Electronic Supplementary Information

Homocoupling of CO and isocyanide mediated by an *C,C'*-bis(silylenyl)- substituted *ortho*-carborane

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1. Experimental Section

General Considerations

All experiments and manipulations were carried out under dry oxygen-free nitrogen using standard Schlenk techniques or in an MBraun inert atmosphere dry-box containing an atmosphere of purified nitrogen. Solvents were dried by standard methods and freshly distilled prior to use. The starting material bis-silylene **1** was prepared according to literature procedure.[S1] The NMR spectra were recorded with Bruker spectrometers ARX200, and AV400 referenced to residual solvent signals as internal standards (^{1}H and ^{13}C{H}) or with an external reference ($SiMe_4$ for ^{29}Si). Abbreviations: s = singlet; d = doublet; t = triplet; sept = septet; m = multiplet; br = broad. Elemental analyses and HR ESI-MS were measured by the analytical service laboratory of the Department of Chemistry of the Technische Universität Berlin. IR spectra were measured with a Nicolet iS5 FT-IR Spectrometer from the company of Thermo Scientific.

Syntheses and Spectroscopic Data

Compound 2

N_2 gas in a 250 mL Schlenk-flask with a yellow solution of **1** (0.30 g, 0.45 mmol) in toluene (10 mL) was exchanged to CO at -20 °C by one freeze-pump-thaw cycle. The reaction mixture was allowed to warm to room temperature, and a brown solution was obtained. After 16 h colorless crystals of **2** were formed with yield of 0.20 g (0.14 mmol, 62%), which are qualified for X-ray diffraction analysis. **Melting point**: 240˚C (decomposed); **^{1}H NMR** (200.13 MHz, 298 K, D_8-THF): δ = 1.30 (s, 18 H; NC(CH_3)$_3$), 1.35 (s, 18 H; NC(CH_3)$_3$), 1.39 (s, 18 H; NC(CH_3)$_3$), 1.46 (s, 18 H; NC(CH_3)$_3$), 7.54 – 7.77 ppm (m, 20 H; H_{arom}); **^{13}C{^{1}H} NMR** (50.61 MHz, 298 K, D_8-THF):): δ = 22.34 (μ-*C*=C-O), 33.01, 33.40, 34.51, 34.86 (NC(CH_3)$_3$), 55.19, 55.80 (NC(CH_3)$_3$), 84.84, 88.51 (cage), 126.90, 129.11, 129.14, 129.28, 129.77, 129.85, 130.53, 131.41, 131.96, 132.16 (HC_{Ph}), 133.73, 135.60 (C_{arom} quaternary Ph), 139.31, 157.64 (N*C*N), 173.78 ppm (C=*C*-O); **^{29}Si{^{1}H} NMR** (99.49 MHz, 298 K, D_8-THF): δ = −62.27, -108.44 ppm; **^{11}B{^{1}H} NMR** (64.17 MHz, 298 K, D_8-THF): δ = −2 ~ -15 ppm (m, b); **ESI-MS: m/z**: 717.50213 (calc. 717.50177 [M/2+H]$^{+}$); **Elemental analysis** calcd for $C_{68}H_{112}N_8B_{20}Si_4O_4$: C 56.95, H 7.87, N 7.81; found: C 56.56, H 7.60, N 7.61; **IR** (cm^{-1}): 2978 (w), 2554 (m), 1608 (m), 1565 (w), 1444 (m), 1414 (m), 1383 (s), 1361 (s), 1256 (w), 1202 (vs), 1075 (m), 1022 (m), 925 (w), 878 (w), 826 (m),796 (s), 764 (s), 729 (vs), 706 (vs), 641 (s), 622 (m).

Compound 3

At -20 °C toluene (10 mL) was added to a mixture of **1** (0.21 g, 0.32 mmol) and XylylNC (Xylyl = 2, 6-$Me_2C_6H_3$) (0.085 g, 0.64 mmol). The reaction mixture was stirred for 16 h. Solvent and volatiles were evacuated under reduced pressure and the residue was washed with small amount of cold n-hexane. It afforded 0.23 g (0.25 mmol, 78%) of **3** as a colorless powder. The X-ray diffraction analysis qualified single crystals were obtained by recrystallization of **3** in toluene at room temperature. **Melting point**: 247 °C (decomposed); **^{1}H NMR** (200.13 MHz, [D_8]THF, 25ºC): δ = 1.12 (s, 18 H; NCMe_3), 1.56 (s, 18 H; NCMe_3), 2.25 (s, 6 H; Me_2-Ph), 2.49 (s, 6 H; *Me*-Ph), 6.24 (t, ^3J (H,H) = 7.42 Hz, 1 H; H_{arom}), 6.45 (d, ^3J (H,H) = 7.42 Hz, 2 H; H_{arom}), 6.60 – 6.68 (m, 3 H; H_{arom}), 7.17 (d, ^3J (H,H) = 7.72 Hz, 1 H; H_{arom}), 7.39 – 7.68 (m, 8 H; H_{arom}), 7.78 (d, ^3J (H,H) = 7.80 Hz, 1 H; H_{arom}); **^{13}C{^{1}H} NMR** (100.61 MHz, [D_8]THF, 25ºC): δ = 22.44, 22.78 (CH_3)$_2$-Ph), 32.39, 33.01, (NCMe_3), 55.82, 56.45 (N*C*Me$_3$), 87.21, 89.52 (cage), 90.01 (Si=*C*), 120.88, 125.89, 127.96, 128.60, 128.88, 128.99, 129.37, 129.65, 129.76, 130.98, 131.50, 131.76, 132.55, 133.37 (HC_{Ph}), 128.65, 133.95, 136.26, 146.61, 149.83, 171.52, 183.30, 192.06 ppm (C_{arom} quaternary Ph, N*C*N, and *C*=N); **^{29}Si{^{1}H} NMR** (79.49 MHz, [D_8]THF, 25ºC): δ = -32.3 (tetrahedral coordinated *Si*), -60.0 (pentacoordinated *Si*); **^{11}B{^{1}H} NMR** (64.17 MHz, 298 K, D_8-THF): δ = −3 ~ -16 ppm (m, b); **HR ESI-MS**: m/z: 924.65247 (calc. 924.66003 $[M+H]^+$); **elemental analysis** calcd (%) for $C_{50}H_{74}N_6Si_2B_{10}$: C 65.03, H 8.08, N 9.10; found: C 64.96, H 7.94, N 9.00; **IR** (cm^{-1}): 2979 (w), 2562 (m), 1602)m), 1575 (s), 1446 (m), 1412 (s), 1392 (vs), 1365 (s), 1250 (m), 1196 (s), 1086 (m), 1023 (w), 939 (vs), 919 (m), 886 (s), 830 (w), 806 (s), 755 (vs), 739 (m), 707 (vs), 666 (w), 643 (m), 621 (m).

2. X-ray Crystallographic Data

Crystals were each mounted on a glass capillary in per-fluorinated oil and measured in a cold N_2 flow. The data were collected on an Oxford Diffraction Supernova, Single source at offset, Atlas at 150 K (Cu- Kα-radiation, λ = 1.5418 Å). The structures were solved by Direct Method and refined on F^2 with the SHELX-97[s2] software package. CCDC 1963423 -1963424 contain the supplementary crystallographic data for this paper. In the crystals of compound **2**, the solvent molecules were strongly disordered and had been treated using the SQUEEZE routine in PLATON. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk./data_request/cif.

Compound 2 (CCDC 1963423)

Table S1. Crystal data and structure refinement for 2.

Empirical formula	C34 H56 B10 N4 O2 Si2	
Formula weight	717.10	
Temperature	150(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.0023(5) Å	α= 97.894(4)°.
	b = 18.1200(8) Å	β= 110.964(4)°.
	c = 19.4694(9) Å	γ = 98.644(3)°.
Volume	4461.6(3) $Å^3$	
Z	4	
Density (calculated)	1.068 Mg/m^3	
Absorption coefficient	0.964 mm^{-1}	
F(000)	1528	
Crystal size	0.270 x 0.120 x 0.080 mm^3	
Theta range for data collection	2.484 to 67.488°.	
Index ranges	-16<=h<=16, -21<=k<=21, -23<=l<=23	
Reflections collected	31323	
Independent reflections	16084 [R(int) = 0.0564]	
Completeness to theta = 67.488°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.04778	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16084 / 0 / 961	

Goodness-of-fit on F^2	0.997
Final R indices [I>2sigma(I)]	R1 = 0.0573, wR2 = 0.1333
R indices (all data)	R1 = 0.1033, wR2 = 0.1582
Extinction coefficient	n/a
Largest diff. peak and hole	0.408 and -0.334 e.Å^{-3}

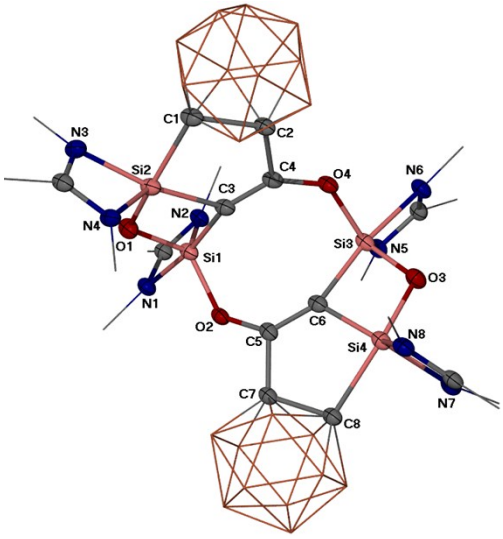

Figure S1. Molecular Structure of **2**. Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms are omitted for clarity.

Table S2. Bond lengths [Å] and angles [°] for 2.

Si(3)-O(3)	1.683(3)
Si(3)-O(4)	1.724(2)
Si(3)-C(6)	1.878(3)
Si(3)-N(5)	1.891(2)
Si(3)-N(6)	1.943(2)
Si(2)-O(1)	1.698(2)
Si(2)-N(4)	1.837(2)
Si(2)-C(3)	1.905(3)
Si(2)-N(3)	1.908(3)
Si(2)-C(1)	2.042(3)
Si(1)-O(1)	1.690(2)
Si(1)-O(2)	1.728(2)
Si(1)-N(2)	1.875(2)
Si(1)-C(3)	1.876(3)

Si(1)-N(1)	1.920(2)
Si(4)-O(3)	1.705(2)
Si(4)-N(8)	1.842(2)
Si(4)-N(7)	1.888(3)
Si(4)-C(6)	1.905(4)
Si(4)-C(8)	2.070(3)
O(4)-C(4)	1.361(3)
O(2)-C(5)	1.346(4)
C(4)-C(3)	1.329(4)
C(4)-C(2)	1.537(3)
C(5)-C(6)	1.337(4)
C(5)-C(7)	1.536(4)
C(7)-C(8)	1.671(5)
C(2)-C(1)	1.678(4)
O(3)-Si(3)-O(4)	122.45(10)
O(3)-Si(3)-C(6)	83.85(13)
O(4)-Si(3)-C(6)	101.37(11)
O(3)-Si(3)-N(5)	110.12(11)
O(4)-Si(3)-N(5)	122.11(12)
C(6)-Si(3)-N(5)	106.88(11)
O(3)-Si(3)-N(6)	90.47(11)
O(4)-Si(3)-N(6)	87.95(10)
C(6)-Si(3)-N(6)	170.64(12)
N(5)-Si(3)-N(6)	68.11(9)
O(1)-Si(2)-N(4)	103.44(11)
O(1)-Si(2)-C(3)	82.46(11)
N(4)-Si(2)-C(3)	128.47(14)
O(1)-Si(2)-N(3)	93.18(11)
N(4)-Si(2)-N(3)	70.24(11)
C(3)-Si(2)-N(3)	161.28(13)
O(1)-Si(2)-C(1)	158.34(11)
N(4)-Si(2)-C(1)	97.96(11)
C(3)-Si(2)-C(1)	86.88(12)
N(3)-Si(2)-C(1)	90.91(12)
O(1)-Si(1)-O(2)	125.16(10)
O(1)-Si(1)-N(2)	111.45(13)
O(2)-Si(1)-N(2)	118.13(10)

O(1)-Si(1)-C(3)	83.53(11)
O(2)-Si(1)-C(3)	100.53(13)
N(2)-Si(1)-C(3)	109.06(11)
O(1)-Si(1)-N(1)	90.24(11)
O(2)-Si(1)-N(1)	86.89(11)
N(2)-Si(1)-N(1)	68.87(10)
C(3)-Si(1)-N(1)	172.19(14)
O(3)-Si(4)-N(8)	101.51(10)
O(3)-Si(4)-N(7)	93.97(11)
N(8)-Si(4)-N(7)	70.41(11)
O(3)-Si(4)-C(6)	82.46(12)
N(8)-Si(4)-C(6)	131.96(11)
N(7)-Si(4)-C(6)	157.63(10)
O(3)-Si(4)-C(8)	162.08(11)
N(8)-Si(4)-C(8)	96.34(11)
N(7)-Si(4)-C(8)	90.48(12)
C(6)-Si(4)-C(8)	86.83(13)
C(4)-O(4)-Si(3)	131.35(17)
C(5)-O(2)-Si(1)	131.42(17)
Si(3)-O(3)-Si(4)	103.93(12)
Si(1)-O(1)-Si(2)	104.08(12)
C(3)-C(4)-O(4)	132.0(2)
C(3)-C(4)-C(2)	116.0(3)
O(4)-C(4)-C(2)	111.6(2)
C(6)-C(5)-O(2)	132.2(3)
C(6)-C(5)-C(7)	116.0(3)
O(2)-C(5)-C(7)	111.5(2)
C(5)-C(7)-C(8)	110.6(2)
C(5)-C(6)-Si(3)	149.3(3)
C(5)-C(6)-Si(4)	120.2(2)
Si(3)-C(6)-Si(4)	89.74(13)
C(4)-C(3)-Si(1)	148.0(2)
C(4)-C(3)-Si(2)	120.47(19)
Si(1)-C(3)-Si(2)	89.89(14)
C(4)-C(2)-C(1)	109.8(2)
C(7)-C(8)-Si(4)	105.59(18)
C(2)-C(1)-Si(2)	106.31(16)

Symmetry transformations used to generate equivalent atoms:

Compound 3 (CCDC 1963424)

Table S3. Crystal data and structure refinement for 3.

Empirical formula	C50 H74 B10 N6 Si2	
Formula weight	923.43	
Temperature	150(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 16.3688(2) Å	α= 90°.
	b = 16.3773(2) Å	β= 96.4510(10)°.
	c = 20.0064(2) Å	γ = 90°.
Volume	5329.29(11) $Å^3$	
Z	4	
Density (calculated)	1.151 Mg/m^3	
Absorption coefficient	0.896 mm^{-1}	
F(000)	1976	
Crystal size	0.270 x 0.210 x 0.070 mm^3	
Theta range for data collection	3.497 to 67.498°.	
Index ranges	-19<=h<=14, -19<=k<=19, -20<=l<=23	
Reflections collected	36977	
Independent reflections	9584 [R(int) = 0.0429]	
Completeness to theta = 67.498°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.39146	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9584 / 0 / 629	
Goodness-of-fit on F^2	1.015	
Final R indices [I>2sigma(I)]	R1 = 0.0426, wR2 = 0.1080	
R indices (all data)	R1 = 0.0538, wR2 = 0.1186	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.347 and -0.248 $e.Å^{-3}$	

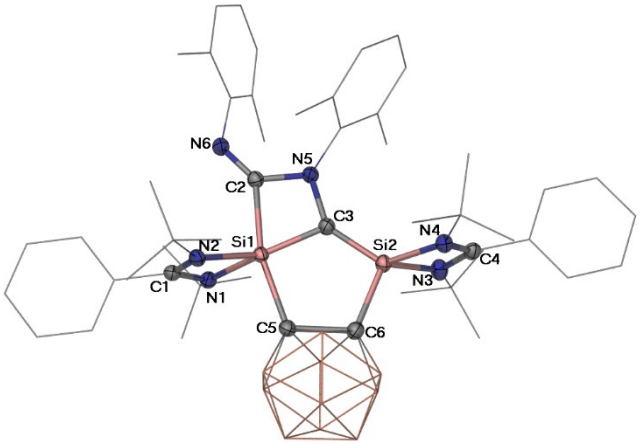

Figure S2. Molecular Structure of **3**. Thermal ellipsoids are drawn at 50% probability level. Hydrogen atoms are omitted for clarity.

Table S4. Bond lengths [Å] and angles [°] for 3.

