

Supplementary Information:

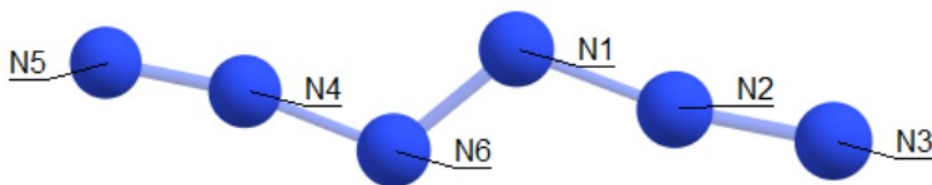


Fig. S1: Molecular structure of N₆ creating from two N₃ molecules.

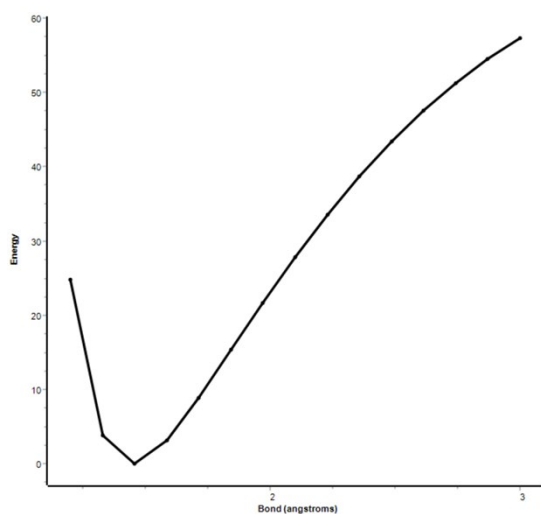


Fig. S2: N₃ to N₆ Saddlepoint Surface Scan. Energies are in kcal/mol

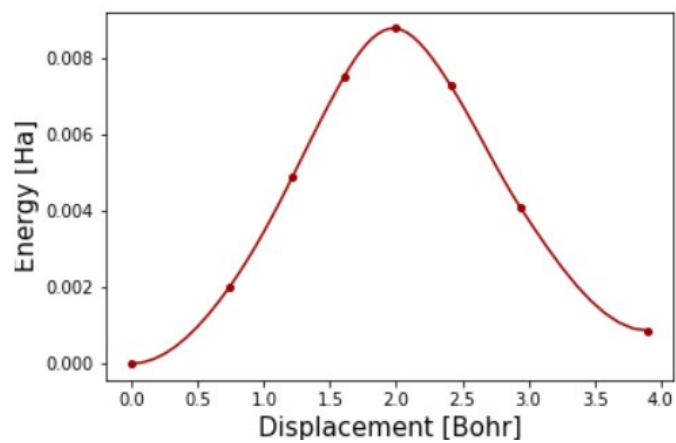


Fig. S3: NEB for EEE N₈^{*} to ZEZ N₈⁻

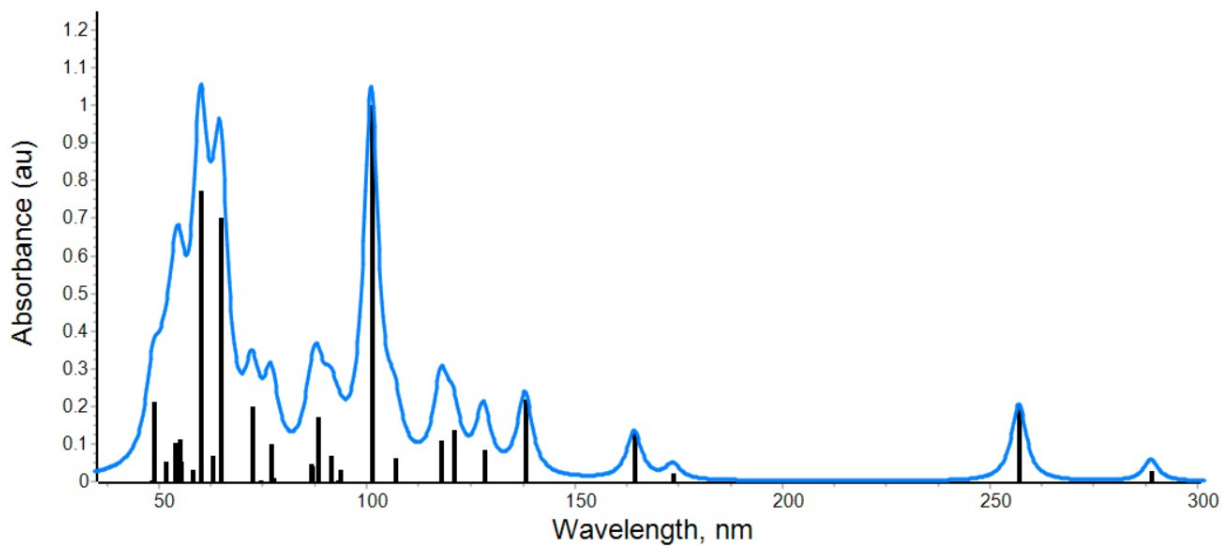


Fig. S4: TD-DFT, CAM-B3LYP functional for N_3^- to N_3^*

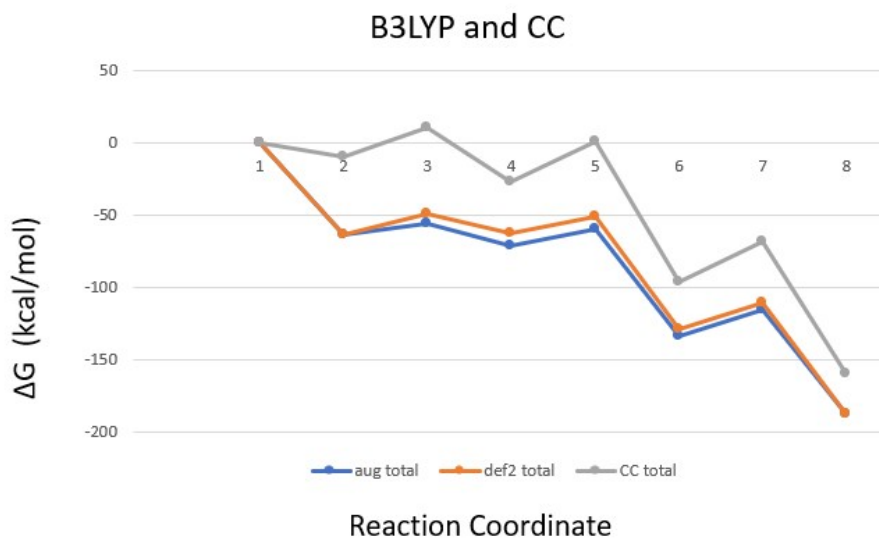


Fig S5: Comparison of single point energies for aug-ss-pVDZ, TZVPP, and Coupled Cluster theory.

Table S1: Vibrational Frequencies of Transition States

Transition State	Vibrational Frequency for Imaginary Mode (1/cm)
N6 to N12	-82.44
N12 to N10	-625.4
N10 to N8	-729.59

Table S2: Single-point energies for def2-TZVPP and aug-ss-pVDZ basis sets, and Coupled Cluster theory

		aug total	def2 total	CC total
	Step			
N3*	1	0	0	0
N6	2	-63.1386	-63.2772	-8.8956
N6toN12TS	3	-55.491	-48.2605	11.07253
N12	4	-70.5789	-61.9227	-26.6616
N12toN10TS	5	-59.6099	-50.5638	1.503936
N10	6	-133.006	-128.615	-95.9427
N10toN8TS	7	-115.295	-110.562	-67.7879
N8*	8	-187.582	-187.557	-158.911

Coordinates for All Mechanism Steps:

Azide Radical:

