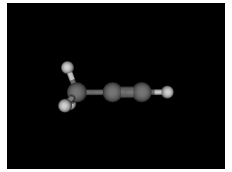
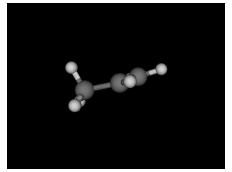
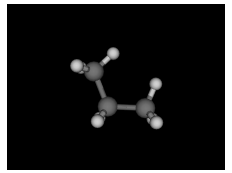
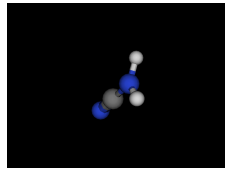
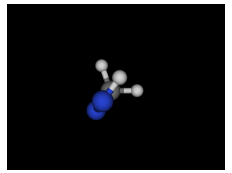
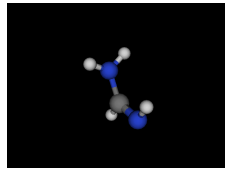
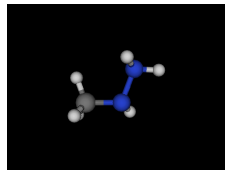
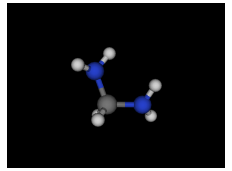
Molecule table

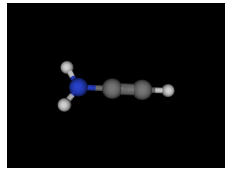
This represents a table of all unique molecules found in the folder **N__3-2022-10-26__23-34-31**.

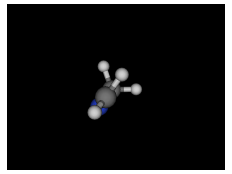
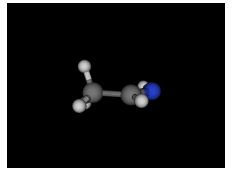
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_C_C	C3H4	Propyne	-115.824	C3H4,H6,-119.2 **CH4,C2H6,-119.372** C3H4,H2,-116.946 **C2H2,CH4,-116.969**	3.05441e-06 6.25074e-06 4.99263e-06	36	
BW	C_C_C	C3H6	Propene	-117.026	C3H6,H4,-119.272 **C2H6,CH4,-119.372** C3H6,H2,-118.145 **CH4,C2H4,-118.183**	0.00016928 0.000612643 1.38112e-05	40	

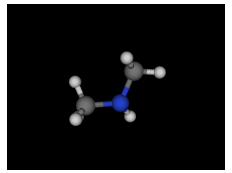
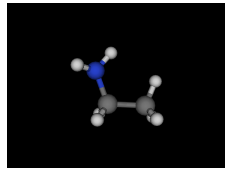
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_C_C	C3H8	Propane	-118.205	C3H8,H2,-119.331 **C2H6,CH4,-119.372** C3H8,H2,-119.331 **C2H6,CH4,-119.372**	0.000187758 0.000264128 7.67988e-06	44	
BW	N_C_N	N2CH2	Cyanamide	-147.843	N2CH2,H6,-151.216 **NH3,NCH5,-151.333** N2CH2,H2,-148.962 **NCH,NH3,-148.986**	0.000436282 5.60864e-05 6.79674e-05	32	

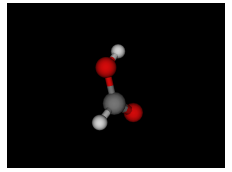
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_N_N	N2CH4	Methyl diazene	-148.934	N2CH4,H4,-151.183 **NCH5,NH3,-151.333** N2CH4,H2,-150.056 **CH4,N2H2,-150.105**	5.8139e-05 6.4087e-05 8.83112e-05	36	
BW	N_C_N	N2CH4	Methyl diazene	-148.989	N2CH4,H4,-151.257 **NCH5,NH3,-151.333** N2CH4,H2,-150.13 **NCH3,NH3,-150.144**	0.000172124 8.64874e-05 0.000327616	36	

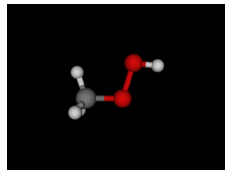
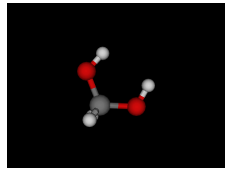
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_N_N	N2CH6	Hydrazine, methyl-	-150.121	N2CH6,H2,-151.23 **CH4,N2H4,-151.3** N2CH6,H2,-151.23 **NCH5,NH3,-151.333**	8.31907e-05 8.00543e-06 8.50122e-05	40	
BW	N_C_N	N2CH6	Hydrazine, methyl-	-150.167	N2CH6,H2,-151.291 **NCH5,NH3,-151.333** N2CH6,H2,-151.291 **NCH5,NH3,-151.333**	0.000238689 0.000331841 4.98121e-06	40	
BW	N_N_N	N3H3	Triazene	-164.901	N3H3,H4,-167.127 **N2H4,NH3,-167.285** N3H3,H2,-166 **N2H2,NH3,-166.089**	0.000167094 0.000109658 3.88978e-05	34	