Si(1)-C(3)	1.8215(16)
Si(1)-N(1)	1.8482(14)
Si(1)-N(2)	1.8719(13)
Si(1)-C(2)	2.0273(16)
Si(1)-C(5)	2.0535(16)
N(1)-C(1)	1.339(2)
C(1)-N(2)	1.332(2)
N(3)-C(4)	1.338(2)
N(3)-Si(2)	1.8540(14)
Si(2)-C(3)	1.7236(16)
Si(2)-N(4)	1.8296(14)
Si(2)-C(6)	1.9049(17)
C(2)-N(6)	1.281(2)
C(2)-N(5)	1.413(2)
C(3)-N(5)	1.474(2)
N(4)-C(4)	1.338(2)
C(5)-C(6)	1.699(2)
C(3)-Si(1)-N(1)	140.67(7)
C(3)-Si(1)-N(2)	145.70(7)
N(1)-Si(1)-N(2)	71.11(6)
C(3)-Si(1)-C(2)	70.68(7)

N(1)-Si(1)-C(2)	96.42(6)
N(2)-Si(1)-C(2)	98.30(6)
C(3)-Si(1)-C(5)	94.27(7)
N(1)-Si(1)-C(5)	95.56(6)
N(2)-Si(1)-C(5)	94.19(6)
C(2)-Si(1)-C(5)	164.95(7)
C(3)-Si(1)-C(1)	167.00(7)
C(2)-Si(1)-C(1)	96.51(6)
C(5)-Si(1)-C(1)	98.54(6)
C(1)-N(1)-Si(1)	90.53(10)
N(2)-C(1)-N(1)	108.16(14)
N(2)-C(1)-Si(1)	54.74(8)
N(1)-C(1)-Si(1)	53.73(8)
C(4)-N(3)-Si(2)	89.85(10)
C(3)-Si(2)-N(4)	125.68(7)
C(3)-Si(2)-N(3)	129.95(7)
N(4)-Si(2)-N(3)	71.70(6)
C(3)-Si(2)-C(6)	101.64(7)
N(4)-Si(2)-C(6)	113.22(7)
N(3)-Si(2)-C(6)	113.30(7)
C(3)-Si(2)-C(4)	137.76(7)
C(6)-Si(2)-C(4)	120.50(6)
C(1)-N(2)-Si(1)	89.72(10)
N(6)-C(2)-N(5)	129.89(14)
N(6)-C(2)-Si(1)	139.44(13)
N(5)-C(2)-Si(1)	90.65(9)
N(5)-C(3)-Si(2)	139.87(12)
N(5)-C(3)-Si(1)	97.32(10)
Si(2)-C(3)-Si(1)	122.34(9)
C(4)-N(4)-Si(2)	90.90(10)
N(4)-C(4)-N(3)	107.43(14)
N(4)-C(4)-Si(2)	53.23(8)
N(3)-C(4)-Si(2)	54.28(8)
C(2)-N(5)-C(3)	101.30(12)
C(6)-C(5)-Si(1)	111.22(10)
C(5)-C(6)-Si(2)	110.30(10)

Symmetry transformations used to generate equivalent atoms:

3. DFT Calculations

DFT calculations were performed at the B97-D/def2-SVP level of theory.[S3-S5] Stationary points on the potential energy surface (PES) were characterized by harmonic vibrational frequency calculations. Transition states, which had one imaginary frequency, were analysed by intrinsic reaction coordinate (IRC) calculations to confirm the corresponding intermediates. Calculations were carried out using the GAUSSIAN 09 program suite.[S6]

Table S5. NBO analysis of the central Si_2CN moiety in **3'**.

2	Occupation	Atom	Polarization	*s*-character	*p*-character	*d*-character
Bond	1.91	Si	28.07%	58.21%	41.28%	0.51%
		C	71.93%	30.20%	69.75%	0.05%
Bond	1.96	Si	70.23%	38.37%	61.60%	0.03%
		C	29.77%	58.14%	41.48%	0.38%
Bond	1.66	Si	19.22%	0.07%	98.45%	1.47%
		C	80.78%	0.01%	99.95%	0.04%
Bond	1.98	C	39.63%	29.61%	70.28%	0.11%
		N	60.37%	39.82%	60.14%	0.04%
Lone Pair	1.81	N	-	23.15%	76.81%	0.04%
Lone Pair	1.48	N	-	0.09%	99.86%	0.05%

Table S6. NBO analysis of the central Si_2CN moiety in **3**.

2	Occupation	Atom	Polarization	*s*-character	*p*-character	*d*-character
Bond	1.90	Si	23.00%	35.26%	63.23%	1.52%
		C	77.00%	32.38%	67.59%	0.03%
Bond	1.91	Si	25.94%	58.28%	38.85%	2.87%
		C	74.06%	42.24%	57.73%	0.03%
Bond	1.79	Si	20.11%	0.11%	98.34%	1.55%
		C	79.89%	0.30%	99.68%	0.02%
Bond	1.97	C	37.14%	24.91%	74.99%	0.11%
		N	62.86%	30.90%	69.08%	0.03%
Lone Pair	1.64	N	-	0.40%	99.59%	0.00%

Table S7. Calculated NPA charges of Si C, and N atoms, Si–C and C-N bond lengths [Å], Wiberg Bond Index (WBI) and Mayer Bond Order (MBO) of the central Si_2CN moiety in **3'** and **3**.

	NPA charge			Bond length [Å]		WBI//MBO	
	Si	C	N	Si-C	C-N	Si–C	C-N
3'	+2.07/+1.89	-1.09	-0.67	1.788/1.772	1.391	0.98/1.06// 1.22/1.23	1.12//1.03
3	+1.94/+1.94	-1.18	-0.49	1.863/1.723	1.453	0.76/1.18// 0.95/1.47	0.94//1.08

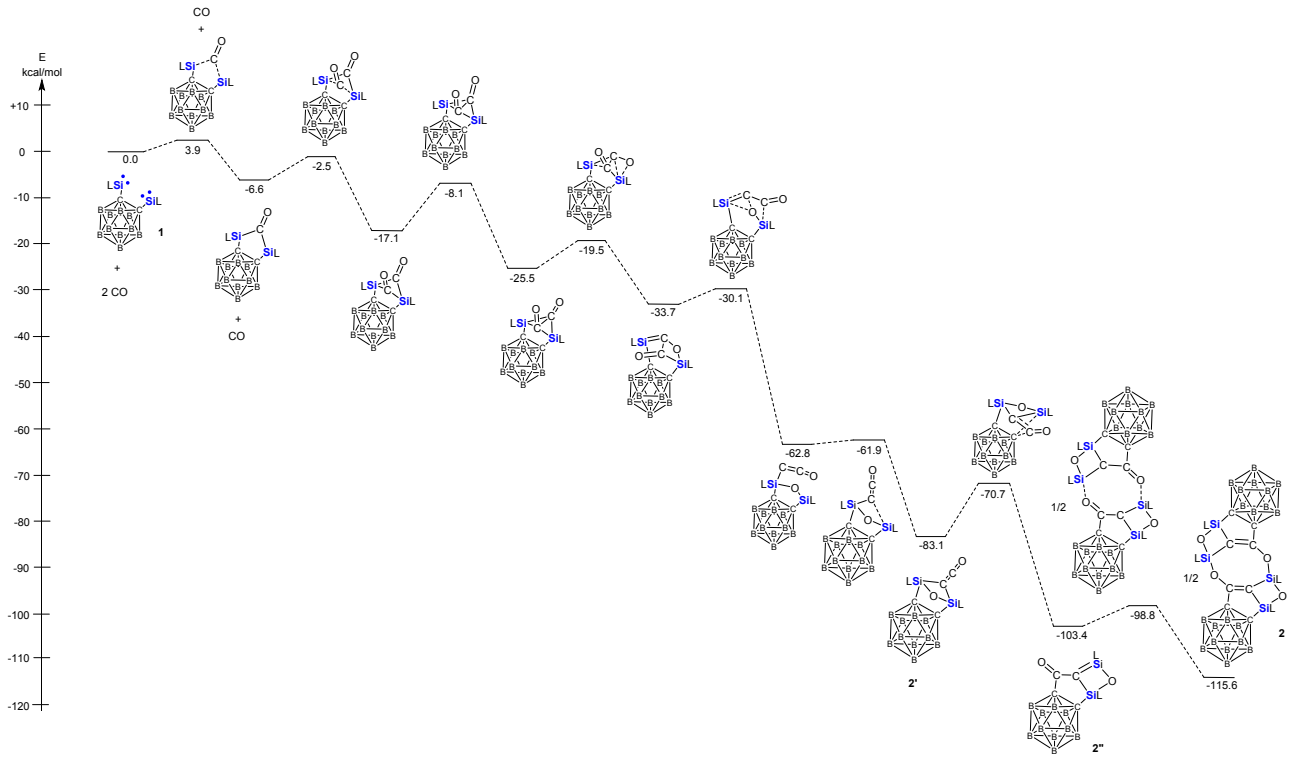

Figure S3. DFT-derived mechanism for the reaction of **1** and CO leading to **2** via **2´** and **2´´**.

Table S8. Cartesian geometry of CO in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	0	0	-0.650852
O	0	0	0.488139

Table S9. Cartesian geometry of **1** in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
Si	-1.659906	0.458737	-1.072174
N	3.279637	-1.224484	-0.388649
C	0.835656	-0.155367	0.756457
B	0.260908	1.400501	1.217868
H	0.410333	2.335921	0.486856
Si	1.660002	-0.458968	-1.072367
N	3.047144	0.86046	-0.926958
C	-0.835443	0.154623	0.756543
B	-0.26072	-1.401635	1.216801
H	-0.410134	-2.336426	0.484974
N	-3.047362	-0.860372	-0.926913
C	-3.93629	0.059895	-0.52482
B	-1.587161	-0.607255	2.111155

H	-2.708219	-1.01729	1.983704
N	-3.279297	1.224552	-0.38828
C	-5.378663	-0.171615	-0.216157
B	1.587309	0.605462	2.111705
H	2.708393	1.015573	1.984566
C	-6.390519	-0.067384	-1.190391
H	-6.122323	0.174153	-2.224834
B	-1.252927	1.132706	2.123697
H	-2.147413	1.918572	2.025611
C	-7.731636	-0.288519	-0.839319
H	-8.515261	-0.206629	-1.603132
B	1.253025	-1.134477	2.122917
H	2.147575	-1.920189	2.024306
C	-8.068895	-0.618434	0.48552
H	-9.117684	-0.792067	0.758023
B	-0.272843	-1.430669	3.00425
H	-0.462866	-2.468996	3.588978
C	-7.060829	-0.726019	1.459525
H	-7.31864	-0.98265	2.494678
B	-0.880141	0.161355	3.570955
H	-1.529591	0.286162	4.580869
C	-5.71912	-0.501881	1.111716
H	-4.924783	-0.572794	1.864064
B	0.272915	1.428149	3.005355
H	0.462895	2.466042	3.590878
C	-3.213535	-2.293111	-1.247786
B	0.880166	-0.164289	3.570905
H	1.52956	-0.289819	4.580762
C	-1.947663	-2.71789	-2.021478
H	-1.873697	-2.160765	-2.974001
H	-1.99269	-3.800039	-2.242673
H	-1.032833	-2.517198	-1.438136
C	-4.436307	-2.543321	-2.161291
H	-5.38836	-2.404986	-1.623534
H	-4.402177	-3.586585	-2.527792
H	-4.413421	-1.865865	-3.035718
C	-3.359095	-3.122954	0.04592
H	-2.479884	-2.989914	0.696334
H	-3.459515	-4.195192	-0.208743
H	-4.26092	-2.810926	0.602943
C	-3.810287	2.604617	-0.336537
C	-2.595668	3.555166	-0.283077
H	-1.992263	3.382465	0.622431
H	-2.947575	4.602848	-0.282698

H	-1.951368	3.402585	-1.170439
C	-4.701553	2.824	0.904201
H	-5.624095	2.221107	0.849562
H	-4.99006	3.890631	0.961608
H	-4.155886	2.556127	1.826025
C	-4.609353	2.912903	-1.624878
H	-3.983884	2.714586	-2.515989
H	-4.91068	3.977772	-1.635987
H	-5.523463	2.297978	-1.682436
C	3.936309	-0.059613	-0.524998
C	5.378597	0.17231	-0.21622
C	6.390474	0.069109	-1.190534
H	6.12237	-0.171971	-2.225104
C	7.731503	0.29065	-0.839366
H	8.515141	0.209543	-1.603249
C	8.068644	0.619958	0.485653
H	9.117358	0.793927	0.758226
C	7.06055	0.726504	1.45975
H	7.31827	0.982658	2.495044
C	5.718936	0.501936	1.111842
H	4.924599	0.572054	1.864263
C	3.811086	-2.604402	-0.337437
C	4.701939	-2.824074	0.903539
H	5.62434	-2.220907	0.849497
H	4.990702	-3.890649	0.960653
H	4.155814	-2.55668	1.825236
C	4.610682	-2.911854	-1.625656
H	3.985494	-2.713153	-2.516881
H	4.912153	-3.976679	-1.637233
H	5.524744	-2.296808	-1.682575
C	2.596787	-3.555428	-0.284912
H	1.992999	-3.383555	0.620495
H	2.949113	-4.602971	-0.285076
H	1.952731	-3.402543	-1.172398
C	3.212767	2.293437	-1.24704
C	4.435263	2.544585	-2.160674
H	5.38748	2.406201	-1.623215
H	4.400716	3.588068	-2.526512
H	4.412401	1.867683	-3.035528
C	3.358383	3.122511	0.047154
H	2.479416	2.988689	0.697738
H	3.45828	4.194956	-0.206854
H	4.260515	2.810479	0.603691
C	1.946575	2.718224	-2.020186

H	1.872627	2.161691	-2.973056
H	1.991104	3.800529	-2.240687
H	1.031961	2.516771	-1.43678

Table S10. Cartesian geometry of transition state (3.9 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-5.745494	0.876307	-1.814484
C	-5.236654	0.247847	-0.658969
C	-6.122288	-0.336042	0.273823
C	-7.506182	-0.280712	0.054095
C	-8.014422	0.347822	-1.098781
C	-7.130341	0.921971	-2.031019
C	-3.782367	0.15367	-0.39494
N	-3.010566	-0.928899	-0.589891
C	-3.233996	-2.215394	-1.293288
C	-3.500654	-3.309813	-0.23859
Si	-1.480877	0.036347	-0.075543
C	-0.765174	-0.502144	1.619781
B	0.225932	0.676434	2.4419
B	1.670539	-0.221127	2.962036
B	0.339322	0.115269	4.124168
B	-1.208628	-0.035052	3.219465
B	-1.364947	-1.731521	2.667232
B	-0.030706	-2.078446	1.54079
B	0.08561	-2.639905	3.22277
B	-0.645702	-1.378155	4.274078
B	1.140487	-1.492887	4.113227
B	1.514459	-1.913184	2.406269
C	0.897557	-0.601053	1.470518
Si	1.389646	0.020263	-0.291335
N	2.944508	-0.936368	-0.78123
C	3.289308	-2.26545	-1.332333
C	2.105325	-3.203213	-1.029161
C	-0.120333	0.499133	-1.192496
O	-0.244014	1.00442	-2.364967
N	2.85766	1.154513	-0.228207
C	3.049255	2.616344	-0.074192
C	1.674832	3.264537	-0.343184
C	3.693266	0.174491	-0.626658
C	5.162629	0.288703	-0.742839
C	5.922303	0.317313	0.450155
C	7.318972	0.423941	0.390762
C	7.971531	0.515865	-0.853694

C	7.214695	0.504766	-2.040829
C	5.818319	0.391353	-1.99013
N	-2.997408	1.111018	0.13919
C	-3.230174	2.562679	0.299332
C	-3.099374	3.229363	-1.088863
C	-2.110074	3.08005	1.22055
C	-4.595943	2.863106	0.94749
C	-1.929192	-2.517497	-2.06617
C	-4.395741	-2.16501	-2.304485
C	4.562803	-2.832739	-0.672057
C	3.456811	-2.163205	-2.86442
C	4.065211	3.170578	-1.093965
C	3.511747	2.924725	1.365359
H	0.270163	1.792861	2.024699
H	-0.178772	-2.719203	0.546115
H	-2.448266	-2.194738	2.43094
H	2.735183	0.33535	2.922751
H	-5.053573	1.305737	-2.547328
H	-2.187988	0.646031	3.371191
H	-7.521649	1.405697	-2.934861
H	2.478746	-2.505546	2.002072
H	-9.097287	0.389242	-1.270404
H	0.031729	-3.820515	3.460345
H	-8.191088	-0.731604	0.783215
H	-1.23788	-1.654125	5.287645
H	-5.718633	-0.82762	1.16719
H	0.469654	0.91981	5.012419
H	1.863182	-1.852477	5.009137
H	-1.681195	-1.683217	-2.749487
H	-2.051153	-3.452467	-2.644023
H	-1.084041	-2.639062	-1.367427
H	-5.378219	-2.067626	-1.814152
H	-4.389331	-3.111036	-2.876841
H	-4.266804	-1.328385	-3.014803
H	-2.66424	-3.363402	0.480427
H	-3.613331	-4.294808	-0.730163
H	-4.429574	-3.08605	0.319417
H	-2.14665	2.580062	2.204157
H	-2.223483	4.16984	1.365477
H	-1.126323	2.884966	0.761345
H	-5.438118	2.608839	0.283489
H	-4.650686	3.944725	1.172636
H	-4.704952	2.301856	1.894371
H	-2.165	2.895145	-1.580679

H	-3.081686	4.330693	-0.980521
H	-3.954818	2.961706	-1.734422
H	5.229577	0.41782	-2.913112
H	7.715994	0.592647	-3.013107
H	9.064452	0.600758	-0.898026
H	7.901819	0.433669	1.320478
H	5.410779	0.236821	1.416577
H	5.458047	-2.240612	-0.926363
H	4.721219	-3.869659	-1.023637
H	4.445818	-2.848793	0.427379
H	2.56326	-1.689877	-3.313502
H	3.578272	-3.175149	-3.295505
H	4.348803	-1.571427	-3.129796
H	1.980396	-3.333704	0.057169
H	2.29468	-4.191122	-1.486889
H	1.168844	-2.790529	-1.44638
H	5.094622	2.838724	-0.880796
H	4.042081	4.275083	-1.044887
H	3.794163	2.862756	-2.121114
H	2.790503	2.518818	2.09674
H	3.5912	4.018684	1.512351
H	4.502316	2.472705	1.55717
H	1.272769	2.951853	-1.325463
H	1.776904	4.365088	-0.311404
H	0.950772	2.954127	0.427593

Table S11. Cartesian geometry of intermediate (-6.6 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-5.976134	0.384078	-1.756996
C	-5.296226	-0.016642	-0.590684
C	-6.022275	-0.490146	0.519724
C	-7.423513	-0.555474	0.464019
C	-8.10204	-0.156272	-0.701023
C	-7.37619	0.311691	-1.811397
C	-3.812314	0.033625	-0.502374
N	-2.985232	-1.011342	-0.645132
C	-3.231755	-2.409514	-1.062774
C	-3.445007	-3.299175	0.180343
Si	-1.458536	0.159709	-0.431487
C	-0.863611	-0.153387	1.401506
B	0.072257	1.129818	2.114019
B	1.502213	0.325002	2.81094
B	0.117838	0.791409	3.856948

