Activation of Ammonia by a Si=O Double Bond and Formation of a Unique Pair of Sila-Hemiaminal and Silanoic Amide Tautomers

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Supporting Information

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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 silylene **1** was prepared according to literature procedure.[1] The NMR spectra were recorded with Bruker spectrometers ARX200, AV400 and with residual solvent signals as internal reference (^{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.

Single-Crystal X-ray Structure Determination

Crystals were each mounted on a glass capillary in per-fluorinated oil and measured in a cold N_2 flow. The data of **2**, **3**, **4** and **5** were collected on an Oxford Diffraction Xcalibur S Sapphire at 150 K (Mo-Kα-radiation, λ = 0.71073 Å). The structures were solved by direct methods and refined on F^2 with the SHELX-97 [2] software package. The positions of the H atoms were calculated and considered isotropically according to a riding model (exception is the hydrogen atoms on nitrogen and oxygen in **4** and **5** which were detected in the difference electron density map and refined).

Compound 2: p-dimethylaminopyridine **(**DMAP) (0.61 g, 5.0 mmol) was added to a solution of silylene **1** (2.24 g, 5.0 mmol) in hexane (50 mL) at room temperature under stirring. Compound **2** was formed as yellow precipitate. After 24 hours the solution was filtrated and the solid subsequently washed with hexane (2 × 5 mL). At -20 ºC compound **2** crystallized from toluene (10 mL) as yellow plates with yield of 2.43 g (4.3 mmol, 86 %). M. p. 120 ºC (decomp.); ^{1}H NMR (200.13 MHz, [D$_6$]benzene, 25ºC): δ = 1.14 (d, ^{3}J (H,H) = 7.0 Hz, 6 H; CHMe_2), 1.16 (d, ^{3}J (H,H) = 7.0 Hz, 6 H; CHMe_2), 1.23 (d, ^{3}J (H,H) = 7.0 Hz, 6 H; CHMe_2), 1.45 (d, ^{3}J (H,H) = 7.0 Hz, 6 H; CHMe_2), 1.59 (s, 3 H; NCMe), 2.11 (s, 6 H; NMe_2 in DMAP), 3.35 (s, 1 H; NCCH_2), 3.51 (sept., ^{3}J (H,H) = 7.0 Hz, 2 H; CHMe$_2$), 3.64 (sept., ^{3}J (H,H) = 7.0 Hz, 2 H; CHMe$_2$), 3.99 (s, 1 H; NCCH_2), 5.58 (s, 1 H; γ-CH), 5.83 - 5.85 (m, 2 H; DMAP), 6.90 – 7.22 ppm (m, br, 6 H; 2,6-iPr$_2$C$_6$H$_3$), 8.50 – 8.52 (m, 2 H; DMAP); ^{13}C{^{1}H} NMR (100.61 MHz, [D$_6$]benzene, 25ºC): δ = 21.4, 24.1, 24.9, 25.4, 25.7 (NCMe, CHMe_2), 28.7, 28.9 (CHMe$_2$), 38.4 (NMe_2 in DMAP), 83.2 (NCH_2), 106.2 (γ-*C*), 106.3 (DMAP), 124.0, 124.5, 127.2, 127.3, 140.8, 140.9, 141.6, 148.2, 148.4, 148.8, 149.2, 154.9 ppm (NCMe, NCCH$_2$, 2,6-iPr$_2$$C_6H_3$, DMAP); ^{29}Si{^{1}H} NMR (79.49 MHz, [D$_6$]benzene, 25ºC): δ = 37.4 ppm (s); EI-MS: m/z (%): 566 (2) [M$^+$], 551 (32) [M$^+$-Me], 523 (8) [M$^+$-iPr], 403 (100) [M$^+$-DMAP-iPr+H]; elemental analysis calcd (%) for $C_{36}H_{50}N_4Si$: C 76.27, H 8.89, N 9.88, found: C 75.83, H 8.77, N 9.91. IR (KBr, cm^{-1}): 445(w), 533(w), 595(w), 702(w), 758(m), 803(s), 883(w), 934(w), 987(m), 1058(s), 1102(s), 1175(s), 1227(m), 1254(w), 1276(w), 1323(m), 1362(m), 1381(s), 1441(s), 1463(m), 1550(s), 1619(s), 2867(m), 2926(m), 2962(s), 3058(w).

Compound 3: To a solution of **2** (0.60 g, 1.0 mmol) in toluene (20 mL) excess of N_2O was bubbled at -20 ºC and the solution was allowed to warm to room temperature slowly. After one hour the reaction was completed and a pale yellow precipitate formed. By cooing of the solution to -20 ºC for 1 hour the solid was isolated by filtration. The collected pale yellow powder amounted to 0.48 g (0.82 mmol, 82 %). X-ray quality crystals were obtained from the solution of **3** in CH_2Cl_2. M.p. 298 ºC (decomposed); ^{1}H NMR (200.13 MHz, [D$_2$]dichloromethane, 25ºC): δ = 0.36 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 0.55 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 1.07 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 1.09 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 1.22 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 1.25 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 1.40 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 1.43 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 1.61 (s, 3 H; NCMe), 2.48 – 2.64 (m, 2 H; CHMe$_2$), 2.92 (s, 1 H; NCCH_2), 3.19 (s, 6 H; NMe_2), 3.69 (s, 1 H; NCCH_2), 3.75 – 3.90 (m, 2 H; CHMe$_2$), 5.38 (s, 1 H; γ-H), 6.61 – 6.65 (m, 2 H; DMAP), 6.99 – 7.31 (m, br, 6 H; 2,6-iPr$_2$C$_6$H$_3$), 8.70 – 8.74 ppm (m, 2 H; DMAP); ^{13}C{^{1}H} NMR (100.61 MHz, [D$_2$]dichloromethane, 25ºC): δ = 21.7, 23.5, 23.6, 23.7, 24.4, 24.6, 24.9, 25.0, 25.5 (NCMe, CHMe_2), 28.3, 28.4, 28.7, 28.8 (CHMe$_2$), 39.6 (NMe_2), 83.6 (NCH_2), 102.9 (γ-*C*), 106.1 (DMAP), 123.4, 123.8, 123.9, 124.2, 126.4, 126.7, 136.9, 137.6, 144.1, 147.5, 147.7, 148.9, 149.2, 150.2, 156.8 ppm (NCMe, NCCH$_2$, DMAP, 2,6-iPr$_2$$C_6H_3$); ^{29}Si{^{1}H} NMR (79.49 MHz, [D$_2$]dichloromethane, 25ºC): δ -71 ppm (s); EI-MS: m/z (%): 582 (5) [M$^+$], 567 (9) [M$^+$-Me], 539 (13) [M$^+$-iPr], 445 (100) [M$^+$-DMAP-Me]; elemental analysis calcd (%) for $C_{36}H_{50}N_4SiO{\cdot}0.4CH_2Cl_2$: C 70.90, H 8.32, N 9.08; found: C 70.50, H 8.32, N 9.05; IR (KBr, cm^{-1}): 457(w), 480(m), 530(w), 584(w), 591(w), 758(m), 800(m), 928(w), 987(w), 1034(s), 1058(s), 1072(s), 1152 (s, $\nu_{Si=O}$), 1176(m), 1225(m), 1321(m), 1354(m), 1379(s), 1442(m), 1463(m), 1553(s), 1626(s), 2867(m), 2926(m), 2962(s), 3059(w).

