCF	N	0.2595	0.3058	0.2870
		O	-0.1730	-0.2039	-0.1914
	MP2	N	0.2034	0.2414	-
		O	-0.1356	-0.1610	-
<i>3s2p1d</i>	SCF	N	0.2307	0.2044	0.2028
		O	-0.1538	-0.1365	-0.1353
	MP2	N	0.1647	0.1416	-
		O	-0.1098	-0.0945	-
<i>4s3p2d</i>	SCF	N	0.2263	0.2057	-
		O	-0.1507	-0.1371	-
	MP2	N	0.1578	-	-
		O	-0.1052	-	-
<i>4s3p2d1f</i>	SCF	N	0.2278	0.1862	-
		O	-0.1519	-0.1241	-
	MP2	N	0.1501	-	-
		O	-0.1000	-	-