B	-1.387396	0.508727	2.916047
B	-1.512031	-1.233613	2.58223
B	-0.129462	-1.705317	1.56937
B	-0.084695	-2.054836	3.30248
B	-0.864484	-0.679487	4.157527
B	0.928345	-0.796682	4.089322
B	1.379761	-1.422469	2.467728
C	0.798956	-0.24908	1.34508
Si	1.424374	0.092341	-0.482267
N	2.988783	-1.072421	-0.546389
C	3.293824	-2.456046	-0.96274
C	2.003238	-3.275149	-0.778665
C	0.008921	1.37466	-1.061719
O	-0.019423	2.196336	-1.966422
N	3.030054	1.08015	-0.252204
C	3.399515	2.518779	-0.306737
C	2.333694	3.313279	0.472162
C	3.795223	-0.008226	-0.45649
C	5.280652	-0.028202	-0.559453
C	6.046012	-0.232315	0.606137
C	7.446701	-0.225483	0.535772
C	8.090739	-0.017076	-0.697543
C	7.328472	0.185114	-1.861356
C	5.925552	0.182155	-1.79355
N	-3.064098	1.120983	-0.23445
C	-3.433855	2.557179	-0.186795
C	-3.467481	3.097316	-1.634014
C	-2.333478	3.297052	0.599246
C	-4.780563	2.792128	0.529775
C	-1.969468	-2.874879	-1.821339
C	-4.439857	-2.5547	-2.015292
C	4.406211	-3.088026	-0.097983
C	3.694071	-2.475975	-2.455512
C	3.391783	2.960367	-1.787214
C	4.770318	2.813432	0.341763
H	0.112163	2.187825	1.576306
H	-0.234425	-2.471252	0.661485
H	-2.584199	-1.731219	2.3787
H	2.5651	0.884998	2.752247
H	-5.405295	0.740228	-2.622037
H	-2.376352	1.190041	2.942997
H	-7.902828	0.619616	-2.723447
H	2.356765	-2.061779	2.183875
H	-9.19718	-0.210192	-0.744474

H	-0.143095	-3.198524	3.681515
H	-7.986793	-0.919049	1.332569
H	-1.498266	-0.831427	5.172802
H	-5.483991	-0.794919	1.42515
H	0.205062	1.706895	4.637304
H	1.608449	-1.031245	5.057812
H	-1.825898	-2.278701	-2.741325
H	-2.077267	-3.940451	-2.096424
H	-1.069073	-2.759588	-1.195223
H	-5.402429	-2.396037	-1.502162
H	-4.437218	-3.582071	-2.424914
H	-4.363501	-1.843037	-2.85788
H	-2.560362	-3.269522	0.83759
H	-3.62182	-4.345147	-0.134702
H	-4.322158	-2.954071	0.757769
H	-2.27603	2.925661	1.635787
H	-2.570832	4.376403	0.618246
H	-1.352088	3.167103	0.116908
H	-5.643587	2.441299	-0.058795
H	-4.902627	3.878326	0.697592
H	-4.788085	2.283782	1.511562
H	-2.484738	2.934559	-2.115747
H	-3.684484	4.182667	-1.629391
H	-4.253765	2.589496	-2.222491
H	5.327067	0.350783	-2.696123
H	7.826809	0.350339	-2.824893
H	9.186759	-0.011161	-0.750993
H	8.038343	-0.381841	1.446497
H	5.535007	-0.391456	1.562937
H	5.390034	-2.628892	-0.289285
H	4.478741	-4.166166	-0.33571
H	4.160838	-2.981395	0.974474
H	2.897772	-2.01181	-3.067879
H	3.837599	-3.519725	-2.79461
H	4.638044	-1.927691	-2.618509
H	1.731301	-3.332828	0.287326
H	2.156989	-4.299485	-1.164586
H	1.167231	-2.807543	-1.330347
H	4.15496	2.400694	-2.360257
H	3.623107	4.040337	-1.863434
H	2.393237	2.781307	-2.227856
H	4.825122	2.374957	1.354911
H	4.879824	3.910191	0.431238
H	5.617228	2.438912	-0.254893

H	1.337761	3.185222	0.022735
H	2.593306	4.387412	0.440142
H	2.298464	2.984948	1.524745

Table S12. Cartesian geometry of transition state (-2.5 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	5.880384	0.052295	-1.895147
C	5.322149	0.019958	-0.602775
C	6.162778	-0.01339	0.527801
C	7.554208	-0.015725	0.36336
C	8.114678	0.018097	-0.92766
C	7.275819	0.052784	-2.055175
C	3.846308	0.012323	-0.435105
N	3.059457	1.087744	-0.332499
C	3.397	2.522916	-0.52937
C	4.778645	2.907261	0.047601
Si	1.468219	-0.058159	-0.292965
C	-0.034344	1.196354	-1.021699
O	0.022301	2.084657	-1.857649
C	0.845809	-0.022576	1.545335
B	1.438836	-0.920824	2.896455
B	0.898657	-0.018117	4.347284
B	-0.902472	0.00552	4.344825
B	-0.02078	-1.460356	3.794542
B	-0.017463	-1.453973	2.025172
B	-1.462162	-0.881708	2.891303
B	-1.43868	0.904297	2.889782
B	0.018647	1.446015	3.790315
B	1.462318	0.865557	2.893184
B	0.020386	1.433232	2.021258
C	-0.841566	-0.000822	1.542895
Si	-1.461791	0.043321	-0.297475
N	-3.063554	1.089007	-0.355866
C	-3.408737	2.518822	-0.582339
C	-4.771465	2.913819	0.029189
N	-3.060622	-1.087158	-0.366858
C	-3.423155	-2.520055	-0.539272
C	-3.433001	-2.841574	-2.051519
C	-3.840483	-0.00427	-0.440373
C	-5.316755	0.001034	-0.604304
C	-5.876016	-0.025152	-1.896701
C	-7.27151	-0.018715	-2.055691
C	-8.109519	0.012549	-0.927439

C	-7.54811	0.038495	0.363211
C	-6.156372	0.034212	0.526626
C	-4.789854	-2.874979	0.087482
C	-2.355979	-3.378372	0.167005
N	3.074977	-1.087979	-0.387041
C	3.426153	-2.519734	-0.595267
C	3.391839	-2.815331	-2.110313
C	2.372456	-3.382631	0.128059
C	4.806568	-2.895721	-0.01356
C	2.338669	3.370674	0.203308
C	3.349625	2.824997	-2.043188
C	-3.41779	2.779728	-2.104688
C	-2.329112	3.386233	0.095725
H	0.023364	2.357334	1.271229
H	-0.017323	-2.379738	1.278576
H	-2.497446	-1.477747	2.759356
H	2.498081	1.460861	2.760563
H	-5.217219	-0.050384	-2.772432
H	-2.457682	1.527252	2.752583
H	-7.704224	-0.038561	-3.063822
H	2.458661	-1.543199	2.765632
H	-9.199625	0.016827	-1.052365
H	-0.03549	-2.509969	4.387562
H	-8.199781	0.062352	1.245639
H	-1.560248	0.016397	5.355632
H	-5.711779	0.054116	1.528397
H	0.03054	2.497679	4.379823
H	1.55407	-0.027824	5.359669
H	-1.375063	-3.274189	-0.31326
H	-2.655819	-4.440187	0.100259
H	-2.268588	-3.099022	1.230801
H	-4.210015	-2.246042	-2.56613
H	-3.657682	-3.913788	-2.208683
H	-2.442736	-2.618991	-2.488294
H	-4.848971	-2.518582	1.132293
H	-4.886899	-3.976438	0.090997
H	-5.640654	-2.465223	-0.478794
H	-2.265417	3.156511	1.173038
H	-2.598527	4.451263	-0.026961
H	-1.345082	3.229471	-0.364995
H	-5.624507	2.454743	-0.495515
H	-4.87612	4.011658	-0.051073
H	-4.819702	2.638903	1.098309
H	-2.427822	2.542636	-2.533037

H	-3.642444	3.844755	-2.306651
H	-4.19573	2.162478	-2.59364
H	5.220506	0.076471	-2.770002
H	7.707875	0.078849	-3.063459
H	9.204686	0.017259	-1.053507
H	8.206311	-0.043629	1.245316
H	5.719123	-0.040145	1.529662
H	5.644096	-2.480476	-0.59575
H	4.895309	-3.997758	-0.033954
H	4.897736	-2.559935	1.035654
H	2.386551	-2.593621	-2.512104
H	3.616947	-3.883519	-2.293388
H	4.149885	-2.205471	-2.637332
H	2.329431	-3.124003	1.198891
H	2.65245	-4.447537	0.028708
H	1.376532	-3.250623	-0.314925
H	4.118857	2.235359	-2.57706
H	3.549464	3.899041	-2.221642
H	2.347904	2.580031	-2.441275
H	4.877452	2.564722	1.093812
H	4.861985	4.009826	0.035035
H	5.615344	2.501289	-0.542947
H	1.337416	3.217174	-0.220418
H	2.597134	4.439173	0.087871
H	2.31801	3.124457	1.277956
C	0.046077	-1.216954	-1.020675
O	-0.006518	-2.100077	-1.863659

Table S13. Cartesian geometry of intermediate (-17.1 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	5.905226	-0.003801	-1.868614
C	5.319114	0.007779	-0.588435
C	6.13412	0.006603	0.560971
C	7.528896	-0.007967	0.427933
C	8.117221	-0.016231	-0.850804
C	7.303749	-0.012337	-1.997323
C	3.840355	0.015387	-0.446492
N	3.071938	1.09095	-0.280448
C	3.419397	2.522271	-0.488156
C	4.79889	2.905854	0.094815
Si	1.462405	-0.066829	-0.323059
C	-0.034814	1.209808	-1.049862
O	0.021848	2.094536	-1.887857

C	0.842113	-0.014131	1.518096
B	1.434633	-0.917283	2.865945
B	0.900803	-0.015281	4.320112
B	-0.900244	0.015416	4.320252
B	-0.025248	-1.45311	3.765989
B	-0.026637	-1.442693	1.996624
B	-1.465904	-0.86788	2.867733
B	-1.434291	0.917825	2.866428
B	0.025728	1.453399	3.766369
B	1.466235	0.868391	2.867747
B	0.026823	1.443557	1.99698
C	-0.841994	0.015152	1.518243
Si	-1.462415	0.067731	-0.322859
N	-3.05213	1.079362	-0.465089
C	-3.400445	2.51822	-0.639653
C	-4.785892	2.884249	-0.061547
N	-3.071744	-1.091103	-0.279793
C	-3.418932	-2.522489	-0.487637
C	-3.385397	-2.809102	-2.005371
C	-3.840398	-0.015826	-0.446234
C	-5.319137	-0.00847	-0.58836
C	-5.905066	0.00347	-1.868627
C	-7.303562	0.011893	-1.997549
C	-8.117207	0.015344	-0.851144
C	-7.529073	0.006728	0.427673
C	-6.13431	-0.007758	0.560917
C	-4.798096	-2.906577	0.095786
C	-2.360455	-3.38374	0.227028
N	3.051813	-1.079529	-0.46492
C	3.399771	-2.518427	-0.63968
C	3.35056	-2.843476	-2.148167
C	2.352042	-3.364862	0.112155
C	4.785056	-2.884946	-0.061465
C	2.361386	3.383674	0.22701
C	3.385354	2.80915	-2.005836
C	-3.351163	2.843575	-2.148062
C	-2.353016	3.364774	0.11249
H	0.028392	2.370332	1.250311
H	-0.028188	-2.369169	1.249623
H	-2.503127	-1.459284	2.73483
H	2.50342	1.459879	2.734941
H	-5.264466	0.005858	-2.758079
H	-2.45177	1.544571	2.732064
H	-7.758213	0.018094	-2.996168

H	2.452072	-1.544016	2.731164
H	-9.209681	0.024677	-0.953138
H	-0.041808	-2.503636	4.357434
H	-8.161755	0.009651	1.324082
H	-1.556942	0.029362	5.331793
H	-5.667938	-0.017627	1.552803
H	0.042435	2.503735	4.358146
H	1.557639	-0.029398	5.331561
H	-1.361494	-3.2258	-0.200312
H	-2.621985	-4.449851	0.097698
H	-2.333252	-3.152674	1.304902
H	-4.155284	-2.208735	-2.526138
H	-3.594492	-3.879681	-2.193686
H	-2.386177	-2.568216	-2.412205
H	-4.887433	-2.574334	1.146153
H	-4.886937	-4.00859	0.072326
H	-5.637397	-2.490267	-0.483215
H	-2.326249	3.089991	1.180205
H	-2.629595	4.431593	0.026051
H	-1.351632	3.237882	-0.319105
H	-5.620062	2.473217	-0.651576
H	-4.876792	3.986071	-0.071577
H	-4.882498	2.539147	0.983833
H	-2.343309	2.624828	-2.544256
H	-3.570167	3.916232	-2.311369
H	-4.105367	2.247112	-2.695668
H	5.26477	-0.005802	-2.758171
H	7.758546	-0.01828	-2.995877
H	9.209708	-0.025641	-0.952645
H	8.161448	-0.011238	1.324433
H	5.667594	0.016175	1.552788
H	5.6194	-2.474062	-0.651348
H	4.875647	-3.98679	-0.071643
H	4.881622	-2.540028	0.983978
H	2.342831	-2.624284	-2.544431
H	3.569219	-3.916173	-2.311698
H	4.10503	-2.247152	-2.695565
H	2.325219	-3.090362	1.179951
H	2.628413	-4.431713	0.025463
H	1.350736	-3.237637	-0.319521
H	4.154826	2.208614	-2.527012
H	3.5947	3.879688	-2.194089
H	2.385889	2.568633	-2.412303
H	4.888432	2.573573	1.145152

H	4.888098	4.007834	0.071314
H	5.637859	2.489236	-0.484436
H	1.362242	3.226137	-0.200043
H	2.623196	4.449733	0.097811
H	2.334419	3.152382	1.304836
C	0.034576	-1.208558	-1.05011
O	-0.022035	-2.092946	-1.888471

Table S14. Cartesian geometry of transition state (-8.1 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	5.83557	0.045271	-1.581703
C	5.129407	-0.033941	-0.366827
C	5.830316	-0.097464	0.854273
C	7.232521	-0.082995	0.856544
C	7.939583	-0.003842	-0.356937
C	7.24015	0.059094	-1.574217
C	3.643092	-0.016952	-0.32525
N	2.874233	1.081387	-0.213525
C	3.237757	2.502588	-0.46343
C	4.521032	2.915289	0.288449
Si	1.315455	0.013408	-0.248863
C	-0.000988	1.063681	-1.662725
O	-0.045493	2.068999	-2.364048
C	0.736387	-0.110809	1.619602
B	1.241091	-1.117466	2.922922
B	0.678249	-0.27088	4.401865
B	-1.115258	-0.151512	4.324842
B	-0.285238	-1.632186	3.724293
B	-0.207252	-1.519097	1.957204
B	-1.657691	-0.919703	2.801091
B	-1.543845	0.851939	2.899042
B	-0.102117	1.269706	3.890242
B	1.352603	0.661292	3.027582
B	-0.024079	1.34763	2.119923
C	-0.918496	-0.010777	1.538804
Si	-1.266806	0.096214	-0.412677
N	-2.867131	1.115408	-0.413867
C	-3.24883	2.547385	-0.52346
C	-4.509121	2.883502	0.303452
N	-2.768994	-1.043476	-0.637052
C	-3.061788	-2.481807	-0.864779
C	-4.073051	-2.67527	-2.017016
C	-3.605152	0.004791	-0.555756

C	-5.092142	-0.068015	-0.501347
C	-5.891611	0.134471	-1.642963
C	-7.290214	0.095911	-1.533034
C	-7.8939	-0.143401	-0.285437
C	-7.095258	-0.351706	0.852614
C	-5.696085	-0.315995	0.74689
C	-3.599335	-3.140284	0.422318
C	-1.735779	-3.150595	-1.270775
N	2.844055	-1.09119	-0.33085
C	3.175523	-2.502009	-0.658436
C	3.606644	-2.587741	-2.14194
C	1.891916	-3.325213	-0.469864
C	4.274052	-3.052418	0.273572
C	2.078983	3.37226	0.042134
C	3.397288	2.710475	-1.984178
C	-3.450552	2.894276	-2.015492
C	-2.074094	3.37875	0.021889
H	0.062776	2.296414	1.412913
H	-0.242758	-2.396834	1.151895
H	-2.71497	-1.446619	2.590447
H	2.419997	1.211738	2.955837
H	-5.417962	0.305799	-2.615245
H	-2.522102	1.534072	2.752577
H	-7.910195	0.251952	-2.424665
H	2.233758	-1.785348	2.787843
H	-8.987585	-0.170642	-0.201004
H	-0.377635	-2.710608	4.255511
H	-7.562134	-0.53883	1.827638
H	-1.813827	-0.165387	5.30782
H	-5.064502	-0.461677	1.631212
H	-0.063657	2.284625	4.539759
H	1.280076	-0.369221	5.442246
H	-1.331104	-2.717078	-2.201336
H	-1.904297	-4.233137	-1.416764
H	-0.980592	-3.022872	-0.480632
H	-5.094857	-2.378161	-1.73047
H	-4.095026	-3.746542	-2.290481
H	-3.761866	-2.095573	-2.906053
H	-2.86066	-3.060983	1.237421
H	-3.80143	-4.211012	0.23066
H	-4.540224	-2.661887	0.746899
H	-1.922246	3.178278	1.094734
H	-2.308198	4.45087	-0.108139
H	-1.14879	3.156878	-0.536064