Compounds 4 and 5: To a pale yellow suspension of **3** (0.43 g, 0.74 mmol) in toluene (20 mL) excess of ammonia was bubbled at 10 ºC under stirring. The suspension was warmed to room temperature slowly. After 30 min the suspension turned clear and colorless. The excess of ammonia was evacuated. To the residue toluene (8 mL) was added. By cooing of the solution at 4 ºC overnight, colorless crystals of **4** and **5** were obtained. The collected crystals amounted to 0.20 g (0.40 mmol, 54%). X-ray quality crystals were obtained both from benzene and THF. M. p. 140 ºC (decomposed). ^{1}H NMR (200.13 MHz, **[D$_6$]-benzene**, 25ºC): for **4**: δ = 0.28 (s, 2 H; NH_2), 0.88 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 0.95 (d, ^{3}J (H,H) = 7.0 Hz, 3 H; CHMe_2), 1.14 – 1.47 (m, 18 H; CHMe_2), 1.55 (s, 3 H; NCMe), 3.17 (s, 1 H; NCCH_2), 3.53 – 3.75 (m, 2 H; CHMe$_2$), 3.86 (s, 1 H; NCCH_2), 3.85 – 4.02 (m, 2 H; CHMe$_2$), 5.38 (s, 1 H; γ-H), 6.90 – 7.20 (m, br, 6 H; 2,6-iPr$_2$C$_6$H$_3$), 9.50 ppm (br, 1 H; OH); for **5**: δ = 0.18 (s, 2 H; NH_2), 1.11 – 1.47 (m, 30 H; NCMe, CHMe_2), 2.50 – 2.64 (m, 2 H; CHMe$_2$), 2.88 – 3.08 (m, 2 H; CHMe$_2$), 4.89 (s, 1 H; γ-H), 6.90 – 7.20 (m, br, 6 H; 2,6-iPr$_2$C$_6$H$_3$); ^{13}C{^{1}H} NMR (100.61 MHz, [D$_6$]benzene, 25ºC) for **4** and **5**: δ = 21.4, 22.2, 22.8, 24.3, 24.4, 24.6, 24.8, 25.0, 25.1, 25.2, 25.3, 25.9, 26.3, 26.7, 28.0, 28.4, 28.5, 28.6, 28.7, 28.9 (NCMe, CHMe$_2$), 82.4 (NCH_2), 97.5 (γ-*C* for **5**), 102.9 (γ-*C* for **4**), 123.5, 123.8, 124.1, 124.6, 125.0, 125.7, 126.9, 127.0, 128.9, 135.2, 137.7, 138.2, 142.2, 142.7, 144.4, 147.2, 148.4, 148.7, 149.8, 150.9, 169.4 ppm (NCMe, NCCH$_2$, 2,6-iPr$_2$$C_6H_3$); ^{29}Si{^{1}H} NMR (79.49 MHz, [D$_6$]benzene, 25ºC): δ = -59 (s), -67 ppm (s); ^{1}H NMR (200.13 MHz, **[D$_8$]-THF**, 25ºC): for **4**: δ = 0.64 (s, 2 H; NH_2), 0.95 (br, 3 H; CHMe_2), 1.06 – 1.25 (m, 21 H; CHMe_2), 1.49 (s, 3 H; NCMe), 2.73 (s, 1 H; NCCH_2), 3.42 – 3.89 (m, 4 H; CHMe$_2$), 3.43 (s, 1 H; NCCH_2), 5.12 (s, 1 H; γ-H), 7.00 – 7.27 (m, br, 6 H; 2,6-iPr$_2$C$_6$H$_3$), 8.34 ppm (br, 1 H; OH); for **5**: δ = 0.39 (s, 2 H; NH_2), 1.06 – 1.25 (m, 24 H; CHMe_2), 1.79 (s, 6 H; NCMe), 2.63 – 2.83 (m, 1 H; CHMe$_2$), 3.10 – 3.30 (m, 3 H; CHMe$_2$), 5.49 (s, 1 H; γ-H), 7.00 – 7.27 (m, br, 6 H; 2,6-iPr$_2$C$_6$H$_3$); **Variant temperature** ^{1}H NMR (400.13 MHz, [D$_8$]-toluene): the signals for **4** split into 2 sets: the singlet at 3.07 ppm (NCH_2) at 25 ºC splits into singlet at 3.18 and 3.40 ppm at -60 ºC; the singlet at 3.76 ppm (NCH_2) at 25 ºC splits into singlet at 3.91 and 4.02 ppm at -60 ºC; and the singlet at 5.30 (γ-H) at 25 ºC splits into singlet at 5.38 and 5.51 ppm at -60 ºC; the signals for **5** keep one set; ESI-MS: m/z: 478.32419 (478.32482 theoretical) [M$^+$+H]; elemental analysis calcd (%) for $C_{29}H_{43}N_3SiO$: C 72.91, H 9.07, N 8.80; found: C 72.89, H 8.96, N 8.98; IR (KBr, cm^{-1}): 439(w), 475(w), 561(w), 729(w), 759(w), 786(w), 803(s), 856(w), 923(m), 966(m), 1054(m), 1072(m), 1102(m), 1177(w), 1260(w), 1226(w), 1250(w), 1317(m), 1382(s), 1441(m), 1484(m), 1550(s), 1604(m), 1635(m), 2866(m), 2927(m), 2963(s), 3057(w), 3400(m, $\nu_{(NH)}$), 3504(w, $\nu_{(NH)}$), 3610(w, $\nu_{(O-H)}$).

