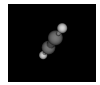
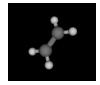
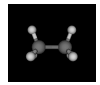
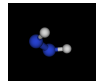
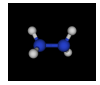
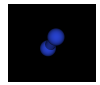
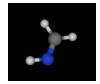
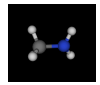
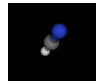
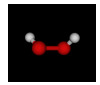
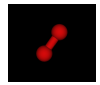
Molecule table

This represents a table of all unique molecules found in the folder **N__2-2021-04-17__20-09-38**.

graph6	elements	chemical formula	molecule name	energy [Ht]	stability	largest force [Ht]	num neg EV	configuration
A_	C_C	C2H2	Acetylene	-76.793	C2H2,H6,-80.1698 **CH4,CH4,-80.3602**	5.47201e-06 1.63543e-06 3.50893e-06	23	
A_	C_C	C2H4	Ethylene	-78.004	C2H4,H4,-80.2564 **CH4,CH4,-80.3602**	3.50865e-06 1.43474e-06 3.48204e-06	27	
A_	C_C	C2H6	Ethane	-79.193	C2H6,H2,-80.319 **CH4,CH4,-80.3602**	8.17247e-07 1.14349e-06 1.14236e-06	31	
A_	N_N	N2H2	Diimide	-109.915	N2H2,H4,-112.178 **NH3,NH3,-112.329**	8.43364e-07 2.76091e-07 4.72403e-07	23	
A_	N_N	N2H4	Hydrazine	-111.123	N2H4,H2,-112.247 **NH3,NH3,-112.329**	0.000158875 8.16602e-05 0.000474671	27	

graph6	elements	chemical formula	molecule name	energy [Ht]	stability	largest force [Ht]	num neg EV	configuration
A_	N_N	N2	Nitrogen	-108.868	N2,H6,-112.236 **NH3,NH3,-112.329**	5.04148e-11 7.26885e-11 1.24928e-10	19	
A_	C_N	NCH3	Methanimine	-93.981	NCH3,H4,-96.2334 **CH4,NH3,-96.3448**	0.000122963 0.000142553 4.40149e-06	25	
A_	C_N	NCH5	Methylamine	-95.169	NCH5,H2,-96.2951 **CH4,NH3,-96.3448**	5.71918e-05 6.65827e-05 0.000113067	29	
A_	C_N	NCH	Hydrogen cyanide	-92.828	NCH,H6,-96.2016 **CH4,NH3,-96.3448**	1.54766e-08 1.83316e-08 6.92125e-09	21	
A_	O_O	O2H2	Hydrogen peroxide	-150.710	O2H2,H2,-151.829 **OH2,OH2,-151.969**	0.00015088 0.000958314 0.000303463	23	
A_	O_O	O2	Oxygen	-149.462	O2,H4,-151.629 **OH2,OH2,-151.969**	6.27918e-09 8.87228e-09 1.78281e-11	19	

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A_	C_O	OCH2	Formaldehyde	-113.808	OCH2,H4,-116.062 **CH4,OH2,-116.165**	1.42976e-10 2.89562e-10 1.72154e-12	23	
A_	C_O	OCH4	Methyl Alcohol	-114.986	OCH4,H2,-116.111 **CH4,OH2,-116.165**	2.50415e-06 4.51661e-06 8.6962e-07	27	
A_	N_O	ONH3	Hydroxylamine	-130.910	ONH3,H2,-132.045 **NH3,OH2,-132.149**	1.92386e-05 2.26754e-05 0.000385189	25	
A_	N_O	ONH	Nitrosyl hydride	-129.714	ONH,H4,-131.966 **NH3,OH2,-132.149**	2.84751e-09 7.08971e-09 1.225e-08	21	