H	-5.428343	2.448552	-0.121695
H	-4.630525	3.982521	0.32199
H	-4.393691	2.527576	1.343614
H	-2.523729	2.680253	-2.578046
H	-3.686088	3.970917	-2.118863
H	-4.288025	2.317115	-2.444529
H	5.286606	0.098589	-2.527934
H	7.787826	0.120592	-2.522866
H	9.036767	0.007927	-0.353065
H	7.775563	-0.131068	1.808635
H	5.270457	-0.154261	1.795082
H	5.257858	-2.598047	0.068309
H	4.362638	-4.143904	0.117432
H	4.007095	-2.8705	1.331028
H	2.810609	-2.174443	-2.786424
H	3.77609	-3.645673	-2.418716
H	4.548352	-2.036844	-2.31245
H	1.575639	-3.325197	0.587139
H	2.085959	-4.36814	-0.77785
H	1.0874	-2.916599	-1.103158
H	4.221101	2.086603	-2.373799
H	3.636143	3.770721	-2.19522
H	2.455689	2.453818	-2.503993
H	4.452064	2.635643	1.356333
H	4.627798	4.014336	0.22107
H	5.428132	2.460866	-0.141971
H	1.142457	3.111186	-0.479938
H	2.308789	4.433543	-0.168724
H	1.946893	3.24644	1.129357
C	0.206232	-0.459918	-1.914706
O	0.434695	-1.200059	-2.858865

Table S15. Cartesian geometry of intermediate (-25.5 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	5.761158	-0.001065	-1.757938
C	5.095512	-0.000426	-0.51842
C	5.836329	0.000363	0.681031
C	7.237501	0.000524	0.637325
C	7.904533	-0.000091	-0.601493
C	7.165592	-0.000898	-1.796812
C	3.61017	-0.000357	-0.425049
N	2.828434	1.086856	-0.336735
C	3.165622	2.506571	-0.618449

C	4.426515	2.968438	0.142993
Si	1.279158	-0.00014	-0.228908
C	-0.000189	0.780131	-1.679636
O	-0.00034	1.688566	-2.505693
C	0.837498	0.000926	1.688683
B	1.455296	-0.889881	3.02411
B	0.899827	0.002298	4.476913
B	-0.900051	0.002711	4.476856
B	-0.00043	-1.453871	3.918602
B	-0.000381	-1.432148	2.145047
B	-1.455841	-0.88922	3.024069
B	-1.455507	0.893432	3.023158
B	0.000207	1.458313	3.917126
B	1.455731	0.892791	3.023226
B	0.000282	1.434873	2.143612
C	-0.837606	0.001287	1.688662
Si	-1.27909	-0.000184	-0.228846
N	-2.828404	1.086781	-0.337028
C	-3.165738	2.50665	-0.617634
C	-4.426339	2.967973	0.144605
N	-2.828236	-1.087476	-0.335436
C	-3.165338	-2.507416	-0.616155
C	-3.349622	-2.677392	-2.140982
C	-3.610095	-0.000418	-0.425219
C	-5.095438	-0.000522	-0.518506
C	-5.761201	-0.000353	-1.757959
C	-7.165641	-0.000313	-1.796693
C	-7.904465	-0.000385	-0.601306
C	-7.237313	-0.000537	0.637451
C	-5.836138	-0.000635	0.68102
C	-4.425801	-2.96898	0.14618
C	-1.973917	-3.363094	-0.156475
N	2.828352	-1.087398	-0.335416
C	3.165534	-2.507495	-0.615084
C	3.3502	-2.67846	-2.139757
C	1.973928	-3.362799	-0.155211
C	4.425796	-2.968546	0.147895
C	1.9745	3.362671	-0.158795
C	3.349313	2.675484	-2.143472
C	-3.349976	2.676584	-2.142485
C	-1.974463	3.362489	-0.1579
H	0.000585	2.348981	1.385361
H	-0.000638	-2.346995	1.387678
H	-2.478325	-1.507055	2.878323

H	2.478268	1.510413	2.876973
H	-5.181481	-0.000288	-2.687591
H	-2.477776	1.511455	2.876715
H	-7.682554	-0.000211	-2.764421
H	2.477541	-1.508125	2.878455
H	-9.001253	-0.00033	-0.634237
H	-0.000678	-2.503789	4.51124
H	-7.810942	-0.000592	1.572643
H	-1.549028	0.003356	5.493276
H	-5.30693	-0.000766	1.641047
H	0.000441	2.508824	4.508715
H	1.548734	0.002678	5.493374
H	-1.053031	-3.045069	-0.671373
H	-2.168949	-4.419308	-0.416053
H	-1.836546	-3.286932	0.934886
H	-4.206178	-2.078794	-2.499957
H	-3.549698	-3.74015	-2.375836
H	-2.429668	-2.365229	-2.668287
H	-4.340644	-2.721144	1.220377
H	-4.512509	-4.067047	0.04733
H	-5.349231	-2.519202	-0.253346
H	-1.837098	3.286287	0.933445
H	-2.169654	4.418697	-0.417392
H	-1.053489	3.044685	-0.672806
H	-5.349656	2.518068	-0.255043
H	-4.513204	4.066029	0.045797
H	-4.341284	2.72011	1.218806
H	-2.430051	2.364246	-2.669739
H	-3.54986	3.739369	-2.377375
H	-4.206639	2.078117	-2.501415
H	5.181339	-0.001694	-2.68751
H	7.68241	-0.001395	-2.76459
H	9.001317	0.000056	-0.634529
H	7.811218	0.00114	1.572464
H	5.307213	0.000846	1.64111
H	5.349308	-2.518912	-0.251603
H	4.512622	-4.066659	0.049686
H	4.340288	-2.720115	1.221929
H	2.430412	-2.366497	-2.667485
H	3.55013	-3.741412	-2.373857
H	4.206959	-2.080272	-2.498915
H	1.836234	-3.285952	0.936048
H	2.16891	-4.419206	-0.414052
H	1.053232	-3.045021	-0.670617

H	4.205793	2.07669	-2.502299
H	3.549238	3.738093	-2.379121
H	2.429175	2.36293	-2.670222
H	4.341967	2.721193	1.217378
H	4.513228	4.066447	0.043511
H	5.349713	2.518411	-0.256794
H	1.053314	3.044499	-0.67309
H	2.169536	4.418705	-0.419103
H	1.837601	3.287229	0.932672
C	0.000105	-0.781394	-1.679313
O	0.000275	-1.690287	-2.504796

Table S16. Cartesian geometry of transition state (-19.5 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-5.836138	-0.000635	0.68102
C	-5.095438	-0.000522	-0.518506
C	-5.761201	-0.000353	-1.757959
C	-7.165641	-0.000313	-1.796693
C	-7.904465	-0.000385	-0.601306
C	-7.237313	-0.000537	0.637451
C	-3.610095	-0.000418	-0.425219
N	-2.828236	-1.087476	-0.335436
C	-3.165338	-2.507416	-0.616155
C	-1.973917	-3.363094	-0.156475
Si	-1.27909	-0.000184	-0.228846
C	0.166329	-0.882907	-1.867792
O	-0.898184	-1.491356	-1.803668
Si	1.279158	-0.000139	-0.228908
N	2.828352	-1.087397	-0.335416
C	3.165534	-2.507494	-0.615084
C	4.425796	-2.968546	0.147895
N	2.828434	1.086857	-0.336735
C	3.165622	2.506572	-0.618448
C	3.349313	2.675485	-2.143472
C	3.61017	-0.000356	-0.425049
C	5.095512	-0.000425	-0.51842
C	5.761158	-0.001064	-1.757938
C	7.165592	-0.000897	-1.796812
C	7.904533	-0.00009	-0.601493
C	7.237501	0.000525	0.637325
C	5.836329	0.000364	0.681031
C	4.426514	2.968439	0.142994
C	1.974499	3.362672	-0.158794

C	-0.000189	0.780132	-1.679636
O	-0.00034	1.688567	-2.505693
C	0.837498	0.000926	1.688683
C	-0.837606	0.001287	1.688662
B	0.000282	1.434873	2.143612
B	1.455731	0.892791	3.023226
B	0.000207	1.458313	3.917126
B	-1.455507	0.893431	3.023158
B	-1.455841	-0.889221	3.024069
B	-0.000381	-1.432148	2.145047
B	-0.00043	-1.453871	3.918602
B	-0.900051	0.00271	4.476856
B	0.899827	0.002298	4.476913
B	1.455296	-0.889881	3.02411
N	-2.828404	1.086781	-0.337028
C	-3.165738	2.50665	-0.617634
C	-1.974463	3.362489	-0.157899
C	-4.426339	2.967973	0.144605
C	-3.349976	2.676585	-2.142485
C	-3.349622	-2.677391	-2.140982
C	-4.425801	-2.96898	0.14618
C	3.3502	-2.678459	-2.139757
C	1.973928	-3.362799	-0.155211
H	0.000584	2.348981	1.385361
H	-0.000637	-2.346995	1.387678
H	-2.478325	-1.507056	2.878323
H	2.478268	1.510413	2.876974
H	-5.181481	-0.000288	-2.687591
H	-2.477776	1.511454	2.876715
H	-7.682554	-0.000211	-2.764421
H	2.477541	-1.508125	2.878455
H	-9.001253	-0.00033	-0.634237
H	-0.000678	-2.50379	4.511239
H	-7.810942	-0.000592	1.572643
H	-1.549028	0.003355	5.493276
H	-5.30693	-0.000766	1.641047
H	0.00044	2.508823	4.508716
H	1.548734	0.002677	5.493374
H	-1.053031	-3.045068	-0.671373
H	-2.168949	-4.419308	-0.416053
H	-1.836546	-3.286932	0.934886
H	-4.206178	-2.078794	-2.499957
H	-3.549698	-3.740149	-2.375836
H	-2.429668	-2.365228	-2.668287

H	-4.340644	-2.721144	1.220377
H	-4.512509	-4.067047	0.04733
H	-5.349231	-2.519202	-0.253346
H	-1.837098	3.286287	0.933446
H	-2.169654	4.418698	-0.417391
H	-1.053489	3.044686	-0.672805
H	-5.349656	2.518068	-0.255043
H	-4.513204	4.066029	0.045798
H	-4.341284	2.72011	1.218806
H	-2.430051	2.364247	-2.669739
H	-3.54986	3.73937	-2.377374
H	-4.206639	2.078118	-2.501415
H	5.181339	-0.001693	-2.68751
H	7.68241	-0.001393	-2.76459
H	9.001317	0.000058	-0.634529
H	7.811218	0.001141	1.572465
H	5.307213	0.000847	1.64111
H	5.349308	-2.518912	-0.251603
H	4.512622	-4.066658	0.049686
H	4.340288	-2.720115	1.221929
H	2.430412	-2.366496	-2.667485
H	3.55013	-3.741411	-2.373857
H	4.206959	-2.080271	-2.498915
H	1.836234	-3.285952	0.936048
H	2.16891	-4.419206	-0.414052
H	1.053232	-3.045021	-0.670617
H	4.205793	2.076691	-2.502299
H	3.549238	3.738094	-2.37912
H	2.429175	2.362931	-2.670222
H	4.341966	2.721194	1.217379
H	4.513227	4.066448	0.043512
H	5.349712	2.518412	-0.256793
H	1.053314	3.0445	-0.67309
H	2.169535	4.418706	-0.419102
H	1.8376	3.28723	0.932673

Table S17. Cartesian geometry of intermediate (-33.7 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	6.103308	-0.685274	-1.336897
C	5.364319	-0.403623	-0.172395
C	6.013836	-0.352065	1.076735
C	7.394233	-0.583495	1.158755

C	8.133701	-0.861438	-0.00536
C	7.487168	-0.909912	-1.252543
C	3.894885	-0.171178	-0.233833
N	3.282014	1.007661	-0.283358
C	3.865535	2.329253	-0.652984
C	5.105576	2.677739	0.198392
Si	1.579882	0.081321	-0.557476
C	0.640987	1.059655	-2.02375
O	0.781939	2.141093	-2.600666
C	0.738891	0.503461	1.175463
B	1.245113	-0.029936	2.742973
B	0.643525	1.220261	3.886968
B	-1.144753	1.258981	3.779542
B	-0.267579	-0.311206	3.674985
B	-0.172511	-0.764018	1.963286
B	-1.645311	0.029146	2.582003
B	-1.583799	1.745247	2.112302
B	-0.171106	2.499104	2.916102
B	1.299396	1.68974	2.293331
B	-0.072699	2.025545	1.199135
C	-0.933509	0.515957	1.090417
Si	-1.607844	-0.016225	-0.649402
N	-3.244098	0.884387	-0.73817
C	-3.721181	2.20595	-1.211907
C	-4.821722	2.778987	-0.29628
N	-2.976152	-1.248149	-0.426189
C	-3.175367	-2.708983	-0.222723
C	-4.257575	-3.250287	-1.18363
C	-3.896251	-0.257945	-0.508034
C	-5.360242	-0.38051	-0.273337
C	-6.274743	-0.572996	-1.326312
C	-7.650907	-0.62809	-1.0548
C	-8.116529	-0.491549	0.265009
C	-7.202377	-0.301355	1.316197
C	-5.825461	-0.24328	1.05033
C	-3.560823	-3.009852	1.239629
C	-1.841881	-3.398202	-0.555518
N	2.948861	-1.145676	-0.259389
C	3.11867	-2.6222	-0.327903
C	3.313354	-3.021051	-1.807517
C	1.834444	-3.275954	0.211371
C	4.30034	-3.133752	0.527071
C	2.80155	3.423249	-0.43847
C	4.224126	2.296011	-2.156732

C	-4.241029	2.053037	-2.658948
C	-2.501991	3.149416	-1.212167
H	0.000077	2.71261	0.227777
H	-0.174915	-1.857352	1.495919
H	-2.686279	-0.567698	2.537403
H	2.361671	2.204442	2.105895
H	-5.906559	-0.689783	-2.351397
H	-2.58312	2.309944	1.765454
H	-8.361334	-0.779259	-1.877017
H	2.259004	-0.672832	2.826246
H	-9.192832	-0.533522	0.474056
H	-0.333139	-1.171142	4.518073
H	-7.561038	-0.192111	2.347146
H	-1.85852	1.533122	4.712616
H	-5.105383	-0.078394	1.860401
H	-0.170388	3.666589	3.216372
H	1.248065	1.476565	4.898671
H	-1.518714	-3.161065	-1.584108
H	-1.965808	-4.491428	-0.452491
H	-1.053667	-3.065222	0.134067
H	-5.26939	-2.915216	-0.903924
H	-4.24503	-4.355238	-1.145413
H	-4.043895	-2.934522	-2.221999
H	-2.771017	-2.661939	1.926761
H	-3.688074	-4.101159	1.368671
H	-4.510883	-2.515593	1.508995
H	-2.127485	3.299447	-0.186735
H	-2.806442	4.13026	-1.61967
H	-1.67845	2.757679	-1.838813
H	-5.751045	2.186591	-0.345726
H	-5.053075	3.810574	-0.620437
H	-4.47217	2.811309	0.751311
H	-3.454964	1.61521	-3.301905
H	-4.514161	3.045811	-3.063048
H	-5.138158	1.409429	-2.691672
H	5.594237	-0.724846	-2.306502
H	8.060717	-1.123615	-2.163207
H	9.214582	-1.039295	0.059985
H	7.896237	-0.544957	2.133624
H	5.429505	-0.131794	1.977653
H	5.283206	-2.89034	0.093936
H	4.224363	-4.23505	0.593366
H	4.248523	-2.719738	1.550508
H	2.452039	-2.673948	-2.408124

H	3.390088	-4.12137	-1.900703
H	4.238823	-2.572546	-2.212708
H	1.677052	-3.001858	1.268882
H	1.931978	-4.374881	0.140744
H	0.962847	-2.955645	-0.376935
H	4.97684	1.514434	-2.36565
H	4.647205	3.272644	-2.460166
H	3.310384	2.112009	-2.75081
H	4.884348	2.553306	1.274637
H	5.366654	3.73716	0.018051
H	5.984502	2.065237	-0.06011
H	1.896257	3.201249	-1.023511
H	3.216709	4.381973	-0.80048
H	2.54629	3.538427	0.625886
C	-0.420016	0.110502	-1.959045
O	0.113005	-0.984498	-1.013915

Table S18. Cartesian geometry of transition state (-30.1 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-5.826045	-0.242637	1.051659
C	-5.35997	-0.381144	-0.271545
C	-6.273901	-0.57467	-1.324849
C	-7.650228	-0.629701	-1.054083
C	-8.116633	-0.492077	0.265318
C	-7.203075	-0.300749	1.316846
C	-3.895962	-0.258183	-0.506127
N	-2.975667	-1.248213	-0.424062
C	-3.174806	-2.708975	-0.220007
C	-1.841113	-3.398366	-0.551156
Si	-1.6073	-0.01657	-0.64935
O	0.109416	-0.983353	-1.013574
C	-0.421783	0.111712	-1.961244
C	0.538758	1.150247	-2.132798
O	0.544603	2.209619	-2.76537
Si	1.682016	0.355964	-0.387282
N	3.165586	-0.685185	0.040327
C	3.485321	-2.135535	0.129358
C	4.706398	-2.429643	1.03028
N	3.194965	1.569758	-0.126473
C	3.56852	2.944431	-0.566677
C	3.99513	2.877065	-2.051493
C	3.990406	0.515818	0.028343
C	5.473863	0.537089	0.155337

C	6.300723	0.312321	-0.961491
C	7.697482	0.329005	-0.815092
C	8.270512	0.562469	0.447033
C	7.443803	0.783458	1.563691
C	6.049221	0.773936	1.41933
C	4.694313	3.548789	0.300144
C	2.330011	3.85598	-0.465698
C	0.709284	0.7421	1.283931
C	-0.9372	0.468422	1.144183
B	-0.34313	2.104623	1.173655
B	1.016903	2.07519	2.332278
B	-0.592998	2.664622	2.84875
B	-1.825314	1.633948	2.055455
B	-1.622245	-0.034189	2.64286
B	-0.013103	-0.606829	2.129493
B	-0.256228	-0.067265	3.800991
B	-1.384628	1.336734	3.766129
B	0.378886	1.605927	3.933388
B	1.22818	0.403487	2.900683
N	-3.369044	0.609507	-0.599985
C	-4.071634	1.872586	-0.930452
C	-3.020391	2.998902	-0.875383
C	-5.207933	2.173271	0.067703
C	-4.623581	1.768213	-2.369941
C	-4.256063	-3.250891	-1.181762
C	-3.561456	-3.009114	1.242212
C	3.842115	-2.642603	-1.285517
C	2.231126	-2.870746	0.633061
H	-0.342374	2.730702	0.15932
H	0.185617	-1.712837	1.740709
H	-2.547465	-0.798771	2.607364
H	1.986496	2.747942	2.143265
H	-5.905266	-0.692362	-2.34966
H	-2.88857	1.998933	1.638044
H	-8.360136	-0.781599	-1.876619
H	2.329843	-0.053305	3.061672
H	-9.193043	-0.533999	0.473827
H	-0.215293	-0.869923	4.700248
H	-7.56238	-0.190575	2.347468
H	-2.174097	1.546321	4.653856
H	-5.106468	-0.076632	1.861953
H	-0.79828	3.832546	3.0655
H	0.888351	2.024734	4.943218
H	-1.516625	-3.161426	-1.579381