Crystallographic data for 2

Empirical formula	$C_{36} H_{50} N_4 Si$	
Formula weight	566.89	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 17.3691(3) Å	α= 90°.
	b = 13.0764(2) Å	β= 111.277(2)°.
	c = 15.8971(3) Å	γ = 90°.
Volume	3364.52(10) $Å^3$	
Z	4	
Density (calculated)	1.119 Mg/m^3	
Absorption coefficient	0.099 mm^{-1}	
F(000)	1232	
Crystal size	0.23 x 0.16 x 0.11 mm^3	
Theta range for data collection	3.01 to 25.00°.	
Index ranges	-20<=h<=20, -15<=k<=15, -18<=l<=18	
Reflections collected	29697	
Independent reflections	5919 [R(int) = 0.0254]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9892 and 0.9776	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5919 / 0 / 381	
Goodness-of-fit on F^2	1.077	
Final R indices [I>2sigma(I)]	R1 = 0.0445, wR2 = 0.1010	
R indices (all data)	R1 = 0.0578, wR2 = 0.1068	
Largest diff. peak and hole	0.323 and -0.288 $e.Å^{-3}$	

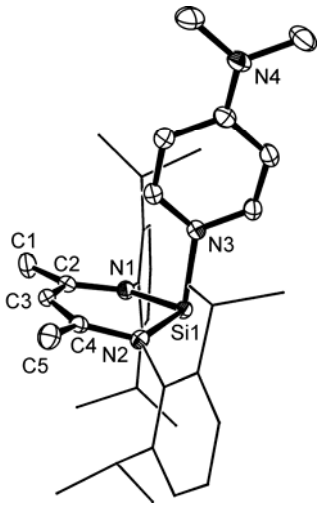


Figure 1. Molecular structure of compound **2** Thermal ellipsoids are drawn at 50% probability level. H atoms are omitted for clarity.

Table 1. Selected interatomic distances and angles of compound **2**

Interatomic distances (Å)		Angles (º)	
Si(1)-N(1)	1.795(1)	N(1)-Si(1)-N(2)	98.08(6)
Si(1)-N(2)	1.795(1)	N(1)-Si(1)-N(3)	96.80(6)
Si(1)-N(3)	2.005(2)	N(2)-Si(1)-N(3)	96.20(6)
N(1)-C(2)	1.406(2)	C(2)-N(1)-Si(1)	125.8(1)
C(1)-C(2)	1.412(2)	C(4)-N(2)-Si(1)	124.3(1)
N(2)-C(4)	1.412(2)	N(1)-C(2)-C(3)	119.3(2)
C(2)-C(3)	1.409(2)	C(3)-C(2)-C(1)	119.0(2)
C(3)-C(4)	1.391(2)	C(4)-C(3)-C(2)	128.3(2)
C(4)-C(5)	1.436(2)	C(3)-C(4)-N(2)	119.8(2)

Crystallographic data for 3

Empirical formula	C_{38} H_{54} Cl_4 N_4 O Si
Formula weight	752.74
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	*P*-1

Unit cell dimensions	a = 9.2101(3) Å	α= 95.548(3)°.
	b = 12.0914(4) Å	β= 104.500(3)°.
	c = 18.2291(7) Å	γ = 94.189(3)°.
Volume	1946.19(12) $Å^3$	
Z	2	
Density (calculated)	1.285 Mg/m^3	
Absorption coefficient	0.370 mm^{-1}	
F(000)	800	
Crystal size	0.34 x 0.28 x 0.24 mm^3	
Theta range for data collection	3.11 to 25.00°.	
Index ranges	-10<=h<=10, -12<=k<=14, -21<=l<=21	
Reflections collected	13903	
Independent reflections	6834 [R(int) = 0.0296]	
Completeness to theta = 25.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9164 and 0.8844	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6834 / 0 / 444	
Goodness-of-fit on F^2	1.118	
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1332	
R indices (all data)	R1 = 0.0668, wR2 = 0.1393	
Largest diff. peak and hole	0.541 and -0.361 $e.Å^{-3}$	

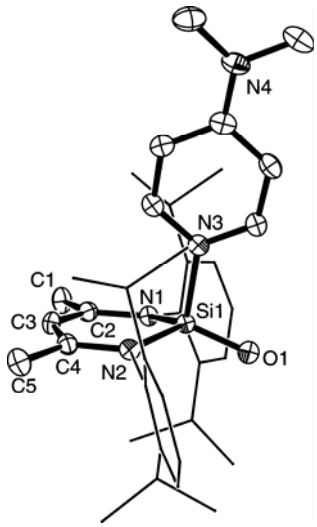


Figure 2. Molecular structure of compound **3**. Thermal ellipsoids are drawn at 50% probability level. H atoms and two dichloromethane molecules are omitted for clarity.

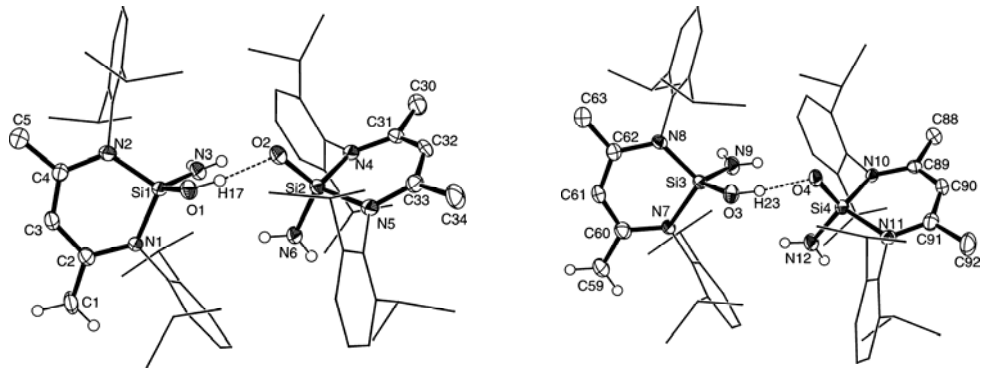
Table 2 Selected interatomic distances and angles of compound **3**

Interatomic distances (Å)		Angles (º)	
Si(1)-O(1)	1.545(2)	O(1)-Si(1)-N(2)	119.8 (1)
Si(1)-N(2)	1.743(2)	O(1)-Si(1)-N(1)	119.2(1)
Si(1)-N(1)	1.746(2)	N(2)-Si(1)-N(1)	103.9(1)
Si(1)-N(3)	1.862(2)	O(1)-Si(1)-N(3)	104.7(1)
N(1)-C(2)	1.412(3)	N(2)-Si(1)-N(3)	102.9(1)
C(1)-C(2)	1.404(4)	N(1)-Si(1)-N(3)	104.2(1)
N(2)-C(4)	1.409(3)	C(2)-N(1)-Si(1)	122.1(2)
C(2)-C(3)	1.416(4)	C(4)-N(2)-Si(1)	122.2(2)
C(3)-C(4)	1.390(4)	C(1)-C(2)-C(3)	119.0(2)
C(4)-C(5)	1.444(4)	C(4)-C(3)-C(2)	129.0(2)

Crystallographic data for 4 and 5

Empirical formula	$C_{143}\ H_{199}\ N_{12}\ O_4\ Si_4$	
Formula weight	2262.50	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 23.9515(9) Å	α= 90°.
	b = 20.8350(7) Å	β= 109.422(5)°.
	c = 28.7818(13) Å	γ = 90°.
Volume	13545.6(9) $Å^3$	
Z	4	
Density (calculated)	1.109 Mg/m^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	4916	
Crystal size	0.23 x 0.15 x 0.12 mm^3	
Theta range for data collection	3.28 to 25.00°.	
Index ranges	-28<=h<=28, -23<=k<=24, -34<=l<=34	
Reflections collected	94373	
Independent reflections	23797 [R(int) = 0.0983]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9881 and 0.9774	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	23797 / 644 / 1706
Goodness-of-fit on F^2	0.889
Final R indices [I>2sigma(I)]	R1 = 0.0589, wR2 = 0.1004
R indices (all data)	R1 = 0.1354, wR2 = 0.1182
Largest diff. peak and hole	0.415 and -0.330 e.Å^{-3}



Mol. Pair 1 ***Mol. Pair 2***

Figure 3. Molecular structures of compounds **4** and **5**. Thermal ellipsoids are drawn at 50% probability level. H atoms (except those for C1, O1, N3, N6 in molecule pair 1, and those for C59, O3, N9, N12 in molecule pair 2) and solvents C_6D_6 molecules are omitted for clarity.