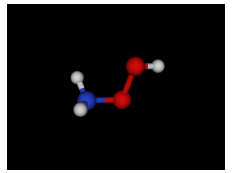
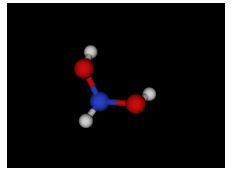
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	N_N_N	N3H5		-166.069	N3H5,H2,-167.191 **N2H4,NH3,-167.285** N3H5,H2,-167.191 **N2H4,NH3,-167.285**	0.000310255 4.64611e-05 0.000938694	38	
BW	C_C_N	NC2H3	Acetonitrile	-131.801	NC2H3,H6,-135.176 **CH4,NCH5,-135.348** NC2H3,H2,-132.922 **C2H2,NH3,-132.954**	0.000188511 0.000249058 0.000440443	34	

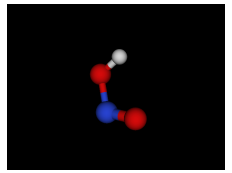
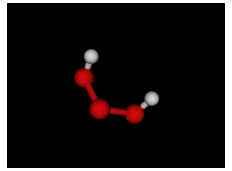
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_N_C	NC2H5	Ethylenimine	-132.993	NC2H5,H4,-135.246 **NCH5,CH4,-135.348** NC2H5,H2,-134.119 **CH4,NCH3,-134.16**	2.85923e-05 2.64795e-05 6.60635e-05	38	
BW	C_C_N	NC2H5	Ethylenimine	-133.008	NC2H5,H4,-135.257 **C2H6,NH3,-135.357** NC2H5,H2,-134.13 **CH4,NCH3,-134.16**	0.000859894 5.95429e-05 4.837e-05	38	

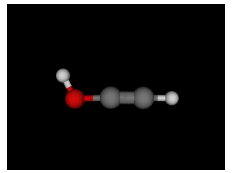
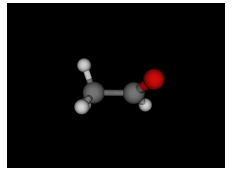
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_N_C	NC2H7	Ethylamine	-134.175	NC2H7,H2,-1.12683 **NCH5,CH4,-135.348** NC2H7,H2,-1.12683 **CH4,NCH5,-135.348**	0.000352871 0.000148494 0.000147472	42	
BW	C_C_N	NC2H7	Ethylamine	-134.184	NC2H7,H2,-135.308 **C2H6,NH3,-135.357** NC2H7,H2,-135.308 **NCH5,CH4,-135.348**	0.000261618 0.000293477 2.34535e-05	42	

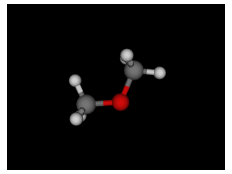
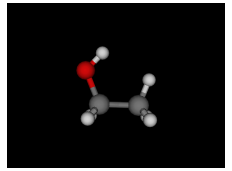
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	O_C_O	O2C	Carbon dioxide	-187.515	O2C,H4,-189.761 **OH2,OCH2,-189.793** O2C,H4,-189.761 **OCH2,OH2,-189.793**	8.1315e-09 4.81542e-09 7.98489e-09	28	
BW	O_C_O	O2CH2	Formic acid	-188.665	O2CH2,H2,-189.786 **OCH2,OH2,-189.793** O2CH2,H4,-190.913 **OCH4,OH2,-190.969**	0.000118911 5.64122e-05 0.000205658	32	

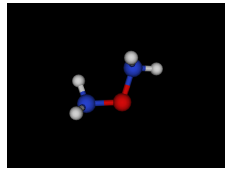
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_O_O	O2CH4	Methyl peroxide	-189.718	O2CH4,H2,-190.838 **CH4,O2H2,-190.883** O2CH4,H2,-190.838 **OCH4,OH2,-190.969**	1.04633e-05 9.9558e-06 1.06615e-06	36	
BW	O_C_O	O2CH4	Methyl peroxide	-189.804	O2CH4,H2,-190.927 **OCH4,OH2,-190.969** O2CH4,H2,-190.927 **OCH4,OH2,-190.969**	9.18448e-05 0.000125801 2.6474e-05	36	

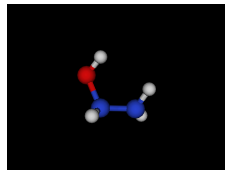
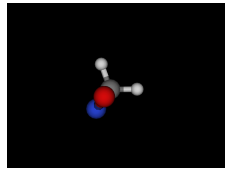
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	N_O_O	O2NH3		-205.657	O2NH3,H2,-206.77 **NH3,O2H2,-206.867** O2NH3,H2,-206.77 **ONH3,OH2,-206.903**	0.000123939 3.39199e-05 0.000222113	34	
BW	O_N_O	O2NH3		-205.697	O2NH3,H2,-206.813 **ONH3,OH2,-206.903** O2NH3,H2,-206.813 **ONH3,OH2,-206.903**	8.94533e-05 0.000123492 7.81283e-06	34	