H	-1.965412	-4.491546	-0.448114
H	-1.053661	-3.065569	0.139365
H	-5.268148	-2.915511	-0.903404
H	-4.243649	-4.355813	-1.142819
H	-4.041175	-2.935717	-2.220059
H	-2.772143	-2.660702	1.929691
H	-3.688697	-4.100356	1.371838
H	-4.511784	-2.514897	1.510575
H	-2.630004	3.115575	0.148432
H	-3.495735	3.949238	-1.17828
H	-2.173344	2.805044	-1.560387
H	-6.032011	1.444144	-0.01139
H	-5.615291	3.178349	-0.148334
H	-4.821687	2.167231	1.102856
H	-3.806662	1.524326	-3.0743
H	-5.069249	2.73553	-2.668534
H	-5.406984	0.992516	-2.438686
H	5.849281	0.12803	-1.942864
H	8.338731	0.158814	-1.689028
H	9.361889	0.573202	0.560989
H	7.888285	0.965992	2.55009
H	5.396714	0.947964	2.282802
H	5.662545	-2.135029	0.569962
H	4.742418	-3.519485	1.214537
H	4.605064	-1.915868	2.003535
H	3.004188	-2.444584	-1.979609
H	4.035002	-3.732381	-1.264499
H	4.749372	-2.136252	-1.662732
H	1.959297	-2.521287	1.644153
H	2.442114	-3.955008	0.677787
H	1.384617	-2.698806	-0.046819
H	4.875389	2.221552	-2.179848
H	4.263906	3.889792	-2.40786
H	3.152062	2.504802	-2.661764
H	4.44819	3.457121	1.374283
H	4.784916	4.623474	0.055423
H	5.673019	3.077198	0.115121
H	1.501084	3.448395	-1.063954
H	2.597297	4.845696	-0.879879
H	2.011489	3.994324	0.578634

Table S19. Cartesian geometry of intermediate (-62.8 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates

C	5.5297	-1.142834	-0.814525
C	5.072077	-0.534594	0.371994
C	5.972883	-0.334163	1.436531
C	7.311857	-0.738186	1.317593
C	7.761422	-1.352279	0.135572
C	6.866412	-1.555764	-0.929133
C	3.653206	-0.066476	0.446792
N	2.615584	-0.741182	1.019115
C	2.664485	-2.106791	1.618802
C	3.683401	-2.169906	2.78454
Si	1.392275	0.63819	0.63006
O	-0.238507	-0.208767	1.249071
C	1.118138	2.093253	1.543664
C	0.631038	2.77917	2.508879
O	0.180512	3.476235	3.380453
C	0.7957	0.198915	-1.275784
B	-0.247467	1.347444	-2.048943
B	-1.499473	0.377641	-2.912091
B	-0.106073	1.057559	-3.805274
B	1.336546	0.931921	-2.746384
B	1.663832	-0.777512	-2.419661
B	0.277884	-1.44363	-1.544557
B	0.429166	-1.758344	-3.284555
B	1.085825	-0.271642	-4.04293
B	-0.669902	-0.61831	-4.14858
B	-1.170476	-1.350514	-2.602563
C	-0.848934	-0.143514	-1.420618
Si	-1.540186	-0.136543	0.336475
N	-3.005357	-1.223557	0.504762
C	-3.36016	-2.669056	0.58289
C	-3.946975	-2.972827	1.977503
N	-3.01415	0.954393	0.520574
C	-3.358454	2.410732	0.469414
C	-3.605557	2.83227	-0.99221
C	-3.805081	-0.132601	0.4947
C	-5.283631	-0.134752	0.369836
C	-5.84495	0.010025	-0.915243
C	-7.239642	0.019678	-1.067387
C	-8.072895	-0.110925	0.057942
C	-7.509573	-0.251451	1.338516
C	-6.115301	-0.264407	1.498001
C	-2.153708	3.163972	1.049419
C	-4.600641	2.719835	1.330813
C	-2.054099	-3.458765	0.402969

C	-4.355672	-3.069009	-0.525834
N	3.198577	1.071138	-0.051125
C	3.960071	2.31817	-0.352201
C	4.945079	2.105466	-1.521853
C	4.713353	2.782871	0.917059
C	2.969904	3.446736	-0.717901
C	3.018748	-3.16472	0.549702
C	1.287136	-2.446216	2.211721
H	-0.494079	2.364049	-1.468118
H	0.363079	-2.221201	-0.645623
H	2.760844	-1.159187	-2.125987
H	-2.631501	0.782472	-2.934133
H	5.618807	0.140485	2.357494
H	2.228768	1.719023	-2.723341
H	8.005389	-0.57258	2.151668
H	-2.077783	-2.110591	-2.397798
H	8.808096	-1.669192	0.043739
H	0.672937	-2.873877	-3.67188
H	7.210367	-2.030331	-1.856715
H	1.819847	-0.304501	-4.998934
H	4.832569	-1.282066	-1.64769
H	-0.243433	1.972572	-4.577147
H	-1.223896	-0.911987	-5.178477
H	0.981681	-1.700539	2.965339
H	1.34552	-3.443333	2.685482
H	0.521432	-2.466728	1.426027
H	4.725324	-2.170589	2.430082
H	3.524493	-3.107028	3.350763
H	3.531741	-1.31626	3.470849
H	2.297369	-3.126285	-0.285018
H	2.982708	-4.173946	1.002732
H	4.033773	-3.007313	0.148269
H	2.396172	3.219338	-1.628606
H	3.552638	4.369246	-0.899573
H	2.261955	3.610524	0.112199
H	5.766411	1.420907	-1.251459
H	5.389434	3.080314	-1.798429
H	4.417206	1.700073	-2.404338
H	3.996777	2.863164	1.75504
H	5.162667	3.777399	0.734308
H	5.52728	2.089409	1.184778
H	-5.67135	-0.353985	2.495474
H	-8.157477	-0.346037	2.218503
H	-9.163207	-0.100864	-0.063102

H	-7.675579	0.128708	-2.067946
H	-5.187643	0.101821	-1.787384
H	-5.346592	-2.609037	-0.378344
H	-4.482033	-4.167206	-0.507192
H	-3.965352	-2.780466	-1.518351
H	-3.247467	-2.646541	2.769587
H	-4.10761	-4.062289	2.077926
H	-4.918593	-2.470267	2.121525
H	-1.601244	-3.250009	-0.579649
H	-2.271385	-4.539418	0.469267
H	-1.331602	-3.199414	1.195092
H	-5.536748	2.354744	0.877167
H	-4.677253	3.817471	1.4324
H	-4.492575	2.288391	2.34296
H	-2.714603	2.638772	-1.611721
H	-3.825645	3.915145	-1.022587
H	-4.466959	2.290058	-1.421429
H	-2.014172	2.943115	2.121354
H	-2.319605	4.250689	0.9412
H	-1.213108	2.902634	0.533505

Table S20. Cartesian geometry of transition state (-61.9 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	6.133299	-0.536474	-0.958744
C	5.047872	-0.18993	-0.129807
C	5.280717	0.171401	1.212381
C	6.586625	0.155475	1.727471
C	7.667133	-0.199522	0.902674
C	7.437076	-0.539881	-0.442737
C	3.644084	-0.135244	-0.622126
N	2.968184	1.003061	-0.915868
C	3.475744	2.408114	-0.989998
C	4.973568	2.491046	-1.372512
Si	1.325517	0.143457	-0.706888
N	2.806282	-1.158006	-0.790052
C	3.163136	-2.604534	-0.883455
C	4.102842	-3.095636	0.241684
O	0.009515	-0.294671	-1.610259
Si	-1.264489	0.668525	-0.720458
N	-3.021865	1.182997	-0.141585
C	-3.730384	2.473366	0.11208
C	-2.692615	3.519396	0.55306
N	-2.617528	-0.748679	-1.060418

C	-2.807095	-2.115014	-1.643625
C	-1.530116	-2.558561	-2.374684
C	-3.559732	0.001313	-0.490472
C	-4.99838	-0.352141	-0.257729
C	-5.448924	-0.869363	0.973318
C	-6.812077	-1.139536	1.17118
C	-7.744024	-0.88165	0.15186
C	-7.30299	-0.354531	-1.073353
C	-5.938926	-0.095354	-1.276717
C	-3.927767	-2.099966	-2.717411
C	-3.156817	-3.147721	-0.550531
C	0.026657	1.931054	-0.455153
C	0.225351	3.203767	-0.594945
O	0.457357	4.369749	-0.648134
C	-0.789531	-0.035903	1.135176
C	0.823724	-0.369775	1.168993
B	1.085903	-1.769997	2.183802
B	0.5709	-1.304221	3.83389
B	-1.178921	-0.903997	3.773647
B	-0.5297	-2.260159	2.792655
B	-0.332433	-1.668607	1.132889
B	-1.715403	-1.119334	2.085997
B	-1.371632	0.509838	2.679403
B	0.043861	0.404386	3.780194
B	1.4445	-0.131002	2.781033
B	0.245437	0.982435	2.124046
C	3.840549	-2.817058	-2.26358
C	1.880366	-3.447654	-0.897624
C	3.271502	3.099239	0.377327
C	2.742519	3.061076	-2.191512
C	-4.789584	2.359604	1.233195
C	-4.393927	2.97533	-1.189974
H	0.489033	2.118455	1.869157
H	-0.483926	-2.314608	0.150579
H	-2.816272	-1.386623	1.708993
H	2.592306	0.203221	2.908747
H	-5.598434	0.309136	-2.234968
H	-2.269996	1.305986	2.724508
H	-8.020144	-0.14534	-1.876928
H	1.988174	-2.51095	1.931435
H	-8.809763	-1.088135	0.312069
H	-0.783961	-3.425404	2.977408
H	-7.145531	-1.545031	2.134443
H	-1.929555	-1.087675	4.701157

H	-4.736956	-1.046652	1.782726
H	0.206321	1.181797	4.688537
H	1.120592	-1.779565	4.797455
H	-1.266898	-1.853186	-3.180746
H	-1.715469	-3.557383	-2.810756
H	-0.680274	-2.616766	-1.690244
H	-4.933042	-2.035908	-2.275585
H	-3.880835	-3.041877	-3.294807
H	-3.779768	-1.256885	-3.418282
H	-2.38101	-3.17604	0.230045
H	-3.230761	-4.149954	-1.013397
H	-4.12665	-2.91743	-0.078048
H	-2.111747	3.17477	1.425005
H	-3.224547	4.450397	0.820526
H	-2.002094	3.764361	-0.264563
H	-5.64928	1.735065	0.946615
H	-5.171522	3.374753	1.449429
H	-4.338786	1.952472	2.155197
H	-3.650541	3.01156	-2.009726
H	-4.785277	3.99856	-1.035835
H	-5.235416	2.330703	-1.493424
H	5.964383	-0.767901	-2.014987
H	8.278206	-0.802475	-1.096355
H	8.687938	-0.207482	1.305036
H	6.757007	0.423122	2.777613
H	4.436359	0.444672	1.853789
H	5.114175	-2.66805	0.165262
H	4.194203	-4.194649	0.158699
H	3.69439	-2.8544	1.237243
H	3.179132	-2.45346	-3.071976
H	4.031717	-3.894899	-2.423158
H	4.804868	-2.288143	-2.326625
H	1.336581	-3.398252	0.05266
H	2.155333	-4.500931	-1.087056
H	1.223566	-3.10892	-1.713948
H	5.654052	2.197792	-0.560707
H	5.185377	3.548508	-1.616107
H	5.188815	1.879299	-2.267828
H	2.302322	2.833042	0.827989
H	3.320549	4.197713	0.270791
H	4.06731	2.774468	1.073937
H	3.145021	2.615286	-3.121928
H	2.938675	4.146499	-2.201676
H	1.655346	2.894255	-2.19198

Table S21. Cartesian geometry of **2'** in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	5.868445	-0.430382	-1.699504
C	5.076074	-0.336398	-0.541167
C	5.680517	-0.332634	0.731311
C	7.076336	-0.422755	0.840763
C	7.870101	-0.516414	-0.316518
C	7.264335	-0.519671	-1.585544
C	3.594121	-0.227474	-0.612587
N	2.899055	0.902713	-0.672837
C	3.3748	2.257736	-1.056601
C	4.662917	2.672998	-0.306087
Si	1.246338	-0.128784	-0.371785
N	2.723372	-1.260321	-0.530165
C	2.982077	-2.713869	-0.293184
C	3.004991	-2.985892	1.224058
O	-0.033689	-1.307037	-0.344418
Si	-1.304071	-0.118983	-0.255258
N	-2.978595	0.899472	-0.500667
C	-3.47771	2.259761	-0.833372
C	-2.382303	3.289588	-0.501243
N	-2.778106	-1.250499	-0.278957
C	-2.920307	-2.733483	-0.29974
C	-2.32284	-3.231543	-1.636073
C	-3.661515	-0.240516	-0.43387
C	-5.144402	-0.371236	-0.445913
C	-5.833637	-0.36161	0.782322
C	-7.23286	-0.455585	0.798887
C	-7.947729	-0.56161	-0.407971
C	-7.258516	-0.578279	-1.63297
C	-5.857414	-0.484174	-1.653377
C	-4.376264	-3.223237	-0.183971
C	-2.122224	-3.312808	0.88607
C	-0.070386	0.867464	-1.343581
C	-0.120506	1.451368	-2.508059
O	-0.164391	1.996052	-3.560281
C	-0.782633	0.442485	1.572388
C	0.890919	0.453996	1.496211
B	1.580433	0.003336	3.013251
B	1.065145	1.275922	4.173269
B	-0.732402	1.254935	4.253156
B	0.179742	-0.28432	4.108982

B	0.110797	-0.800142	2.424798
B	-1.320817	-0.030949	3.141595
B	-1.359158	1.673136	2.627191
B	0.111514	2.491957	3.26318
B	1.536722	1.702956	2.497076
B	0.042867	1.967501	1.574485
C	4.310203	-3.190983	-0.923719
C	1.843542	-3.518552	-0.956457
C	2.28774	3.29209	-0.710539
C	3.615887	2.271991	-2.583727
C	-4.739357	2.645241	-0.024837
C	-3.777539	2.321691	-2.349091
H	-0.006017	2.634982	0.596942
H	0.111591	-1.918636	2.026175
H	-2.33823	-0.668317	3.237657
H	2.546592	2.256313	2.155631
H	-5.314096	-0.506607	-2.605209
H	-2.407166	2.206252	2.379104
H	-7.812119	-0.666198	-2.576143
H	2.615611	-0.609224	3.017788
H	-9.042609	-0.632582	-0.393175
H	0.22671	-1.117116	4.980284
H	-7.767846	-0.443665	1.756701
H	-1.347556	1.544873	5.249688
H	-5.268524	-0.270188	1.717611
H	0.110909	3.669981	3.522509
H	1.762012	1.578288	5.110664
H	-2.908372	-2.83478	-2.488201
H	-2.355466	-4.337203	-1.673908
H	-1.275245	-2.898479	-1.730582
H	-4.854703	-2.868881	0.744986
H	-4.35179	-4.32803	-0.161902
H	-4.997331	-2.912117	-1.039906
H	-1.057662	-3.055932	0.791662
H	-2.230912	-4.413494	0.896383
H	-2.501928	-2.90771	1.841794
H	-2.180951	3.309757	0.580204
H	-2.735899	4.288906	-0.813782
H	-1.442481	3.068447	-1.027538
H	-5.639066	2.101411	-0.354209
H	-4.928221	3.725949	-0.164021
H	-4.577492	2.456528	1.052019
H	-2.872544	2.081299	-2.936008
H	-4.106736	3.342185	-2.622067

H	-4.582851	1.616973	-2.620773
H	5.39059	-0.44503	-2.685488
H	7.880919	-0.594642	-2.489977
H	8.961691	-0.586007	-0.229345
H	7.545704	-0.417251	1.832403
H	5.053199	-0.248639	1.626635
H	3.827438	-2.427194	1.706497
H	3.159138	-4.06577	1.409945
H	2.053149	-2.678573	1.687149
H	4.378156	-2.88942	-1.984934
H	4.327815	-4.295265	-0.876363
H	5.197814	-2.818285	-0.38903
H	0.869235	-3.268717	-0.513286
H	2.047943	-4.597077	-0.823993
H	1.799811	-3.297716	-2.039763
H	4.538401	2.518716	0.780864
H	4.840195	3.749522	-0.486874
H	5.554403	2.122702	-0.646616
H	1.324537	3.043732	-1.178434
H	2.616477	4.280455	-1.079855
H	2.141079	3.354356	0.378205
H	4.40511	1.55083	-2.862292
H	3.940171	3.280274	-2.903862
H	2.686827	2.017608	-3.126143

Table S22. Cartesian geometry of transition state (-70.7 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	5.334562	-1.187617	0.313191
C	4.146932	-1.947297	0.322283
C	4.204026	-3.337907	0.532845
C	5.443377	-3.967832	0.729842
C	6.628311	-3.211548	0.712914
C	6.571343	-1.822247	0.501475
C	2.851696	-1.221408	0.192272
N	2.249657	-0.57712	1.180422
C	2.34644	-0.825541	2.647237
C	1.778623	-2.236963	2.930198
N	2.133882	-1.027243	-0.948215
C	2.538601	-1.409918	-2.339121
C	1.418295	-1.038913	-3.326634
Si	0.97998	0.174545	-0.07833
O	-0.354171	-0.339044	0.989957
Si	-1.593718	-0.128373	-0.075374