Table 3 Selected interatomic distances of compounds **4** and **5**

Interatomic distances (Å) (*Mol. Pair 1*)		Interatomic distances (Å) (*Mol. Pair 2*)	
Si(1)-O(1)	1.607(2)	Si(3)-O(3)	1.607(2)
Si(2)-O(2)	1.545(2)	Si(4)-O(4)	1.546(2)
C(1)-C(2)	1.383(3)	C(59)-C(60)	1.404(4)
C(33)-C(34)	1.516(4)	C(91)-C(92)	1.508(4)
C(4)-C(5)	1.463(3)	C(62)-C(63)	1.432(3)
C(30)-C(31)	1.499(4)	C(88)-C(89)	1.494(4)
Si(1)-N(3)	1.681(3)	Si(3)-N(9)	1.676(3)
Si(1)-N(2)	1.736(2)	Si(3)-N(8)	1.737(2)
Si(1)-N(1)	1.742(2)	Si(3)-N(7)	1.746(2)
N(1)-C(2)	1.405(3)	N(7)-C(60)	1.400(3)
Si(2)-N(6)	1.677(2)	Si(4)-N(12)	1.683(2)
Si(2)-N(5)	1.793(2)	Si(4)-N(11)	1.795(2)
Si(2)-N(4)	1.817(2)	Si(4)-N(10)	1.805(2)
N(2)-C(4)	1.410(3)	N(8)-C(62)	1.408(3)
C(2)-C(3)	1.429(4)	C(60)-C(61)	1.413(4)
C(3)-C(4)	1.365(3)	N(10)-C(89)	1.348(3)

N(4)-C(31)	1.341(3)	N(10)-C(89)	1.348(3)
C(31)-C(32)	1.397(4)	C(89)-C(90)	1.396(4)
C(32)-C(33)	1.370(4)	C(90)-C(91)	1.377(4)
N(5)-C(33)	1.353(3)	N(11)-C(91)	1.351(3)

Table 4 Selected angles of compounds **4** and **5**

Angles (°) (Mol. Pair 1)		***Angles (°) (Mol. Pair 2)***	
O(1)-Si(1)-N(3)	107.4(2)	O(3)-Si(3)-N(9)	108.1(2)
O(2)-Si(2)-N(6)	113.8(1)	O(4)-Si(4)-N(12)	114.1(1)
O(1)-Si(1)-N(2)	113.3(1)	O(3)-Si(3)-N(8)	114.2(1)
N(3)-Si(1)-N(2)	111.6(1)	N(9)-Si(3)-N(8)	110.4(1)
O(1)-Si(1)-N(1)	112.1(1)	O(3)-Si(3)-N(7)	110.0(1)
N(3)-Si(1)-N(1)	111.2(1)	N(9)-Si(3)-N(7)	112.2(1)
N(2)-Si(1)-N(1)	101.4(1)	N(8)-Si(3)-N(7)	102.0(1)
C(2)-N(1)-Si(1)	124.5(2)	C(60)-N(7)-Si(3)	124.9(2)
O(2)-Si(2)-N(5)	116.8(1)	O(4)-Si(4)-N(11)	114.5(1)
N(6)-Si(2)-N(5)	107.1(1)	N(12)-Si(4)-N(11)	108.3(1)
O(2)-Si(2)-N(4)	111.2(1)	O(4)-Si(4)-N(10)	112.4(1)
N(6)-Si(2)-N(4)	109.2(1)	N(12)-Si(4)-N(10)	108.4(1)
N(5)-Si(2)-N(4)	97.4(1)	N(11)-Si(4)-N(10)	97.8(1)
C(4)-N(2)-Si(1)	122.5(2)	C(62)-N(8)-Si(3)	123.8(2)
C(1)-C(2)-N(1)	121.2(2)	N(7)-C(60)-C(59)	120.8(2)
C(1)-C(2)-C(3)	120.3(3)	C(59)-C(60)-C(61)	120.6(3)
N(1)-C(2)-C(3)	118.5(2)	N(7)-C(60)-C(61)	118.7(2)
C(3)-C(4)-N(2)	121.1(2)	C(61)-C(62)-N(8)	119.8(2)
C(3)-C(4)-C(5)	120.5(3)	C(61)-C(62)-C(63)	120.6(3)
N(2)-C(4)-C(5)	118.4(2)	N(8)-C(62)-C(63)	119.6(2)
C(33)-N(5)-Si(2)	123.3(2)	C(91)-N(11)-Si(4)	123.2(2)
N(4)-C(31)-C(32)	121.1(3)	N(10)-C(89)-C(90)	121.5(3)
N(4)-C(31)-C(30)	121.1(3)	N(10)-C(89)-C(88)	120.0(3)
C(32)-C(31)-C(30)	117.8(3)	C(90)-C(89)-C(88)	118.5(3)
C(33)-C(32)-C(31)	126.5(3)	C(91)-C(90)-C(89)	126.3(3)
N(5)-C(33)-C(32)	122.3(3)	N(11)-C(91)-C(90)	122.0(3)
N(5)-C(33)-C(34)	118.7(3)	N(11)-C(91)-C(92)	119.4(3)
C(32)-C(33)-C(34)	119.0(3)	C(90)-C(91)-C(92)	118.6(3)
C(4)-C(3)-C(2)	127.6(3)	C(62)-C(61)-C(60)	128.9(3)
C(31)-N(4)-Si(2)	124.4(2)	C(89)-N(10)-Si(4)	123.6(2)

Computational Details

Structure optimizations as well as computed dissociation and reaction energies used the gradient-corrected BP86[3,4] functional in conjunction with the resolution-of-identity[5] (RI) approximation and def2-TZVP[6,7,8] orbital and auxiliary basis sets. Additional optimizations employed the COSMO[9] polarizable continuum model, as implemented in Turbomole, using a dielectric constant of ε=2.38 for toluene. Where available, X-ray crystal structure data was used as starting point for the calculations. All structures were fully optimized without restrictions and without imposing any structural simplifications. All calculations were done with the Turbomole program, version 5.10.[10] Table 5 contains the Cartesian coordinates for optimized structures **3**, **4**, **5** and the **4-5** dimer in the gas phase and in toluene, respectively.