N 1.105350000 0.013400000 -0.092010000
 N 2.290140000 0.013400000 -0.092010000
 N 3.474950000 0.013400000 -0.092010000

N6:

N 0.965225000 0.553455000 -0.249708000
 N 2.107429000 0.126799000 -0.112684000

N	3.149043000	-0.179023000	-0.014149000
N	-1.063382000	-0.090661000	-0.070402000
N	-2.105334000	0.217050000	-0.158995000
N	0.079139000	-0.521251000	0.050288000

N6 to N12 TS:

N	4.92095367993796	-0.97840539898874	0.44222265292877
N	3.95351641747798	-0.56029269005302	0.85473102335250
N	2.81772790795973	-0.27192854076957	1.32216914454285
N	2.68514686254232	1.13142442940902	1.42023253287303
N	1.60573539058246	1.50463564769842	1.90215613593268
N	0.77130178145777	0.52523177664367	2.45715174853024
N	-0.34431049360878	0.52761248974984	1.91881348623023
N	-1.21076600719656	-0.34208412951333	2.65888093550757
N	-1.88267322617817	-1.14979830985734	2.02424190529131
N	-1.59264410812149	-1.31393177826565	0.57421445836582
N	-1.97704133463985	-0.34169623446418	-0.10401341917962
N	-2.31265687021341	0.47538273841092	-0.82384060437548

N12:

N	1.382489000	-0.354864000	-0.456367000
N	0.446781000	-0.964107000	-1.231734000
N	2.494582000	-0.623834000	-0.840373000
N	-0.683348000	-0.646654000	-0.769684000
N	3.402405000	0.029278000	-0.017464000
N	-1.700844000	-0.447565000	-0.467347000
N	7.495211000	0.665188000	0.850633000

N	6.538981000	0.072855000	0.089159000
N	8.609937000	0.286369000	0.395300000
N	5.433003000	0.391909000	0.452651000
N	9.615191000	0.032316000	0.093713000
N	4.518272000	-0.255250000	-0.367548000

N12 to N10 TS:

N	1.29254	-1.34437	-1.69112
N	0.37548	-0.86532	-1.085
N	2.57015	-1.43393	-1.8057
N	0.6689	0.10264	0.13624
N	3.14267	-0.6515	-0.81973
N	0.09831	0.69811	0.88541
N	6.74985	0.78927	0.99348
N	6.18078	0.00413	0.00466
N	8.01112	0.73012	0.91804
N	4.93073	0.07964	0.10015
N	9.13782	0.79961	1.00478
N	4.39427	-0.72277	-0.91027

N10:

N	1.506354000	-1.071609000	-1.258509000
N	0.436463000	-1.046869000	-1.107324000
N	2.725763000	-1.185522000	-1.543813000
N	3.416565000	-0.442594000	-0.631209000
N	7.130705000	0.805987000	0.931966000
N	6.441426000	0.068433000	0.012896000
N	8.349933000	0.546278000	0.771337000
N	5.255069000	0.240443000	0.131813000

N	9.419767000	0.398897000	0.723741000
N	4.602846000	-0.529650000	-0.821112000

N10 to N8 TS:

N	1.40649	-1.086531	-1.36533
N	0.27251	-1.110173	-1.39305
N	2.65483	-1.188249	-1.49594
N	3.30046	-0.418533	-0.52638
N	7.12897	0.759012	0.95457
N	6.42036	0.085693	0.10628
N	8.64672	0.473752	0.59466
N	5.16855	0.232098	0.2917
N	9.74866	0.576311	0.72392
N	4.5373	-0.539584	-0.68065

ZEZ N8

N	-1.027722000	-1.153156000	-0.000251000
N	-0.465008000	-0.231091000	-0.000419000
N	0.091147000	0.898079000	-0.000783000
N	1.462611000	0.801121000	-0.000729000
N	1.919794000	-0.310573000	-0.001070000
N	3.291099000	-0.408015000	-0.000908000
N	3.847789000	0.720882000	0.000864000
N	4.411499000	1.642313000	0.002506000