N	-2.893434	-1.415007	-0.087624
C	-3.017457	-2.691314	-0.839237
C	-3.420936	-2.378522	-2.296669
N	-3.162128	0.683484	0.40759
C	-3.490514	2.015532	0.990957
C	-5.002177	2.224677	1.161122
C	-3.820765	-0.471898	0.222692
C	-5.282334	-0.701547	0.311411
C	-5.819417	-1.349147	1.441212
C	-7.201798	-1.575362	1.520034
C	-8.043987	-1.16941	0.469308
C	-7.50441	-0.528433	-0.659768
C	-6.123885	-0.287199	-0.739493
C	-2.902858	3.067397	0.0286
C	-2.785097	2.08632	2.36246
C	0.543191	3.12697	-0.625131
C	1.658753	1.974069	-0.102455
B	2.77277	2.608521	1.074455
B	3.696541	3.865653	0.216845
B	2.542052	5.119086	-0.33088
B	2.298952	4.313034	1.26218
B	1.021138	3.059754	1.027563
B	0.896405	4.607458	0.182495
B	1.401504	4.350176	-1.487825
B	3.136298	3.876673	-1.495362
B	3.279682	2.336285	-0.605948
B	1.837232	2.647289	-1.647991
C	-0.546323	0.345606	-1.411971
C	-0.853204	1.200054	-2.370276
O	-1.194302	1.894456	-3.247535
C	2.74106	-2.942059	-2.41954
C	3.82378	-0.677237	-2.779826
C	1.476447	0.202912	3.401255
C	3.796654	-0.718894	3.16872
C	-4.035626	-3.641315	-0.183294
C	-1.613828	-3.331332	-0.806968
H	1.650362	1.964976	-2.624233
H	0.261304	2.670463	1.878947
H	-0.021844	5.345435	0.458225
H	4.02287	1.426903	-0.866299
H	-5.153421	-1.669474	2.250889
H	0.849978	4.901829	-2.41033
H	-7.622618	-2.071831	2.403007
H	3.2046	1.894019	1.932149

H	-9.124061	-1.3514	0.531646
H	2.419963	4.879202	2.323505
H	-8.160247	-0.20969	-1.479166
H	2.849796	6.284687	-0.420641
H	-5.697123	0.222898	-1.611152
H	3.862261	4.124045	-2.429522
H	4.841616	4.097743	0.530961
H	-3.193131	1.322202	3.051921
H	-2.943396	3.086325	2.805714
H	-1.697025	1.933888	2.251154
H	-5.530666	2.166716	0.193804
H	-5.15714	3.235608	1.578589
H	-5.450194	1.490521	1.854163
H	-1.809322	2.93772	-0.125838
H	-3.066654	4.076225	0.448962
H	-3.405617	3.009973	-0.955655
H	-0.870301	-2.670909	-1.292358
H	-1.632083	-4.291868	-1.352764
H	-1.293877	-3.515978	0.235112
H	-4.423955	-1.914312	-2.329807
H	-3.44952	-3.309888	-2.892315
H	-2.688663	-1.687931	-2.755613
H	-3.802641	-3.783678	0.888138
H	-3.979568	-4.623883	-0.687057
H	-5.068217	-3.266449	-0.277958
H	3.277931	-3.923405	0.539961
H	5.48318	-5.051526	0.897298
H	7.59637	-3.704968	0.866547
H	7.492989	-1.227365	0.490794
H	5.274094	-0.103024	0.166059
H	4.43116	-1.548583	2.81789
H	3.77384	-0.752291	4.273972
H	4.248189	0.239272	2.856681
H	0.744828	-2.306509	2.544635
H	1.763864	-2.42396	4.020841
H	2.400409	-3.017329	2.456215
H	1.808373	1.233002	3.2062
H	1.568938	0.002627	4.484634
H	0.418863	0.111084	3.112069
H	3.675989	0.414972	-2.746803
H	4.069256	-0.972012	-3.817559
H	4.680409	-0.940023	-2.137499
H	0.458249	-1.507121	-3.050056
H	1.716853	-1.396899	-4.328851

H	1.279579	0.051767	-3.379749
H	3.645928	-3.270817	-1.885015
H	2.85329	-3.234441	-3.48017
H	1.862509	-3.470733	-2.00254

Table S23. Cartesian geometry of intermediate (-103.4 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-3.660264	-3.649908	-0.551681
C	-3.835667	-2.263269	-0.38069
C	-5.130463	-1.708209	-0.428859
C	-6.242148	-2.53931	-0.636432
C	-6.065982	-3.92361	-0.809249
C	-4.774051	-4.477028	-0.768193
C	-2.673788	-1.345261	-0.208437
N	-2.117937	-0.634502	-1.185959
C	-2.101766	-0.874939	-2.646991
C	-1.240696	0.241698	-3.272348
Si	-0.953504	0.200858	0.092919
N	-2.046351	-1.039854	0.951651
C	-2.38658	-1.451259	2.339273
C	-3.757498	-0.887673	2.767892
Si	1.585302	0.082812	0.228446
N	2.972156	-1.02549	0.779599
C	3.003752	-2.463894	1.16012
C	4.274203	-2.825828	1.952719
N	3.142199	0.625162	-0.63046
C	3.618172	1.939218	-1.153808
C	4.13385	2.786496	0.028374
C	3.834678	-0.341509	-0.000342
C	5.287981	-0.610383	-0.121601
C	6.151001	-0.276878	0.94132
C	7.524975	-0.539832	0.831907
C	8.036158	-1.150357	-0.327365
C	7.172793	-1.488899	-1.384672
C	5.800446	-1.213164	-1.287673
C	4.715831	1.755528	-2.219798
C	2.391689	2.615866	-1.791617
C	0.39754	1.148612	0.978181
C	0.286163	2.549313	1.220268
O	1.119629	3.379576	1.590882
O	0.441262	-0.818677	-0.578302
C	-1.145121	3.065514	0.81471
C	-2.083333	1.874045	0.121185

B	-2.462413	2.444247	1.714137
B	-2.080019	4.191233	1.715021
B	-3.142079	4.973858	0.5039
B	-2.722551	4.305914	-1.112121
B	-1.433295	4.606584	0.101595
B	-1.42494	3.111336	-0.886229
B	-3.103226	2.55441	-1.087681
B	-3.738304	2.130199	0.513108
B	-3.775124	3.623669	1.515322
B	-4.174246	3.702954	-0.235519
C	2.898089	-3.313746	-0.125024
C	1.763534	-2.700488	2.040303
C	-2.391508	-2.993016	2.459101
C	-1.285065	-0.907222	3.268905
C	-1.432603	-2.239133	-2.9328
C	-3.519195	-0.838969	-3.256595
H	1.975931	1.987892	-2.601885
H	2.68772	3.591478	-2.216379
H	1.608667	2.795314	-1.037365
H	-2.783464	4.944785	-2.133675
H	-3.517189	6.110686	0.650446
H	-1.598282	4.666222	2.707548
H	-4.123369	-1.703351	-2.933721
H	-3.435792	-0.871441	-4.359229
H	-4.042452	0.090103	-2.969996
H	-5.253075	-0.625849	-0.309561
H	3.333523	2.929924	0.778721
H	4.448379	3.781394	-0.339109
H	5.009566	2.299807	0.498573
H	-0.308956	-1.350297	3.015748
H	-1.534355	-1.173025	4.312497
H	-1.187121	0.185929	3.191357
H	-2.233331	1.748008	2.655049
H	5.740049	0.185861	1.845814
H	5.6607	1.389666	-1.785099
H	4.914463	2.736328	-2.689569
H	4.384437	1.052842	-3.007195
H	-7.247862	-2.10224	-0.669877
H	-0.512258	5.368618	-0.009348
H	5.121801	-1.458983	-2.112311
H	-0.52509	2.818157	-1.621539
H	-4.451769	1.174222	0.663552
H	1.811828	-2.08026	2.953818
H	1.712394	-3.763793	2.336762

H	0.844648	-2.445072	1.482714
H	-3.760858	0.212364	2.706726
H	-3.966846	-1.18705	3.812131
H	-4.564627	-1.282798	2.126916
H	-6.935524	-4.571621	-0.977246
H	-3.388303	1.893337	-2.045417
H	-2.651636	-4.075858	-0.51249
H	-4.592636	3.769912	2.39012
H	-5.295489	3.913432	-0.628786
H	-1.685427	1.233273	-3.089088
H	-1.169837	0.081794	-4.363716
H	-0.222032	0.216434	-2.845452
H	8.197776	-0.27165	1.655805
H	-3.252334	-3.444105	1.939773
H	-2.456374	-3.270644	3.527885
H	-1.45711	-3.415222	2.043847
H	-0.439898	-2.271388	-2.450716
H	-1.316365	-2.375861	-4.024929
H	-2.054841	-3.06674	-2.54876
H	-4.632348	-5.556524	-0.904553
H	5.181166	-2.777097	1.327645
H	4.173225	-3.860552	2.329926
H	4.398754	-2.148776	2.817849
H	7.570132	-1.96441	-2.28993
H	9.109919	-1.36111	-0.40781
H	1.98933	-3.030304	-0.687281
H	2.843599	-4.387986	0.134031
H	3.786291	-3.156616	-0.76496

Table S24. Cartesian geometry of transition state (-98.8 kcal/mol) in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-6.371155	-4.396577	0.848101
C	-6.099947	-3.425297	-0.136543
C	-6.824402	-3.431476	-1.344097
C	-7.811336	-4.404835	-1.567097
C	-8.075594	-5.378163	-0.587576
C	-7.35319	-5.372849	0.618848
C	-5.074583	-2.382078	0.151917
N	-3.774123	-2.40761	-0.218072
C	-3.010936	-3.450867	-0.947172
C	-2.908898	-4.745249	-0.113987
Si	-3.417771	-0.819926	0.677962
O	-3.86825	0.477117	-0.468348

Si	-2.299048	1.1289	-0.603856
N	-2.272994	2.970469	-0.372133
C	-2.543115	3.153033	-1.686638
C	-2.81969	4.460012	-2.341513
C	-1.787094	5.12862	-3.026485
C	-2.028913	6.385862	-3.600974
C	-3.301061	6.975961	-3.499708
C	-4.33492	6.303375	-2.82443
C	-4.095673	5.04841	-2.242932
C	-1.718608	-0.028715	0.640474
C	-0.892378	-0.004716	1.771517
C	-1.534538	-0.839962	2.943397
B	-0.665452	-1.888914	3.98948
B	-1.678694	-2.520714	2.656841
C	-3.036222	-1.448396	2.553913
B	-2.942236	-0.138462	3.661142
B	-3.047069	-0.863621	5.286174
B	-3.245057	-2.641285	5.077373
B	-4.043457	-1.509978	3.948555
B	-3.269786	-2.972569	3.312376
B	-1.773238	-3.273302	4.261771
B	-1.635828	-1.961338	5.489296
B	-1.450031	-0.4105	4.609812
O	0.172245	0.605422	2.038572
Si	2.376609	1.115081	0.627798
N	2.584969	1.952128	2.290625
C	2.943762	1.524846	3.663691
C	1.938521	2.100211	4.677446
N	2.417071	2.962972	0.377915
C	2.476	3.876185	-0.786444
C	2.177941	5.345818	-0.424305
C	2.648845	3.144586	1.696046
C	2.936716	4.442417	2.360872
C	1.900967	5.13364	3.01724
C	2.159132	6.382348	3.604817
C	3.449349	6.937269	3.544615
C	4.484982	6.241942	2.894571
C	4.229669	4.997438	2.29862
C	3.883746	3.76885	-1.413584
C	1.430351	3.372649	-1.799057
C	1.735948	-0.022362	-0.599685
Si	3.424262	-0.851968	-0.67862
N	5.275987	-1.379855	-0.887959
C	5.029102	-2.480957	-0.183446

C	6.015286	-3.565889	0.092123
C	6.236278	-4.547141	-0.895485
C	7.173985	-5.567796	-0.673926
C	7.901764	-5.609758	0.528275
C	7.687561	-4.627905	1.511382
C	6.745231	-3.609731	1.295776
O	3.913642	0.412326	0.483061
C	0.881477	0.008225	-1.70565
O	-0.180859	0.631208	-1.957448
C	1.488054	-0.810217	-2.899927
C	3.006118	-1.408267	-2.570839
B	1.661725	-2.495974	-2.661367
B	0.599791	-1.845119	-3.942365
B	1.518946	-1.860291	-5.474901
B	2.919668	-0.746441	-5.287441
B	1.336828	-0.336186	-4.548239
B	2.858592	-0.067388	-3.642075
B	3.969136	-1.414541	-3.998627
B	3.235976	-2.906219	-3.379609
B	1.715822	-3.203639	-4.289425
B	3.1507	-2.526023	-5.133532
N	3.727818	-2.467715	0.184464
C	2.940693	-3.482128	0.930711
C	2.808802	-4.785875	0.115774
C	4.38481	1.969143	3.998798
C	2.878748	-0.014995	3.670005
C	3.592437	-3.782626	2.301097
C	1.550869	-2.881546	1.203788
C	6.5591	-0.694837	-1.152777
C	6.22021	0.621602	-1.88248
C	7.243929	-0.338933	0.187372
C	7.496749	-1.55561	-2.024483
N	-2.519088	1.960499	-2.277231
C	-2.997829	1.533981	-3.612741
C	-2.124564	2.159613	-4.717988
C	-4.483382	1.92245	-3.780472
C	-2.873643	0.000578	-3.668162
N	-5.284426	-1.285212	0.875959
C	-6.536957	-0.54138	1.126327
C	-7.140405	-0.083735	-0.221827
C	-6.15558	0.712274	1.941985
C	-7.560022	-1.383411	1.917056
C	-3.667489	-3.75571	-2.313742
C	-1.609025	-2.880863	-1.222591

C	-2.292528	3.915185	0.766981
C	-1.461749	3.278261	1.896449
C	-3.751642	4.088449	1.243996
C	-1.679283	5.280179	0.399443
H	-0.713622	5.120832	-0.102262
H	-1.507564	5.85606	1.327647
H	-2.327977	5.881799	-0.257751
H	-6.607505	-2.676581	-2.107798
H	-1.923433	2.338705	2.239137
H	-1.419503	3.973906	2.754816
H	-0.43737	3.043672	1.561535
H	-1.66628	-1.975922	-1.848283
H	-1.014164	-3.634064	-1.765268
H	-1.081608	-2.607657	-0.296996
H	1.679035	2.357663	-2.141045
H	1.424413	4.039881	-2.680439
H	0.422518	3.338942	-1.350761
H	-5.810931	-4.373948	1.789426
H	3.374879	-0.093431	-6.193999
H	0.957617	-2.016985	-6.531221
H	-0.582	-1.936249	-3.793103
H	-1.220485	-2.963766	1.653702
H	-8.845369	-6.140065	-0.764334
H	7.844098	-2.449754	-1.479374
H	8.384142	-0.957902	-2.306652
H	6.979721	-1.876965	-2.946107
H	5.670804	-4.500655	-1.832722
H	1.272905	5.418233	0.19537
H	2.013616	5.909662	-1.360855
H	3.00731	5.824463	0.120832
H	1.625801	-1.967011	1.813626
H	0.949445	-3.616584	1.763258
H	1.019808	-2.620734	0.276961
H	-0.799715	4.662407	-3.094745
H	-4.365271	4.568817	0.460894
H	-3.782923	4.722675	2.15026
H	-4.19185	3.104313	1.487778
H	-3.891976	-3.309771	5.845745
H	-8.373183	-4.404125	-2.509619
H	1.236635	-2.966841	-1.656567
H	0.898143	4.694508	3.051588
H	-1.8184	-0.297589	-3.588957
H	-3.274995	-0.360305	-4.632693
H	-3.453883	-0.460594	-2.848603

H	4.658295	4.085149	-0.68994
H	3.951793	4.41472	-2.309552
H	4.088364	2.727854	-1.71877
H	7.338263	-6.33049	-1.445317
H	0.525908	-1.944687	3.883927
H	0.653697	0.614047	-4.81246
H	5.029074	4.449005	1.786878
H	-3.287945	0.946729	3.283523
H	3.198427	1.012304	-3.243598
H	3.905008	-3.751169	-2.847622
H	-0.80002	0.53896	4.939316
H	1.857106	-0.347232	3.425262
H	3.146017	-0.391399	4.673648
H	3.587341	-0.428367	2.929057
H	2.355048	-4.586012	-0.869196
H	2.166432	-5.499895	0.664926
H	3.796556	-5.255749	-0.036909
H	8.63609	-6.40715	0.699109
H	-3.908271	-3.813053	2.737242
H	-3.539137	-0.240611	6.194735
H	-5.223891	-1.352612	3.821628
H	-4.898116	4.516405	-1.720001
H	-7.557511	-6.128617	1.387529
H	5.15084	-1.24284	-3.909493
H	6.566556	-2.848858	2.063173
H	-1.35089	-4.391027	4.43177
H	-1.220965	6.905946	-4.130634
H	1.30269	-4.321796	-4.476658
H	-3.488395	7.958789	-3.950214
H	3.781381	-3.163648	-5.940381
H	-7.931224	-2.234086	1.320901
H	-8.425001	-0.747363	2.184636
H	-7.10526	-1.770384	2.846423
H	5.708442	0.430302	-2.839537
H	7.152596	1.179114	-2.087227
H	5.570111	1.2413	-1.24137
H	-6.378481	0.475908	-0.793253
H	-8.01599	0.568025	-0.037689
H	-7.477856	-0.951559	-0.815031
H	-5.719606	0.435783	2.915467
H	-7.058467	1.325026	2.119037
H	-5.423387	1.315297	1.376184
H	1.35009	6.922864	4.111722
H	-1.106598	-2.138077	6.559106