Table 5. Cartesian coordinates of RI-BP86/def2-TZVP optimized structures in gas phase and toluene.

3 gas phase				**3 toluene**				**4 gas phase**			
O	0.096254	0.522152	-1.940944	O	0.138629	0.590733	-1.929335	H	-6.229484	-0.417077	-1.659595
Si	0.077660	0.292400	-0.408915	Si	0.088053	0.305916	-0.404790	C	-5.238182	-0.305562	-1.217131
N	1.562756	0.152869	0.533812	N	1.569902	0.193705	0.550323	H	-4.030162	3.674953	-1.513892
C	1.648382	0.510746	1.897938	C	1.642989	0.550733	1.914792	H	-5.389857	1.831466	-1.047390
C	0.403897	0.857444	2.582232	C	0.395164	0.899641	2.588840	H	-4.825424	-2.414667	-1.246090
C	-0.776020	1.243714	2.022011	C	-0.791101	1.258945	2.023081	H	-1.871042	-2.906748	-2.279634
N	-0.980017	1.259648	0.626996	N	-1.002536	1.239946	0.630125	H	-3.218414	-3.891354	-1.692569
C	-1.941770	1.640865	2.891478	C	-1.953813	1.664837	2.891911	H	0.405488	-0.090452	-2.774233
H	-2.811644	0.991252	2.702592	H	-2.816048	0.998040	2.731810	H	-2.454518	3.041362	-1.981465
H	-2.273645	2.668853	2.687992	H	-2.300839	2.682737	2.663745	C	-4.761240	0.955733	-0.874455
H	-1.670823	1.567082	3.951414	H	-1.670819	1.624443	3.950351	C	-4.444007	-1.425770	-0.985394
H	0.461779	0.863617	3.670447	H	0.452764	0.931415	3.676655	C	-3.016610	3.472547	-1.136783
C	2.823095	0.543855	2.586517	C	2.813000	0.583244	2.614039	H	1.542772	-3.007609	-1.953955
H	3.779757	0.327784	2.117948	H	3.773398	0.361120	2.156150	C	-2.244701	-3.465602	-1.408803
H	2.819292	0.825648	3.637325	H	2.798975	0.865235	3.665124	H	-0.278916	-1.392493	-1.956721
C	2.763612	-0.332611	-0.115997	C	2.785431	-0.267579	-0.089976	N	-0.090282	-0.395923	-1.943734
C	3.207803	-1.660462	0.123613	C	3.243855	-1.593498	0.134441	H	-2.560673	4.437872	-0.873008
C	4.360757	-2.113033	-0.531276	C	4.414157	-2.019697	-0.508958	H	-1.563552	-4.308139	-1.220045
C	5.071373	-1.291498	-1.401813	C	5.130773	-1.173058	-1.350784	H	-0.595582	2.432949	-1.509675
C	4.638494	0.012695	-1.612909	C	4.685550	0.130604	-1.544513	H	2.825599	-4.073433	-1.352130
C	3.497920	0.522012	-0.974606	C	3.525738	0.612214	-0.918531	H	1.158235	-4.314607	-0.803639
H	4.707689	-3.133134	-0.354206	H	4.770823	-3.038569	-0.344734	C	1.901970	-3.548447	-1.067275
H	5.963061	-1.665666	-1.908011	H	6.036458	-1.526443	-1.847220	C	-3.492301	1.126232	-0.301645
H	5.201065	0.661965	-2.286162	H	5.254298	0.799845	-2.192760	C	-3.166903	-1.310665	-0.420867
C	2.499915	-2.621794	1.072679	C	2.537719	-2.579855	1.058388	H	-4.978225	3.231832	0.860147
H	1.607915	-2.109886	1.458581	H	1.633577	-2.087786	1.441250	O	0.129814	2.095509	-0.958430
C	2.043980	-3.902247	0.349725	C	2.111053	-3.855571	0.309754	C	-3.047414	2.532313	0.083612
H	1.415845	-3.674610	-0.522305	H	1.488317	-3.624450	-0.565198	C	-2.360329	-2.576178	-0.157693
H	1.469698	-4.546295	1.033309	H	1.538633	-4.518120	0.976439	C	-2.685528	-0.019277	-0.090466
H	2.905355	-4.486490	-0.006836	H	2.986547	-4.419894	-0.044797	H	4.597684	-2.762089	-0.963279
C	3.381329	-2.983880	2.282993	C	3.410865	-2.948973	2.273004	H	2.406766	2.742415	-2.194532
H	2.835737	-3.649198	2.969986	H	2.863502	-3.628109	2.944729	H	6.158742	-0.947264	-1.600802
H	4.295858	-3.507966	1.966474	H	4.333057	-3.461012	1.958632	H	-3.971251	-3.718177	0.789773
H	3.672859	-2.083734	2.839499	H	3.688825	-2.053509	2.844432	Si	0.002312	0.505231	-0.495977
C	2.815618	2.247076	-2.697812	C	2.893107	2.375073	-2.622697	C	4.306362	-1.721654	-0.807649
H	3.679397	2.016764	-3.340460	H	3.787310	2.175479	-3.232996	C	5.186993	-0.704849	-1.167293
H	2.567499	3.308904	-2.847338	H	2.633240	3.436162	-2.754380	C	-3.934302	3.127963	1.192843
H	1.955727	1.640717	-3.012516	H	2.058369	1.764150	-2.991541	H	-1.347740	-2.264047	0.138379
C	3.130948	1.979265	-1.216367	C	3.146369	2.070135	-1.136412	H	-2.027696	2.463635	0.485208
H	2.218290	2.191892	-0.642701	H	2.206241	2.253094	-0.598805	H	4.134090	3.169534	-2.079387
C	4.236737	2.917280	-0.694776	C	4.214826	3.008991	-0.543557	H	-3.571443	4.127201	1.476627
H	5.180744	2.769393	-1.241064	H	5.182761	2.888384	-1.053799	C	-2.949626	-3.378491	1.018988
H	4.433760	2.749582	0.373592	H	4.368126	2.813598	0.527378	C	2.134201	-2.595828	0.119176
H	3.938473	3.967874	-0.828467	H	3.906353	4.058903	-0.659852	C	3.051791	-1.436245	-0.253202
C	-1.871921	2.269131	0.087741	C	-1.942040	2.197296	0.074921	C	3.171341	3.188431	-1.546281
C	-3.143015	1.913137	-0.424179	C	-3.222937	1.784264	-0.365292	C	4.819011	0.621894	-0.969402
C	-3.991606	2.926810	-0.890519	C	-4.111228	2.749756	-0.861484	H	5.512384	1.416683	-1.250538
C	-3.616873	4.265609	-0.845277	C	-3.765002	4.096491	-0.913762	N	-1.372644	0.118549	0.505254
C	-2.361192	4.604762	-0.350730	C	-2.502138	4.492614	-0.481530	H	-2.336427	-4.269097	1.223542
C	-1.465337	3.628683	0.105932	C	-1.570202	3.565266	0.004678	H	1.161898	-2.170350	0.406542
H	-2.058326	5.653357	-0.332394	H	-2.225732	5.547442	-0.533036	H	2.900337	4.241557	-1.379952
H	-4.296219	5.040818	-1.203731	H	-4.473508	4.833714	-1.295568	H	-3.918578	2.492515	2.088057
H	-4.970235	2.658359	-1.292815	H	-5.098149	2.437114	-1.208077	C	2.689963	-0.078616	-0.049052
C	-3.617521	0.470969	-0.518123	C	-3.678001	0.332503	-0.338059	C	3.580164	0.965549	-0.407141
H	-2.888096	-0.145576	0.023912	H	-2.896471	-0.244113	0.173725	H	-2.985019	-2.767831	1.930803
C	-3.632638	0.007829	-1.987489	C	-3.817763	-0.220116	-1.769088	H	3.653361	-3.823295	1.112865
H	-2.643826	0.144775	-2.448030	H	-2.880723	-0.100062	-2.330463	N	1.396874	0.224641	0.530160
H	-3.915968	-1.053798	-2.059347	H	-4.081214	-1.288562	-1.750097	H	1.983012	-4.197272	1.596229
H	-4.362093	0.589537	-2.571590	H	-4.609891	0.311531	-2.318131	C	2.670385	-3.379934	1.332497
C	-4.987279	0.250656	0.147528	C	-4.984548	0.139979	0.452797	C	3.262515	2.442777	-0.201975
H	-5.258080	-0.815840	0.120436	H	-5.244621	-0.928081	0.506100	H	-3.413159	-0.101833	2.302950
H	-4.983159	0.575762	1.197981	H	-4.894741	0.520846	1.480380	H	2.277939	2.511352	0.278769
H	-5.785507	0.804009	-0.368610	H	-5.827501	0.661709	-0.023930	C	-1.302131	0.098178	1.924547