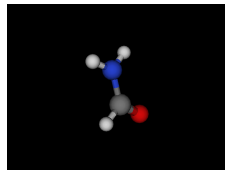
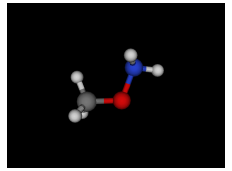
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	O_N_O	O2NH	Nitrous acid	-204.521	O2NH,H4,-206.759 **ONH3,OH2,-206.903** O2NH,H2,-205.632 **ONH,OH2,-205.697**	3.82768e-05 1.26726e-05 3.58129e-05	30	
BW	O_O_O	O3H2	H2O3	-225.435	O3H2,H2,-226.548 **O2H2,OH2,-226.687** O3H2,H2,-226.548 **O2H2,OH2,-226.687**	0.000142479 0.000200573 8.54525e-05	32	

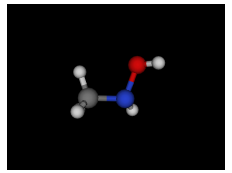
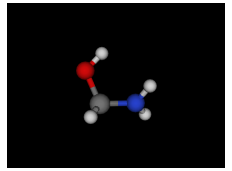
graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_C_O	OC2H2	Ketene	-151.599	OC2H2,H6,-154.974 **CH4,OCH4,-155.164** OC2H2,H2,-152.72 **C2H2,OH2,-152.774**	6.26837e-06 4.04401e-06 6.19414e-07	32	
BW	C_C_O	OC2H4	Acetaldehyde	-152.842	OC2H4,H2,-153.964 **CH4,OCH2,-153.988** OC2H4,H4,-155.091 **C2H6,OH2,-155.177**	2.12841e-05 3.57823e-05 6.21758e-05	36	

graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_O_C	OC2H6	Ethanol	-153.991	OC2H6,H2,-1.12683 **CH4,OCH4,-155.164** OC2H6,H2,-1.12683 **OCH4,CH4,-155.164**	0.000281644 9.74098e-05 1.18303e-06	40	
BW	C_C_O	OC2H6	Ethanol	-154.004	OC2H6,H2,-155.128 **C2H6,OH2,-155.177** OC2H6,H2,-155.128 **OCH4,CH4,-155.164**	8.7824e-05 0.000119335 5.33254e-06	40	

graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	N_N_O	ON2H2	H2N2O	-184.732	ON2H2,H4,-186.976 **N2H4,OH2,-187.105** ON2H2,H2,-185.849 **ONH,NH3,-185.877**	7.0579e-05 3.57105e-05 5.96597e-05	32	
BW	N_O_N	ON2H4	NH2NHOH	-185.858	ON2H4,H2,-1.12683 **ONH3,NH3,-187.083** ON2H4,H2,-1.12683 **NH3,ONH3,-187.083**	0.000171145 0.000831858 2.86559e-05	36	

graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	N_N_O	ON2H4	NH2NHOH	-185.887	ON2H4,H2,-187.019 **N2H4,OH2,-187.105** ON2H4,H2,-187.019 **ONH3,NH3,-187.083**	0.000590097 0.000266079 0.000548946	36	
BW	C_N_O	ONCH3	Formamide	-168.738	ONCH3,H2,-169.853 **CH4,ONH,-169.892** ONCH3,H4,-170.98 **NCH5,OH2,-171.153**	2.48086e-06 6.45682e-06 2.17276e-06	34	

graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	N_C_O	ONCH3	Formamide	-168.855	**ONCH3,H2,-169.978** OCH2,NH3,-169.973 ONCH3,H4,-171.104 **NCH5,OH2,-171.153**	2.66022e-06 1.70585e-06 2.84655e-05	34	
BW	C_O_N	ONCH5	Hydroxylamine, O-methyl-	-169.926	ONCH5,H2,-1.12683 **CH4,ONH3,-171.098** ONCH5,H2,-1.12683 **OCH4,NH3,-171.149**	0.000273851 0.000123065 2.06991e-05	38	

graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	C_N_O	ONCH5	Hydroxylamine, O-methyl-	-169.933	ONCH5,H2,-171.046 **NCH5,OH2,-171.153** ONCH5,H2,-171.046 **CH4,ONH3,-171.098**	0.000278884 0.000190954 1.89431e-05	38	
BW	N_C_O	ONCH5	Hydroxylamine, O-methyl-	-169.990	ONCH5,H2,-171.114 **NCH5,OH2,-171.153** ONCH5,H2,-171.114 **OCH4,NH3,-171.149**	0.000195697 0.000512039 2.20815e-05	38	

graph6	elements	chemical formula	molecule name	energy [Ht]	dissociation	largest force [Ht]	num neg EV	configuration
BW	N_C_O	ONCH	Isocyanic acid	-167.635	ONCH,H2,-168.752 **NCH,OH2,-168.806** ONCH,H6,-171.005 **NH3,OCH4,-171.149**	7.47316e-06 1.04523e-05 5.62005e-06	30