

# Matt Anderson and Eddie Pluhar

X-N-H angle (°)	Bond-length (Å)	RHF/6-31G* E (Ha)	Relative E (kcal/mol)	Dipole Moment (D)	
50.00	1.031	-56.143064	25.91	2.753	
51.00	1.029	-56.148155	22.72	2.723	
52.00	1.027	-56.152845	19.77	2.691	
53.00	1.025	-56.157147	17.07	2.657	
54.00	1.023	-56.161074	14.61	2.621	
55.00	1.021	-56.164640	12.37	2.584	
56.00	1.020	-56.167858	10.35	2.545	
57.00	1.018	-56.170741	8.54	2.505	
58.00	1.016	-56.173302	6.94	2.463	
59.00	1.015	-56.175556	5.52	2.419	
60.00	1.013	-56.177516	4.29	2.374	
61.00	1.012	-56.179197	3.24	2.326	
62.00	1.011	-56.180611	2.35	2.277	
63.00	1.009	-56.181775	1.62	2.226	
64.00	1.008	-56.182702	1.04	2.173	
65.00	1.007	-56.183408	0.60	2.118	
66.00	1.005	-56.183907	0.28	2.061	
67.00	1.004	-56.184215	0.09	2.002	
68.00	1.003	-56.184348	0.01	1.940	
68.32	1.003	-56.184356	0.00	1.920	Minimum
69.00	1.002	-56.184322	0.02	1.877	
70.00	1.001	-56.184153	0.13	1.810	
71.00	1.000	-56.183856	0.31	1.741	
72.00	0.999	-56.183449	0.57	1.670	
73.00	0.998	-56.182948	0.88	1.596	
74.00	0.997	-56.182368	1.25	1.520	
75.00	0.996	-56.181727	1.65	1.441	
76.00	0.995	-56.181039	2.08	1.359	
77.00	0.994	-56.180320	2.53	1.275	
78.00	0.993	-56.179586	2.99	1.188	
79.00	0.993	-56.178850	3.46	1.099	
80.00	0.992	-56.178128	3.91	1.008	
81.00	0.991	-56.177431	4.35	0.914	
82.00	0.991	-56.176772	4.76	0.818	
83.00	0.990	-56.176163	5.14	0.720	
84.00	0.990	-56.175614	5.49	0.621	
85.00	0.989	-56.175133	5.79	0.520	
86.00	0.989	-56.174729	6.04	0.417	
87.00	0.989	-56.174407	6.24	0.314	
88.00	0.989	-56.174174	6.39	0.210	
89.00	0.989	-56.174033	6.48	0.105	
90.00	0.989	-56.173985	6.51	0.000	Transition State
91.00	0.989	-56.174033	6.48	0.105	
92.00	0.989	-56.174174	6.39	0.210	
93.00	0.989	-56.174407	6.24	0.314	
94.00	0.989	-56.174729	6.04	0.417	
95.00	0.989	-56.175133	5.79	0.520	
96.00	0.990	-56.175614	5.49	0.621	
97.00	0.990	-56.176163	5.14	0.720	
98.00	0.991	-56.176772	4.76	0.818	
99.00	0.991	-56.177431	4.35	0.914	
100.00	0.992	-56.178128	3.91	1.008	
101.00	0.993	-56.178850	3.46	1.099	
102.00	0.993	-56.179586	2.99	1.188	
103.00	0.994	-56.180320	2.53	1.275	
104.00	0.995	-56.181039	2.08	1.359	
105.00	0.996	-56.181727	1.65	1.441	

# Inversion Scan Data

106.00	0.997	-56.182368	1.25	1.520
107.00	0.998	-56.182948	0.88	1.596
108.00	0.999	-56.183449	0.57	1.670
109.00	1.000	-56.183856	0.31	1.741
110.00	1.001	-56.184153	0.13	1.810
111.00	1.002	-56.184322	0.02	1.877
111.68	1.003	-56.184356	0.00	1.920 Minimum
112.00	1.003	-56.184348	0.01	1.940
113.00	1.004	-56.184215	0.09	2.002
114.00	1.005	-56.183907	0.28	2.061
115.00	1.007	-56.183408	0.60	2.118
116.00	1.008	-56.182702	1.04	2.173
117.00	1.009	-56.181775	1.62	2.226
118.00	1.011	-56.180611	2.35	2.277
119.00	1.012	-56.179197	3.24	2.326
120.00	1.013	-56.177516	4.29	2.374
121.00	1.015	-56.175556	5.52	2.419
122.00	1.016	-56.173302	6.94	2.463
123.00	1.018	-56.170741	8.54	2.505
124.00	1.020	-56.167858	10.35	2.545
125.00	1.021	-56.164640	12.37	2.584
126.00	1.023	-56.161074	14.61	2.621
127.00	1.025	-56.157147	17.07	2.657
128.00	1.027	-56.152845	19.77	2.691
129.00	1.029	-56.148155	22.72	2.723
130.00	1.031	-56.143064	25.91	2.753

NH<sub>3</sub> Relative Energy vs X-N-H Bond Angle