C -0.084498 4.077228 0.572596	C -0.194492 4.073738 0.420462	C -2.408955 -0.021522 2.709515
H 0.505718 3.179549 0.800949	H 0.425954 3.203321 0.673587	H 2.780579 -2.736360 2.215386
C 0.651683 4.843685 -0.541327	C 0.496189 4.815789 -0.737764	C 1.236318 0.221465 1.929353
H 1.677324 5.082567 -0.224036	H 1.518977 5.100671 -0.450320	H 5.291826 3.154454 0.251067
H 0.148826 5.793125 -0.778487	H -0.041695 5.737974 -1.003932	C 4.293554 3.130936 0.713124
H 0.703580 4.249174 -1.462996	H 0.551922 4.183529 -1.633757	C 0.015272 0.192657 2.532237
C -0.151438 4.924954 1.856629	C -0.265113 4.971240 1.670482	H 3.993509 4.171366 0.906715
H -0.620077 4.374617 2.683870	H -0.705270 4.442052 2.526883	H -2.292698 -0.050076 3.790679
H -0.729268 5.847617 1.694104	H -0.871652 5.869758 1.479350	H 3.192254 -0.513424 2.523366
H 0.860497 5.214130 2.176412	H 0.743372 5.301408 1.960549	H 4.390160 2.620590 1.681630
N -0.685871 -1.468636 -0.241878	N -0.635673 -1.458382 -0.284279	C 2.483468 0.290336 2.768608
C -0.885671 -2.153181 -1.396599	C -0.819575 -2.142318 -1.444276	H 3.018255 1.238420 2.606801
C -1.469052 -3.402628 -1.428199	C -1.379278 -3.400397 -1.486550	H 0.008668 0.232638 3.620435
C -1.899103 -4.022438 -0.224753	C -1.801728 -4.037630 -0.287014	H 2.225402 0.215805 3.830963
C -1.681780 -3.284666 0.972443	C -1.602407 -3.301187 0.916627	
C -1.080410 -2.046134 0.920512	C -1.026072 -2.052424 0.874308	
H -0.554168 -1.611577 -2.285813	H -0.496000 -1.599459 -2.333743	
H -1.593017 -3.888404 -2.392834	H -1.491026 -3.881321 -2.454973	
N -2.483546 -5.252259 -0.214659	N -2.360302 -5.274099 -0.286412	
H -1.973983 -3.677794 1.942949	H -1.891060 -3.704418 1.883953	
H -0.898576 -1.464220 1.825716	H -0.862453 -1.475304 1.785693	
C -2.916675 -5.852037 1.042407	C -2.791399 -5.890233 0.966092	
C -2.677850 -5.981997 -1.463106	C -2.543828 -5.999323 -1.541589	
H -3.364545 -6.828629 0.835156	H -3.212950 -6.875898 0.748958	
H -2.070814 -6.002791 1.732130	H -1.947331 -6.022269 1.660796	
H -3.672176 -5.229792 1.548213	H -3.565325 -5.286899 1.465840	
H -3.149461 -6.944531 -1.243217	H -2.992502 -6.973180 -1.325564	
H -3.331804 -5.429797 -2.156802	H -3.212371 -5.454904 -2.226756	
H -1.719270 -6.177181 -1.969468	H -1.582484 -6.167573 -2.051115	
4 toluene	**5 gas phase**	**5 toluene**
H -6.228299 -0.409499 -1.664386	H 3.639787 -4.248540 -1.090223	H 3.732064 -4.220036 -1.104950
C -5.237762 -0.298753 -1.219622	H 4.186240 -2.710549 -1.797070	H 4.243690 -2.667087 -1.805213
H -4.029233 3.670913 -1.539071	H -3.637682 -4.231845 -1.147580	H -3.703197 -4.228616 -1.118503
H -5.378353 1.841154 -1.072990	H 5.019346 -3.384844 -0.385453	H 5.089968 -3.326402 -0.392809
H -4.837255 -2.411051 -1.223268	C 4.031242 -3.249232 -0.850421	C 4.100613 -3.212900 -0.861025
H -1.862013 -2.929941 -2.236385	H 2.208441 -0.002810 -3.804071	H 2.201919 -0.013763 -3.804080
H -3.230770 -3.892205 -1.658679	H -0.001739 -0.313806 -3.593415	H -0.002157 -0.350560 -3.590670
H 0.430880 -0.148748 -2.760180	H -4.174413 -2.687608 -1.847031	H -4.213902 -2.680595 -1.829111
H -2.441673 3.051801 -1.999592	H -2.199962 0.004842 -3.804390	H -2.196264 -0.035665 -3.803069
C -4.754829 0.964086 -0.888698	H -3.022001 -1.094982 -2.670273	H -3.030109 -1.115079 -2.658834
C -4.450707 -1.421544 -0.972321	H 2.605213 -4.331017 1.198302	H 2.683492 -4.334283 1.176866
C -3.014156 3.478471 -1.160630	C -4.029108 -3.233632 -0.902990	C -4.078454 -3.222298 -0.881370
H 1.541355 -2.990741 -1.982459	H 2.964998 -1.182714 -2.707589	H 2.982425 -1.175073 -2.705441
C -2.255358 -3.476161 -1.366250	H -5.021803 -3.370804 -0.448423	H -5.072265 -3.338586 -0.423423
H -0.283096 -1.423183 -1.933754	C 2.478652 -0.196938 -2.760263	C 2.477299 -0.198873 -2.760238
N -0.102825 -0.424231 -1.941225	C -2.478316 -0.142484 -2.755197	C -2.476359 -0.169178 -2.752755
H -2.567126 4.447808 -0.896081	H 2.060911 -2.495403 -0.373597	H 2.114942 -2.500074 -0.390961
H -1.586620 -4.324538 -1.159983	C -0.000093 -0.248392 -2.507981	C 0.000063 -0.283989 -2.505334
H -0.530597 2.377624 -1.617947	C 3.056397 -2.515119 0.090641	C 3.107321 -2.503885 0.080044
H 2.833458 -4.056451 -1.397634	C 2.894616 -3.291290 1.410647	C 2.958154 -3.291413 1.394782
H 1.169074 -4.312168 -0.844815	H 3.833593 -3.310682 1.985280	H 3.898734 -3.301283 1.966844
C 1.907931 -3.539725 -1.103765	H -2.619043 -4.337308 1.145661	H -2.670271 -4.332606 1.170819
C -3.486347 1.134072 -0.313214	H -2.062232 -2.486782 -0.402596	H -2.101362 -2.498466 -0.393991
