

Compounds	Functional_Used	Basis_Set	Formation_Energy (kJ/mol)	Deviation Formation Energy	CPU_Time_Sum	Geometry_A	Bond_Length (Ang)
NH3	B3LYP_B3LYP	6-31+G*_6-31+G*	-39.83094374	0.88094374	33.6	107.68	1.018
NH3	B3LYP_B3LYP	6-31+G*_6-311+G*	-38.58772362	-0.36227638	33.8	107.68	1.018
NH3	B3LYP_B3LYP	6-311+G*_6-31+G*	-39.04273413	0.09273413	46.7	108	1.01399
NH3	B3LYP_B3LYP	6-311+G*_6-311+G*	-37.29418063	-1.65581937	46.1	108	1.01399
NH3	B3LYP_HFexch	6-31+G*_6-31+G*	-33.58840718	-5.36159282	32.6	107.68	1.018
NH3	B3LYP_HFexch	6-31+G*_6-311+G*	-34.92813201	-4.02186799	34.4	107.68	1.018
NH3	B3LYP_HFexch	6-311+G*_6-31+G*	-31.34384303	-7.60615697	48.8	108	1.01399
NH3	B3LYP_HFexch	6-311+G*_6-311+G*	-32.31036487	-6.63963513	48.7	108	1.01399
NH3	B3LYP_xpbe96_cpbe96	6-31+G*_6-31+G*	-47.01229846	8.06229846	34.3	107.68	1.018
NH3	B3LYP_xpbe96_cpbe96	6-31+G*_6-311+G*	-45.30234227	6.35234227	35.7	107.68	1.018
NH3	B3LYP_xpbe96_cpbe96	6-311+G*_6-31+G*	-46.66231896	7.71231896	48.2	108	1.01399
NH3	B3LYP_xpbe96_cpbe96	6-311+G*_6-311+G*	-44.4756626	5.5256626	48.7	108	1.01399
NH3	HFexch_B3LYP	6-31+G*_6-31+G*	-37.78575303	-1.16424697	8.5	108.12	1.00204
NH3	HFexch_B3LYP	6-31+G*_6-311+G*	-35.15130964	-3.79869036	9.4	108.12	1.00204
NH3	HFexch_B3LYP	6-311+G*_6-31+G*	-37.72231646	-1.22768354	10.7	108.23	0.99864
NH3	HFexch_B3LYP	6-311+G*_6-311+G*	-34.57870883	-4.37129117	12.2	108.23	0.99864
NH3	HFexch_HFexch	6-31+G*_6-31+G*	-27.81721836	-11.13278164	7.1	108.12	1.00204
NH3	HFexch_HFexch	6-31+G*_6-311+G*	-28.33731461	-10.61268539	6.9	108.12	1.00204
NH3	HFexch_HFexch	6-311+G*_6-31+G*	-26.83908624	-12.11091376	10.1	108.23	0.99864
NH3	HFexch_HFexch	6-311+G*_6-311+G*	-26.9409624	-12.0090376	9.7	108.23	0.99864
NH3	HFexch_xpbe96_cpbe96	6-31+G*_6-31+G*	-46.23419862	7.28419862	10.4	108.12	1.00204
NH3	HFexch_xpbe96_cpbe96	6-31+G*_6-311+G*	-43.23656332	4.28656332	12.8	108.12	1.00204
NH3	HFexch_xpbe96_cpbe96	6-311+G*_6-31+G*	-46.42701365	7.47701365	12.2	108.23	0.99864
NH3	HFexch_xpbe96_cpbe96	6-311+G*_6-311+G*	-42.94157538	3.99157538	11.1	108.23	0.99864
NH3	xpbe96_cpbe96_B3LYP	6-31+G*_6-31+G*	-40.84405565	1.89405565	37.3	107.07	1.02575
NH3	xpbe96_cpbe96_B3LYP	6-31+G*_6-311+G*	-39.99836519	1.04836519	36.4	107.07	1.02575
NH3	xpbe96_cpbe96_B3LYP	6-311+G*_6-31+G*	-39.61290936	0.66290936	45.4	107.42	1.02187
NH3	xpbe96_cpbe96_B3LYP	6-311+G*_6-311+G*	-38.35598502	-0.59401498	50.7	107.42	1.02187
NH3	xpbe96_cpbe96_HFexch	6-31+G*_6-31+G*	-36.11382954	-2.83617046	37.9	107.07	1.02575
NH3	xpbe96_cpbe96_HFexch	6-31+G*_6-311+G*	-37.61551004	-1.33448996	35.8	107.07	1.02575
NH3	xpbe96_cpbe96_HFexch	6-311+G*_6-31+G*	-33.57705251	-5.37294749	45.9	107.42	1.02187
NH3	xpbe96_cpbe96_HFexch	6-311+G*_6-311+G*	-34.77483042	-4.17516958	46.5	107.42	1.02187
NH3	xpbe96_cpbe96_xpbe96_cpbe96	6-31+G*_6-31+G*	-47.53632027	8.58632027	37.6	107.07	1.02575
NH3	xpbe96_cpbe96_xpbe96_cpbe96	6-31+G*_6-311+G*	-46.1827511	7.2327511	39.4	107.07	1.02575
NH3	xpbe96_cpbe96_xpbe96_cpbe96	6-311+G*_6-31+G*	-46.67443679	7.72443679	54	107.42	1.02187
NH3	xpbe96_cpbe96_xpbe96_cpbe96	6-311+G*_6-311+G*	-44.93126697	5.98126697	48	107.42	1.02187