H	4.525308	-4.360053	2.198417
H	2.887896	-4.380262	2.908651
H	3.80155	-2.840549	2.840951
H	-2.255114	3.254577	-4.765695
H	-2.413994	1.734889	-5.697339
H	-1.062848	1.920401	-4.529626
H	-2.439996	-4.543599	0.863156
H	-2.293152	-5.486012	-0.658279
H	-3.908998	-5.182569	0.05484
H	-4.616712	-4.304739	-2.203894
H	-2.97821	-4.382204	-2.909734
H	-3.84948	-2.817411	-2.869729
H	6.534046	0.21598	0.826762
H	8.133598	0.291398	-0.003363
H	7.577456	-1.24985	0.713137
H	8.252934	-4.65572	2.451331
H	2.035746	3.197224	4.754012
H	2.129947	1.666604	5.676613
H	0.916267	1.838147	4.361169
H	5.493646	6.671194	2.849857
H	-5.331314	6.756647	-2.750566
H	3.649525	7.912304	4.006384
H	5.080809	1.621524	3.212466
H	4.687267	1.518924	4.962682
H	4.462707	3.065953	4.095472
H	-5.073661	1.499022	-2.946886
H	-4.864881	1.513455	-4.734766
H	-4.61414	3.018463	-3.800593

Table S25. Cartesian geometry of **2** in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	4.597032	6.754263	2.823451
C	3.283634	6.459819	3.230319
C	2.687148	5.245105	2.858463
C	3.400342	4.320519	2.071882
C	4.717912	4.61386	1.670101
C	5.314456	5.827124	2.046526
C	2.75469	3.0428	1.659065
N	2.199921	2.790732	0.444071
C	2.108507	3.719276	-0.719861
C	3.428524	3.730148	-1.520984
Si	1.916724	0.948964	0.892903
C	1.425538	0.029075	-0.671894

C	0.592648	-0.076163	-1.735441
C	1.16737	-0.81828	-2.951431
B	2.500947	0.005549	-3.684516
B	3.659487	-1.276592	-4.082452
B	2.881042	-2.387605	-5.251464
B	1.483779	-3.155222	-4.420716
B	2.995103	-2.81591	-3.510746
B	1.414532	-2.5032	-2.77157
B	0.3104	-1.857719	-4.019636
B	0.980269	-0.297471	-4.583851
B	1.218349	-1.782855	-5.558256
B	2.573709	-0.617585	-5.347241
Si	3.101973	-0.861216	-0.696883
C	2.707958	-1.359344	-2.647204
O	0.606046	0.45545	1.984976
C	-0.59277	-0.076459	1.735467
C	-1.167523	-0.818748	2.951326
B	-0.980196	-0.298338	4.583844
B	-1.218413	-1.78392	5.557917
B	-1.484145	-3.155987	4.420078
B	-2.995495	-2.816228	3.510323
B	-3.659602	-1.276944	4.082441
B	-2.573616	-0.618397	5.347295
B	-2.500904	0.005121	3.684706
C	-2.708218	-1.359503	2.647097
B	-1.414946	-2.503588	2.771078
B	-0.310612	-1.858557	4.019203
O	3.399478	0.09632	0.744878
N	2.640099	1.961513	2.402456
C	3.201882	1.64215	3.734119
C	4.71144	1.965639	3.801
N	3.555483	-2.568588	-0.080631
C	2.909203	-3.686563	0.641032
C	3.699644	-4.079962	1.910756
N	4.976284	-1.185197	-0.971009
C	6.186021	-0.365448	-1.177344
C	6.811051	-0.02044	0.195491
C	4.844759	-2.393884	-0.424349
C	5.940476	-3.396786	-0.282457
C	6.194005	-4.280492	-1.350513
C	7.246296	-5.205677	-1.261696
C	8.051838	-5.250637	-0.110573
C	7.799465	-4.369518	0.955846
C	6.746357	-3.445346	0.871587

C	-1.425654	0.029011	0.671935
Si	-1.916753	0.949288	-0.892654
N	-2.64009	1.962092	-2.40208
C	-3.201619	1.643125	-3.733922
C	-4.711045	1.967183	-3.801182
Si	-3.102236	-0.861005	0.696859
N	-4.976612	-1.184867	0.970907
C	-6.186325	-0.36513	1.17741
C	-5.704489	0.941539	1.830846
O	-3.399679	0.096911	-0.744656
N	-3.555892	-2.56823	0.080355
C	-2.909745	-3.686085	-0.641616
C	-3.70033	-4.079132	-1.911359
O	-0.606118	0.455908	-1.984866
N	-2.199394	2.791068	-0.443707
C	-2.108279	3.719256	0.720531
C	-3.428529	3.729838	1.521248
C	-2.754183	3.04339	-1.65866
C	-3.399434	4.321346	-2.071366
C	-2.685807	5.2459	-2.857591
C	-3.281876	6.460857	-3.229316
C	-4.595284	6.755573	-2.822674
C	-5.313141	5.828463	-2.046115
C	-4.717014	4.614953	-1.669817
C	-4.84516	-2.393486	0.424098
C	-5.940939	-3.396288	0.281957
C	-6.746761	-3.444534	-0.87214
C	-7.799913	-4.368631	-0.956673
C	-8.052382	-5.249992	0.109521
C	-7.24689	-5.205358	1.26069
C	-6.194554	-4.280249	1.349783
C	1.541031	-3.157516	1.09436
C	2.751419	-4.917224	-0.275869
C	-1.771424	5.168216	0.286845
C	-0.996417	3.213511	1.65425
C	0.996387	3.213856	-1.653454
C	1.771807	5.168077	-0.285539
C	-1.541572	-3.157022	-1.094933
C	-2.751964	-4.916971	0.27499
C	-7.217726	-1.061409	2.088321
C	-6.811386	-0.01993	-0.195363
C	7.217448	-1.061596	-2.088326
C	5.704159	0.941292	-1.83061
C	3.018177	0.127683	3.96292

C	2.430968	2.411724	4.828691
B	-2.881219	-2.388346	5.251128
C	-3.018372	0.128621	-3.96284
C	-2.430147	2.412607	-4.828163
H	-0.977156	5.178304	-0.476171
H	-1.41315	5.727208	1.171082
H	-2.648301	5.702013	-0.112716
H	-6.537648	-2.765283	-1.705322
H	-1.265152	2.240587	2.085734
H	-0.867606	3.931692	2.484662
H	-0.03993	3.120038	1.120416
H	-1.66364	-2.332182	-1.816398
H	-0.968852	-3.96208	-1.584046
H	-0.962842	-2.775697	-0.241744
H	1.265057	2.241143	-2.085448
H	0.867249	3.932391	-2.483508
H	0.040087	3.120054	-1.119358
H	-5.573481	-4.225845	2.250356
H	2.991174	0.083365	-6.235693
H	0.652592	-1.926504	-6.613659
H	-0.868752	-1.997926	-3.869068
H	-1.020858	-3.016689	1.775442
H	-8.876407	-5.971631	0.042346
H	7.649302	-1.955	-1.606677
H	8.041061	-0.355688	-2.306473
H	6.748095	-1.362426	-3.042034
H	5.57289	-4.22584	-2.251043
H	0.977639	5.177881	0.477591
H	1.413453	5.727483	-1.169481
H	2.64878	5.701634	0.114145
H	1.663109	-2.332728	1.815884
H	0.968291	-3.962596	1.583413
H	0.962322	-2.77612	0.241186
H	-1.658383	5.013955	-3.159902
H	-4.28335	4.013442	0.883871
H	-3.35335	4.463775	2.346151
H	-3.617381	2.73955	1.9659
H	-3.530747	-2.973715	6.082108
H	-8.423248	-4.402014	-1.859033
H	1.020275	-3.016525	-1.776114
H	1.659732	5.013371	3.160972
H	-1.951511	-0.138697	-3.956856
H	-3.447771	-0.142687	-4.94473
H	-3.532591	-0.441244	-3.169071

H	4.283552	4.013559	-0.883807
H	3.353048	4.46437	-2.345605
H	3.617275	2.740028	-1.966049
H	7.439294	-5.88944	-2.097754
H	0.868511	-1.998876	3.868514
H	0.252652	0.628742	-4.811194
H	5.276101	3.880634	1.077196
H	-2.789792	1.088324	3.262595
H	2.789971	1.088615	-3.26215
H	3.699314	-3.648832	-3.009552
H	-0.252413	0.627714	4.811334
H	1.951231	-0.139286	3.95715
H	3.447708	-0.14385	4.94469
H	3.53204	-0.442279	3.168992
H	2.151964	-4.670467	-1.167409
H	2.248274	-5.731519	0.279207
H	3.740977	-5.281128	-0.606273
H	8.87583	-5.972332	-0.043614
H	-3.699881	-3.648927	3.009009
H	-2.990904	0.082405	6.235948
H	-4.832304	-1.044797	3.983993
H	-5.275524	3.881753	-1.077179
H	-7.439961	-5.889315	2.096573
H	4.83221	-1.044621	-3.983834
H	6.537339	-2.766263	1.704928
H	-1.118156	-4.28423	4.640847
H	-2.718947	7.180537	-3.83689
H	1.117634	-4.283357	-4.64177
H	-5.060512	7.705882	-3.11357
H	3.530548	-2.972882	-6.082525
H	-7.649547	-1.954785	1.606592
H	-8.041367	-0.355551	2.306528
H	-6.748368	-1.362308	3.042005
H	5.211692	0.744556	-2.797904
H	6.559484	1.621007	-1.997642
H	4.989598	1.439738	-1.153992
H	-6.028131	0.384833	-0.86213
H	-7.612657	0.73281	-0.065778
H	-7.257331	-0.914867	-0.661969
H	-5.211917	0.744697	2.798064
H	-6.559859	1.621149	1.998082
H	-4.990053	1.440172	1.154239
H	2.721035	7.179519	3.838175
H	-0.652586	-1.927899	6.613238

H	4.630359	-4.619732	1.67293
H	3.068469	-4.746652	2.527241
H	3.93973	-3.180548	2.507478
H	-2.605312	3.49996	-4.752721
H	-2.767643	2.077227	-5.827221
H	-1.347715	2.20919	-4.73793
H	-2.152357	-4.670488	1.166504
H	-2.248983	-5.731189	-0.280346
H	-3.741511	-5.280851	0.605445
H	-4.631043	-4.61893	-1.673585
H	-3.069241	-4.745687	-2.528077
H	-3.940436	-3.17955	-2.507821
H	6.027791	0.384246	0.862297
H	7.61234	0.732303	0.066027
H	7.25697	-0.915451	0.661983
H	8.422848	-4.403146	1.858163
H	2.606397	3.499038	4.753345
H	2.76868	2.076121	5.827603
H	1.348449	2.208615	4.738771
H	6.342832	6.048493	1.734423
H	-6.341525	6.05005	-1.734194
H	5.062589	7.704375	3.114463
H	5.237018	1.480914	2.957453
H	5.12419	1.569295	4.747737
H	4.906538	3.050648	3.773177
H	-5.237043	1.482601	-2.957817
H	-5.123694	1.571073	-4.74806
H	-4.905722	3.052267	-3.773333

Table S26. Cartesian geometry of dimethylphenyl isocyanide in Figure 3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-0.237355	-1.245729	0.000016
C	0.445187	0.000237	0.000043
C	-0.2386	1.245507	0.000005
C	-1.644989	1.216343	-0.000011
C	-2.344203	-0.001164	0.000011
C	-1.64376	-1.217984	0.000004
N	1.831037	0.0009	0.00002
C	3.01921	0.001467	-0.000007
C	0.53209	2.543451	-0.000019
C	0.534635	-2.5429	-0.000025
H	-2.192637	2.167491	-0.000037
H	-3.441507	-0.001732	0.000004

H	-2.190477	-2.169664	-0.000008
H	1.193105	2.612174	-0.886494
H	-0.152887	3.409562	-0.000434
H	1.192522	2.612576	0.886864
H	1.195448	-2.61121	0.886631
H	-0.149481	-3.409695	-0.000018
H	1.195372	-2.611168	-0.886744

Table S27. Cartesian geometry of transition state (3.3 kcal/mol) in Figure 3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	5.99498	0.804788	-0.073904
C	5.170517	-0.338252	-0.051101
C	5.737991	-1.625485	-0.144521
C	7.128502	-1.763652	-0.274634
C	7.953257	-0.624577	-0.29639
C	7.384456	0.658495	-0.190126
C	3.697226	-0.219315	0.032061
N	2.938738	-0.570632	1.081548
C	3.281569	-0.782473	2.514842
C	3.53258	-2.281349	2.771882
N	2.867098	0.132867	-0.972746
C	3.152532	0.668685	-2.327173
C	3.390102	2.189704	-2.235259
Si	1.394395	-0.287785	0.097457
C	0.711488	-2.019961	-0.458605
B	-0.360773	-1.997749	-1.84364
B	-1.816866	-2.890953	-1.334336
B	-0.545042	-3.683644	-2.339779
B	1.055348	-3.072836	-1.770894
B	1.273967	-3.593065	-0.076855
B	0.004781	-2.814968	0.904466
B	-0.178622	-4.519753	0.422267
B	0.465919	-4.689686	-1.247217
B	-1.306331	-4.574655	-0.975296
B	-1.587727	-3.404362	0.353069
C	-0.967687	-1.909617	-0.226617
Si	-1.446408	-0.090597	0.272267
N	-3.087582	-0.30124	1.160288
C	-3.541356	-0.663138	2.521473
C	-2.298742	-1.18855	3.266306
C	0.234762	1.177703	1.025552
N	0.670595	2.416655	1.464296
C	0.668441	3.782289	1.375004

C	-0.182161	4.526701	0.479735
C	-0.041554	5.922432	0.372535
C	0.87581	6.630815	1.165553
C	1.606421	5.927068	2.142949
C	1.493924	4.5359	2.287983
C	-1.096096	3.786056	-0.471753
C	2.399733	3.799551	3.24835
N	-2.862843	0.062361	-0.985958
C	-3.077242	0.607753	-2.34989
C	-1.868854	1.510407	-2.661543
C	-3.750447	-0.340127	-0.062078
C	-5.198295	-0.570243	-0.281231
C	-5.598879	-1.757997	-0.929275
C	-6.961609	-2.011635	-1.145273
C	-7.928766	-1.080565	-0.724384
C	-7.527847	0.107283	-0.085357
C	-6.167097	0.363875	0.139272
C	1.895811	0.409814	-3.172291
C	4.351231	-0.03798	-2.997411
C	2.070801	-0.296836	3.339915
C	4.51557	0.048771	2.923306
C	-4.636871	-1.748523	2.494514
C	-4.059063	0.600191	3.245665
C	-4.358517	1.465231	-2.446849
C	-3.152153	-0.549916	-3.367704
H	-0.409498	-1.018922	-2.519937
H	0.205468	-2.380614	1.997983
H	2.377659	-3.701964	0.385089
H	-2.890419	-2.505145	-1.711784
H	5.542569	1.798403	0.014703
H	2.004644	-2.82928	-2.468561
H	8.026245	1.548266	-0.198431
H	-2.501162	-3.389395	1.129775
H	9.040487	-0.736359	-0.393175
H	-0.111918	-5.387978	1.255784
H	7.569581	-2.764722	-0.358623
H	1.006187	-5.701038	-1.61988
H	5.085777	-2.506464	-0.131432
H	-0.736945	-3.947889	-3.500062
H	-2.05741	-5.500153	-1.157805
H	1.827943	0.751335	3.085418
H	2.307589	-0.392567	4.415666
H	1.178623	-0.90775	3.120863
H	5.4485	-0.341627	2.483862

H	4.613853	0.010158	4.023666
H	4.384965	1.103462	2.620318
H	2.642887	-2.875097	2.499636
H	3.750751	-2.441361	3.844588
H	4.394904	-2.64407	2.182769
H	1.686287	-0.669953	-3.247032
H	2.04241	0.817497	-4.188377
H	1.029425	0.915019	-2.714525
H	5.316777	0.249278	-2.551439
H	4.37151	0.249471	-4.065048
H	4.240919	-1.136215	-2.933377
H	2.53435	2.694257	-1.752213
H	3.522167	2.601938	-3.25356
H	4.300356	2.410159	-1.652026
H	-5.849119	1.29604	0.61864
H	-8.278897	0.839926	0.235691
H	-8.994089	-1.279276	-0.895953
H	-7.269115	-2.939709	-1.643148
H	-4.837798	-2.480571	-1.246912
H	-5.578876	-1.36355	2.068464
H	-4.838894	-2.081704	3.529583
H	-4.309035	-2.620555	1.902313
H	-3.295478	1.399122	3.216442
H	-4.278548	0.357989	4.30271
H	-4.987561	0.972568	2.780353
H	-1.859839	-2.043305	2.728771
H	-2.586326	-1.515842	4.281535
H	-1.530328	-0.397884	3.346436
H	-5.275395	0.855524	-2.397852
H	-4.350569	1.991619	-3.419075
H	-4.384571	2.223052	-1.643071
H	-2.223935	-1.14515	-3.35055
H	-3.296523	-0.141748	-4.385838
H	-4.002555	-1.215162	-3.134487
H	-1.834215	2.393864	-1.998225
H	-1.928778	1.851888	-3.711088
H	-0.932941	0.948338	-2.527084
H	2.283293	6.473357	2.816463
H	0.984637	7.718058	1.061778
H	-0.700791	6.468581	-0.31982
H	2.869007	2.932751	2.75091
H	3.181261	4.468174	3.657391
H	1.820963	3.385185	4.101195
H	-0.727773	3.775725	-1.515861