C -3.174459 -1.307003 -0.404664	H 3.225270 0.537606 -2.434786	H 3.209656 0.551744 -2.438799
H -4.964868 3.247709 0.842017	H -3.180143 0.644490 -2.451820	H -3.169622 0.628806 -2.458400
O 0.137093 2.074156 -0.980092	C 1.253772 -0.182417 -1.885227	C 1.254354 -0.204572 -1.884022
C -3.038149 2.541916 0.062259	C -1.252787 -0.164693 -1.881572	C -1.251810 -0.195682 -1.879357
C -2.377229 -2.574948 -0.124068	C -3.061502 -2.509726 0.053279	C -3.098014 -2.506458 0.067860
C -2.686779 -0.014066 -0.087818	H 2.095773 -2.843750 2.014522	H 2.157129 -2.856740 2.005510
H 4.603576 -2.749571 -0.992560	C -2.911976 -3.300219 1.366291	C -2.957127 -3.292166 1.384736
H 2.416331 2.760873 -2.170364	H 5.385052 -1.715046 1.161536	H 5.415444 -1.662063 1.165590
H 6.162908 -0.925329 -1.608526	C 3.496133 -1.077209 0.347516	C 3.515447 -1.058705 0.347561
H -4.002366 -3.706081 0.812006	H -3.857006 -3.326835 1.930609	H -3.904522 -3.310017 1.945263
Si 0.002814 0.489467 -0.501588	N 1.383867 -0.114489 -0.544694	N 1.383488 -0.136994 -0.542839
C 4.310315 -1.711374 -0.825757	C 4.760177 -0.854964 0.915668	C 4.772933 -0.814324 0.921833
C 5.190402 -0.689043 -1.173017	N -1.380974 -0.103898 -0.541952	N -1.379580 -0.131543 -0.537785
C -3.920801 3.140989 1.173690	H -2.120755 -2.857499 1.983442	H -2.168257 -2.849730 2.005543
H -1.365603 -2.266741 0.179298	O -0.012402 -2.023709 1.028206	O 0.001360 -2.057066 1.024648
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C -2.983615 -3.365227 1.052387	H -5.398773 -1.719549 1.109832	H -5.422937 -1.676779 1.124862
C 2.141236 -2.600054 0.092988	H 2.913609 2.761162 -2.121535	H 2.887425 2.766551 -2.114314
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C 3.174116 3.204766 -1.512410	Si 0.000002 -0.533887 0.596555	Si 0.001178 -0.563017 0.594715
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H 5.513707 1.434126 -1.231412	C 5.232774 0.427523 1.172587	C 5.218461 0.477125 1.185728
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H	-2.373835	-4.254329	1.273173	C	3.161172	1.370159	0.310137	C	3.131234	1.381444	0.316472
H	1.168720	-2.181003	0.389098	C	-2.899613	3.448553	-1.111250	C	-2.852345	3.430341	-1.145183
H	2.897325	4.254967	-1.336405	C	2.892715	3.382621	-1.216188	C	2.842658	3.388830	-1.210276
H	-3.906077	2.506630	2.070132	H	-1.318515	2.285392	-0.244597	H	-1.284674	2.263740	-0.259225
C	2.691001	-0.078653	-0.049931	H	-2.272477	4.332222	-1.302357	H	-2.213097	4.302607	-1.347762
C	3.580309	0.970940	-0.395052	H	1.318764	2.279888	-0.266970	H	1.277822	2.260693	-0.274256
H	-3.030826	-2.745890	1.958123	C	-3.158895	1.372462	0.328773	C	-3.136732	1.377545	0.321655
H	3.665812	-3.839913	1.061771	C	4.435037	1.528260	0.870302	C	4.400056	1.562905	0.882340
N	1.396087	0.216434	0.531149	H	-3.915144	3.801713	-0.878115	H	-3.863114	3.799685	-0.916078
H	1.998334	-4.217231	1.552836	C	-5.241690	0.422252	1.155273	C	-5.232774	0.462902	1.158530
C	2.685220	-3.397741	1.294306	H	2.275027	4.267581	-1.430151	H	2.208394	4.259993	-1.431938
C	3.260646	2.445605	-0.175107	H	3.919411	3.727068	-1.022075	H	3.859272	3.755216	-1.003330
H	-3.415172	-0.072144	2.306615	C	2.333525	2.613232	-0.003263	C	2.284908	2.610303	-0.002227
H	2.274605	2.507550	0.303551	C	-2.323665	2.618387	0.052339	C	-2.287154	2.610545	0.031392
C	-1.302195	0.108033	1.925562	H	-6.233751	0.561185	1.588110	H	-6.222128	0.619427	1.591771
C	-2.410148	0.001072	2.712759	C	-4.437691	1.525066	0.878988	C	-4.412837	1.552227	0.872827
H	2.803102	-2.764339	2.183821	H	4.807017	2.533093	1.077471	H	4.752145	2.574324	1.092054
C	1.237233	0.210624	1.928987	N	-0.019933	0.644592	1.842011	N	-0.031374	0.598197	1.854649
H	5.288023	3.151794	0.291302	H	0.194166	1.628929	1.734503	H	0.141648	1.591066	1.747278
C	4.288142	3.126123	0.749892	H	-4.807502	2.527772	1.100132	H	-4.768729	2.561604	1.086286
C	0.015820	0.192539	2.533556	H	0.095436	0.322111	2.796766	H	0.136891	0.279559	2.803495
H	3.987094	4.165254	0.949234	C	2.222030	3.555088	1.209684	C	2.148947	3.550051	1.209880
H	-2.292547	-0.023465	3.794321	C	-2.175204	3.494665	1.309154	C	-2.133940	3.505001	1.275008
H	3.178065	-0.557788	2.526546	H	-1.479892	4.325744	1.117965	H	-1.430645	4.326064	1.071384
H	4.379388	2.609139	1.715547	H	1.877226	3.023478	2.107794	H	1.797829	3.015308	2.103783
C	2.484827	0.260336	2.768823	H	1.518154	4.373001	0.997207	H	1.438973	4.360034	0.987889
H	3.037412	1.197550	2.604254	H	3.190967	4.014157	1.454058	H	3.110358	4.019011	1.464976
H	0.011256	0.227891	3.622192	H	-1.797657	2.908099	2.157254	H	-1.763689	2.931688	2.135713
H	2.225038	0.193740	3.831303	H	-3.136981	3.936565	1.607978	H	-3.092861	3.960156	1.562958
4-5 dimer gas phase								**4-5 dimer toluene**			
C	1.965275	-4.762028	-0.634938					C	2.764982	3.746269	-1.150727
C	0.968405	-4.119185	-1.410274					C	1.420809	4.137792	-0.940848
C	1.211341	-3.726851	-2.748456					C	0.671041	4.781444	-1.956813
C	2.478613	-3.992702	-3.287668					C	1.297465	5.017482	-3.188195
C	3.470620	-4.623311	-2.544879					C	2.616959	4.636820	-3.416628
C	3.210267	-5.001863	-1.231105					C	3.336034	4.008776	-2.404806
N	-0.352126	-3.895635	-0.825511					N	0.805391	3.910635	0.365041
C	-1.277047	-4.870860	-0.962962					C	0.914315	4.887066	1.293487
C	-0.941258	-6.116649	-1.737408					C	0.340904	4.785825	2.564621
C	0.172232	-3.049175	-3.636077					C	-0.398618	3.707074	3.063269
C	0.651241	-1.663890	-4.101043					C	-0.904147	3.806020	4.476237
C	1.748825	-5.227589	0.802741					C	-0.769565	5.253161	-1.776836
C	2.772102	-4.592980	1.763016					C	-1.709078	4.608304	-2.813106
Si	-0.664690	-2.252457	-0.063539					C	3.627748	3.076187	-0.086295
N	0.397148	-2.077024	1.256241					C	4.106279	1.689024	-0.545618
O	-0.653579	-1.044316	-1.056888					Si	0.030775	2.269823	0.651234
N	-2.348680	-2.605044	0.600642					N	-1.283254	2.116665	-0.422468
C	-2.963814	-1.525206	1.364834					O	1.014109	1.051884	0.621929
C	-3.727501	-0.543396	0.686459					N	-0.643542	2.601211	2.332232
C	-4.269853	0.502259	1.448485					C	-1.397940	1.509963	2.939804
C	-4.088568	0.570786	2.826377					C	-0.710448	0.536416	3.706423
C	-3.363771	-0.423974	3.476835					C	-1.460300	-0.519425	4.246205
C	-2.788829	-1.489040	2.770389					C	-2.836831	-0.606447	4.059006
C	-4.027019	-0.583167	-0.809403					C	-3.497199	0.379951	3.331192
C	-3.422784	0.620858	-1.550554					C	-2.802568	1.455330	2.759952
C	-2.062710	-2.578613	3.554066					C	0.783854	0.595402	4.010960
C	-3.046562	-3.413102	4.399421					C	1.542056	-0.594738	3.400058
C	-3.072874	-3.707532	0.329721					C	-3.600039	2.532447	2.030259
C	-2.559940	-4.776049	-0.415618					C	-4.467273	1.947716	0.902045
C	-4.495347	-3.816720	0.808829					C	1.045246	0.663891	5.529780
C	-0.951961	-2.008117	4.452232					C	-4.483119	3.338057	3.005197
C	-5.544987	-0.657895	-1.074176					C	1.682447	6.140458	0.975124
C	1.799750	-6.763228	0.930511					C	-0.892392	6.788346	-1.853077
C	-0.190243	-3.915631	-4.858796					C	4.838887	3.947970	0.301780
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Si	0.769085	2.279309	-0.131991					Si	0.140003	-2.280242	-0.767396
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N	2.300567	2.528059	0.697478					C	-0.520706	-3.655498	-3.154948
C	2.813358	1.444065	1.503281					C	-1.112172	-3.745620	-4.383854
C	2.533373	1.411975	2.893800					N	0.863524	-3.875290	-0.468524
C	3.042028	0.351463	3.656124					C	0.910567	-4.869752	-1.457376
C	3.823799	-0.646281	3.077060					C	0.294320	-4.750314	-2.666790
C	4.120655	-0.584971	1.717954					C	1.394497	-4.179968	0.844402
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C	2.678635	3.374789	4.480350					C	2.408346	-4.809379	3.387391
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H	-6.048145	0.272554	-0.772838			H	2.353302	0.742571	-3.911005
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H	3.991634	-5.495487	-0.650815			H	-0.504532	-7.127839	0.676356
H	0.744508	-4.905122	1.113460			H	-0.867691	-7.143880	2.416283
H	1.042427	-7.259372	0.308351			H	-2.909626	-4.704558	2.280022
H	1.624826	-7.064928	1.973898			H	-1.719806	-4.986159	3.563474
H	2.784022	-7.152017	0.631266			H	-1.705393	-3.447869	2.677731
H	3.787895	-4.962269	1.559502			H	3.176731	-3.135615	-0.795199
H	2.533444	-4.853545	2.805256			H	5.560713	-3.782924	-0.919226
H	2.789847	-3.499447	1.668982			H	5.543664	-4.352990	0.762241
H	-0.736403	-2.886745	-3.040657			H	4.609872	-5.217220	-0.474110
H	0.677974	-4.057408	-5.519437			H	4.907508	-1.488701	-0.136033
H	-0.978090	-3.423728	-5.447715			H	3.397545	-1.220737	0.761187
H	-0.556412	-4.913868	-4.578641			H	4.788955	-2.005210	1.561125
H	0.857379	-1.010876	-3.245747			H	1.594263	-6.828835	-1.991032
H	-0.128051	-1.185768	-4.711271			H	2.770729	-5.895153	-1.036388
H	1.559609	-1.739210	-4.717794			H	1.375516	-6.609079	-0.236181
H	0.615055	-2.767253	1.963360			H	-1.733370	-2.957346	-4.799374
H	0.971713	-1.241646	1.332364			H	-0.960250	-4.643777	-4.979603

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