H	-1.212353	2.735776	-0.146424
H	-2.098467	4.258004	-0.497674

Table S28. Cartesian geometry of **3'** in Figure 3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	5.847836	-1.546788	0.047979
C	5.179887	-0.304521	0.020851
C	5.917885	0.896139	0.009638
C	7.319725	0.850407	0.016303
C	7.988707	-0.387252	0.029288
C	7.250284	-1.584502	0.045152
C	3.698657	-0.298002	0.022951
N	2.913529	-0.593199	1.070476
C	3.208169	-0.703143	2.524674
C	4.379161	0.2103	2.941289
Si	1.403681	-0.394441	0.021953
C	0.107224	0.726054	0.471846
N	0.846933	1.840478	0.855242
C	0.63986	-2.105419	-0.436777
B	-0.408742	-2.094997	-1.823513
B	-1.884471	-2.936828	-1.29948
B	-0.636269	-3.799901	-2.263698
B	0.970466	-3.218717	-1.706295
B	1.16694	-3.682326	0.007641
B	-0.087096	-2.836556	0.953862
B	-0.31455	-4.549801	0.529902
B	0.337546	-4.797137	-1.127954
B	-1.431635	-4.619319	-0.875156
B	-1.687177	-3.395759	0.409302
C	-1.011645	-1.929323	-0.207221
Si	-1.469876	-0.084365	0.240668
N	-3.078758	-0.260626	1.194602
C	-3.499204	-0.567065	2.580705
C	-3.920264	0.734351	3.299416
N	-2.904148	0.357819	-0.875432
C	-3.091255	0.965291	-2.217377
C	-3.422854	-0.129277	-3.252408
C	-3.790237	0.088707	0.104107
C	-5.26288	0.114579	-0.02253
C	-5.895567	-0.941503	-0.716257
C	-7.291006	-0.952288	-0.854407
C	-8.06476	0.090305	-0.310874
C	-7.433762	1.147442	0.371518

C	-6.039253	1.16243	0.51785
C	-1.75731	1.647834	-2.584953
C	-4.202209	2.037436	-2.210183
C	-2.265939	-1.150912	3.298756
C	-4.650946	-1.592805	2.613958
N	2.893539	-0.059121	-1.033959
C	3.223087	0.297182	-2.437631
C	4.354837	-0.589934	-2.997209
C	3.602861	1.790925	-2.522307
C	1.950968	0.063762	-3.269228
C	3.521936	-2.173629	2.865588
C	1.939977	-0.23468	3.269349
H	-0.431793	-1.137025	-2.531625
H	0.118458	-2.364672	2.030095
H	2.264318	-3.796868	0.484905
H	-2.944381	-2.5467	-1.703756
H	5.389329	1.854253	0.027627
H	1.933574	-3.029003	-2.400453
H	7.892188	1.786304	0.016765
H	-2.614342	-3.332079	1.165766
H	9.085471	-0.41878	0.03156
H	-0.279356	-5.38909	1.394337
H	7.768196	-2.551671	0.056095
H	0.854317	-5.833064	-1.464415
H	5.264181	-2.474764	0.054743
H	-0.830238	-4.097546	-3.4155
H	-2.213242	-5.524467	-1.029343
H	1.665231	0.785529	2.941973
H	2.132587	-0.25115	4.35767
H	1.089919	-0.903932	3.055494
H	5.348416	-0.144115	2.553701
H	4.435796	0.219441	4.045288
H	4.202482	1.242989	2.590192
H	2.683517	-2.827861	2.567108
H	3.683166	-2.278219	3.95508
H	4.437019	-2.509274	2.343282
H	1.674918	-1.002751	-3.273695
H	2.130075	0.388356	-4.309832
H	1.111022	0.651272	-2.859693
H	5.325775	-0.374293	-2.521529
H	4.45422	-0.396722	-4.081479
H	4.113681	-1.659414	-2.852964
H	2.793363	2.422515	-2.114525
H	3.770906	2.06411	-3.580985

H	4.530072	1.997832	-1.962894
H	-5.544229	2.00038	1.020158
H	-8.031316	1.969553	0.785263
H	-9.156275	0.080863	-0.421274
H	-7.776962	-1.779895	-1.386233
H	-5.287316	-1.756151	-1.126397
H	-5.580978	-1.176283	2.191873
H	-4.846249	-1.878838	3.664504
H	-4.378018	-2.501	2.047722
H	-3.11339	1.487284	3.240247
H	-4.125127	0.518615	4.364991
H	-4.837227	1.156366	2.854613
H	-1.966164	-2.107269	2.842398
H	-2.509976	-1.327018	4.361833
H	-1.413135	-0.44868	3.242197
H	-5.206794	1.597515	-2.099358
H	-4.170291	2.581112	-3.172381
H	-4.035627	2.765348	-1.395131
H	-2.621429	-0.886197	-3.287201
H	-3.52604	0.32765	-4.254607
H	-4.373515	-0.630286	-2.997165
H	-1.506137	2.45703	-1.87595
H	-1.835965	2.073161	-3.60202
H	-0.933773	0.915646	-2.569079
C	0.624796	3.150855	0.551835
C	1.795095	3.984893	0.374621
C	1.660171	5.322039	-0.020212
C	0.394493	5.912545	-0.208956
C	-0.748275	5.146351	0.07157
C	-0.661887	3.799869	0.469949
C	3.15557	3.388079	0.645215
H	2.570994	5.918306	-0.179037
H	0.304996	6.960226	-0.523117
H	-1.744086	5.613059	0.019033
C	-1.902106	3.083366	0.949802
H	3.275181	2.429329	0.110019
H	3.967011	4.082573	0.352286
H	3.27042	3.145282	1.722859
H	-2.377948	2.467719	0.161626
H	-1.65578	2.412697	1.794231
H	-2.668687	3.804697	1.29379

Table S29. Cartesian geometry of transition state (-15.1 kcal/mol) in Figure 3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
C	-6.211512	0.971912	0.431901
C	-5.599034	-0.22812	0.018952
C	-6.391573	-1.314609	-0.405695
C	-7.788842	-1.201029	-0.410398
C	-8.401776	-0.002259	-0.000616
C	-7.611543	1.082202	0.418408
C	-4.118017	-0.349088	-0.008267
N	-3.345231	-0.113592	-1.07998
C	-3.69289	0.584548	-2.346517
C	-2.473173	0.448472	-3.273412
Si	-1.780185	-0.533585	-0.086566
C	-1.216999	-2.293622	-0.623274
B	-2.000436	-3.273165	-1.796706
B	-1.493791	-4.955883	-1.423849
B	0.288765	-5.043066	-1.604845
B	-0.682311	-4.033144	-2.734625
B	-0.526069	-2.337431	-2.198731
C	0.457301	-2.357491	-0.779244
B	-0.293028	-3.194812	0.532455
B	-1.846762	-3.810017	-0.100941
B	-0.429488	-4.898651	0.031611
B	1.029775	-3.939195	-0.397044
B	0.866588	-3.422345	-2.085528
N	-3.327423	-0.736679	1.006605
C	-3.73975	-1.190849	2.366797
C	-4.759011	-2.351315	2.315156
C	-0.281336	0.251189	0.482416
N	0.064733	1.560799	0.814511
C	-0.863165	2.604538	0.652527
C	-1.619392	2.960492	1.819536
C	-2.475177	4.071787	1.798295
C	-2.580798	4.877898	0.649252
C	-1.848718	4.532765	-0.490638
C	-1.018402	3.38813	-0.526765
C	-1.413562	2.162757	3.08335
C	-0.395778	3.019756	-1.852058
Si	1.244489	-0.619783	-0.187988
C	1.892389	1.503304	-0.259898
N	2.730482	2.352	-0.499058
C	3.020203	3.709253	-0.402323
C	2.814234	4.39998	0.826101
C	3.142159	5.767561	0.871053
C	3.654145	6.433427	-0.253292

C	3.872918	5.725628	-1.446323
C	3.580207	4.353561	-1.54032
C	2.299552	3.67405	2.045517
C	3.86066	3.575807	-2.806008
N	2.44348	-1.129576	1.168975
C	2.469826	-1.205998	2.654321
C	1.166229	-0.588214	3.180592
N	3.033253	-1.108361	-0.92333
C	3.784731	-0.989246	-2.188786
C	4.444934	-2.331831	-2.576294
C	3.460353	-1.357281	0.305974
C	4.828825	-1.838866	0.653552
C	5.888783	-0.940829	0.889196
C	7.169034	-1.427183	1.195646
C	7.399056	-2.812799	1.270632
C	6.342721	-3.710869	1.038945
C	5.061209	-3.226785	0.73089
C	4.881963	0.103199	-2.097005
C	2.761999	-0.534594	-3.252724
C	2.557241	-2.678878	3.111947
C	3.647384	-0.395627	3.244051
C	-4.904396	-0.060847	-3.05455
C	-3.980371	2.069316	-2.047377
C	-2.473234	-1.683715	3.083031
C	-4.354304	-0.014491	3.157006
H	2.110482	-4.045903	0.115444
H	1.804146	-3.199941	-2.788741
H	-0.517727	-1.349604	-2.866291
H	-0.165573	-2.76705	1.636483
H	-0.3903	-5.774181	0.860053
H	-2.794093	-3.811842	0.631808
H	-3.057861	-2.899271	-2.231553
H	5.702234	0.137261	0.83966
H	-0.808708	-4.281607	-3.907773
H	7.989115	-0.721559	1.379065
H	0.867739	-6.037074	-1.968351
H	8.400914	-3.191503	1.509647
H	-2.226105	-5.887969	-1.646873
H	6.515507	-4.792966	1.094105
H	4.234922	-3.92045	0.539137
H	4.465923	1.031361	-1.667468
H	5.259234	0.322321	-3.114261
H	5.737816	-0.233799	-1.489771
H	1.923539	-1.243002	-3.337839

H	3.259101	-0.454944	-4.236661
H	2.361218	0.458242	-2.982732
H	5.312807	-2.5352	-1.924223
H	4.803232	-2.283205	-3.621917
H	3.735866	-3.168622	-2.477198
H	1.706126	-3.257863	2.712291
H	2.530849	-2.724498	4.217396
H	3.496521	-3.147296	2.77153
H	4.61981	-0.888014	3.084449
H	3.49737	-0.293355	4.335247
H	3.673679	0.616829	2.801388
H	1.078006	0.470708	2.885121
H	1.144111	-0.676134	4.282308
H	0.301165	-1.113282	2.755019
H	2.979188	6.315448	1.808531
H	3.888906	7.504011	-0.1983
H	4.287331	6.238434	-2.32432
H	2.96623	3.02878	-3.155217
H	4.642576	2.811077	-2.629098
H	4.200526	4.247708	-3.614508
H	3.048034	2.939573	2.408545
H	1.376893	3.108297	1.81616
H	2.094124	4.385624	2.865131
H	-3.037662	4.329138	2.707092
H	-3.226214	5.765894	0.649233
H	-1.94245	5.139778	-1.402524
H	0.075344	2.025099	-1.817383
H	0.364654	3.761114	-2.159024
H	-1.170583	3.005124	-2.641921
H	-1.447953	1.081375	2.873623
H	-2.168383	2.416533	3.850372
H	-0.406506	2.357592	3.501758
H	-5.905404	-2.240373	-0.733474
H	-8.401843	-2.049182	-0.739762
H	-9.495411	0.085994	-0.008795
H	-8.084986	2.018788	0.738321
H	-5.589364	1.812389	0.760282
H	-4.756195	-1.15108	-3.163513
H	-4.993562	0.381795	-4.064355
H	-5.850086	0.123693	-2.520452
H	-4.896332	2.17389	-1.440936
H	-4.135845	2.618233	-2.995678
H	-3.143228	2.532727	-1.500645
H	-1.554357	0.78952	-2.767761

H	-2.631572	1.062243	-4.178457
H	-2.339479	-0.602555	-3.57791
H	-2.045719	-2.556892	2.565501
H	-2.731782	-1.97685	4.116386
H	-1.713585	-0.888801	3.12624
H	-3.666662	0.845449	3.176733
H	-4.54347	-0.338162	4.197817
H	-5.316245	0.299688	2.719107
H	-5.742686	-2.019459	1.946356
H	-4.897921	-2.740932	3.340925
H	-4.392735	-3.174342	1.678586

Table S30. Cartesian geometry of **3** in Figure S3 in Angstrom [Å].

Atomtype	X coordinates	Y coordinates	Z coordinates
Si	1.375958	-0.556954	-0.17263
N	2.631943	-1.019641	1.125502
C	3.618343	-1.115182	0.208327
B	1.369963	-3.926881	-0.251634
H	2.442028	-3.925759	0.28917
N	-3.285615	-1.058399	1.022198
Si	-1.740711	-0.785763	-0.058472
N	3.09613	-0.896265	-0.99679
C	1.496801	1.455378	-0.135199
B	1.19717	-3.471417	-1.952266
H	2.143061	-3.1728	-2.616178
C	-0.309458	0.148155	0.191968
B	-0.285828	-2.516397	-2.120881
H	-0.369826	-1.55352	-2.822144
N	-3.275592	-0.342093	-1.028294
C	-4.068364	-0.636439	0.018737
B	-0.025327	-3.271581	0.630608
H	0.04892	-2.808979	1.725168
N	0.133261	1.531461	0.221893
C	0.682977	-2.40947	-0.694511
B	-0.00468	-4.996886	0.183529
H	0.096078	-5.841493	1.038679
N	2.389877	2.364588	-0.305464
C	-1.009412	-2.495092	-0.550815
B	-1.509924	-4.041427	0.001516
H	-2.471964	-4.107552	0.7155
C	5.042914	-1.45371	0.484544
B	-1.681112	-3.567713	-1.71197
H	-2.761763	-3.299393	-2.172055

C	6.000108	-0.449424	0.727012
H	5.686459	0.599914	0.733815
B	-0.281548	-4.233083	-2.610516
H	-0.371111	-4.526047	-3.776904
C	7.338001	-0.799902	0.965155
H	8.080772	-0.014604	1.153814
B	0.751301	-5.125358	-1.439012
H	1.417216	-6.077257	-1.764335
C	7.724809	-2.152401	0.96356
H	8.771583	-2.42425	1.149948
B	-1.033971	-5.18662	-1.284628
H	-1.679547	-6.184541	-1.490899
C	6.769655	-3.155232	0.721741
H	7.067299	-4.211294	0.715971
C	5.430301	-2.808392	0.481112
H	4.679145	-3.580235	0.277355
C	3.763021	-0.604569	-2.286776
C	4.641083	0.663256	-2.17669
H	4.076307	1.47117	-1.680372
H	4.940504	0.989479	-3.191072
H	5.561757	0.456362	-1.60521
C	2.622555	-0.331711	-3.289381
H	1.966035	-1.2115	-3.390551
H	3.044094	-0.085491	-4.280732
H	2.018074	0.528761	-2.944282
C	4.634376	-1.785816	-2.765162
H	5.496613	-1.93386	-2.092518
H	5.023159	-1.55837	-3.77573
H	4.058242	-2.724765	-2.813122
C	2.691031	-1.138174	2.601067
C	2.837224	-2.617504	3.014619
H	1.996998	-3.214719	2.623342
H	2.850319	-2.697349	4.118402
H	3.781849	-3.036529	2.624536
C	3.850032	-0.306564	3.197464
H	4.833401	-0.762768	3.000958
H	3.718121	-0.246774	4.294173
H	3.836759	0.719365	2.785877
C	1.371388	-0.560407	3.145212
H	1.284374	0.506265	2.880047
H	1.350687	-0.659056	4.245848
H	0.502186	-1.082511	2.71769
C	2.251773	3.745989	-0.126224
C	1.957281	4.311517	1.148667

C	1.804449	5.704917	1.261572
H	1.552838	6.128003	2.243832
C	1.971639	6.548346	0.152962
H	1.835011	7.632629	0.253796
C	2.349564	5.991163	-1.079516
H	2.5275	6.642819	-1.946409
C	2.520452	4.603824	-1.233823
C	3.005273	4.029586	-2.546374
H	2.364589	3.203726	-2.904085
H	4.01968	3.59999	-2.429364
H	3.047014	4.81105	-3.327915
C	1.8985	3.429326	2.371189
H	2.911896	3.055327	2.626696
H	1.273647	2.539534	2.201129
H	1.50246	3.979705	3.243808
C	-0.728381	2.656095	0.34125
C	-1.458018	2.85277	1.551292
C	-2.291295	3.980703	1.662954
H	-2.84709	4.133558	2.59829
C	-2.396744	4.91604	0.621335
H	-3.030186	5.804742	0.737431
C	-1.697129	4.696469	-0.570635
H	-1.796297	5.403341	-1.405162
C	-0.883773	3.559139	-0.74504
C	-0.303551	3.304243	-2.11706
H	0.420553	2.477228	-2.128764
H	0.201429	4.208459	-2.497533
H	-1.119287	3.051693	-2.822648
C	-1.336357	1.900761	2.717981
H	-1.382758	0.847432	2.388049
H	-2.134428	2.091253	3.458326
H	-0.36818	2.017892	3.238332
C	-5.550219	-0.535298	0.032944
C	-6.317582	-1.607624	-0.467443
H	-5.811285	-2.502844	-0.846293
C	-7.717012	-1.519698	-0.478903
H	-8.310636	-2.356697	-0.866923
C	-8.356561	-0.36185	0.000997
H	-9.451526	-0.293789	-0.012369
C	-7.591372	0.70801	0.496959
H	-8.085664	1.613366	0.870593
C	-6.189737	0.623575	0.516195
H	-5.587619	1.453987	0.901882
C	-3.583161	0.438723	-2.255599

C	-4.75638	-0.179063	-3.044639
H	-4.578482	-1.256122	-3.220857
H	-4.829484	0.32794	-4.024946
H	-5.720009	-0.053599	-2.524182
C	-3.900297	1.897752	-1.86387
H	-4.833262	1.952067	-1.27649
H	-4.036609	2.507429	-2.776947
H	-3.077572	2.33525	-1.271683
C	-2.321937	0.398458	-3.136349
H	-1.438996	0.75075	-2.57567
H	-2.473142	1.050512	-4.01535
H	-2.130026	-0.629272	-3.487158
C	-3.663775	-1.539784	2.376515
C	-2.367738	-2.008952	3.060223
H	-1.942132	-2.877559	2.53415
H	-2.589586	-2.300063	4.102544
H	-1.616294	-1.200626	3.070051
C	-4.281924	-0.385524	3.195933
H	-3.602204	0.482992	3.213651
H	-4.446746	-0.725483	4.235548
H	-5.255827	-0.077092	2.780259
C	-4.656737	-2.71971	2.304882
H	-5.645112	-2.397829	1.93646
H	-4.790255	-3.137561	3.320266
H	-4.267278	-3.516952	1.647711

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