Supplementary Information

Crystal Structure of New 1-Phenyl Substituted Tribenzsilatranes

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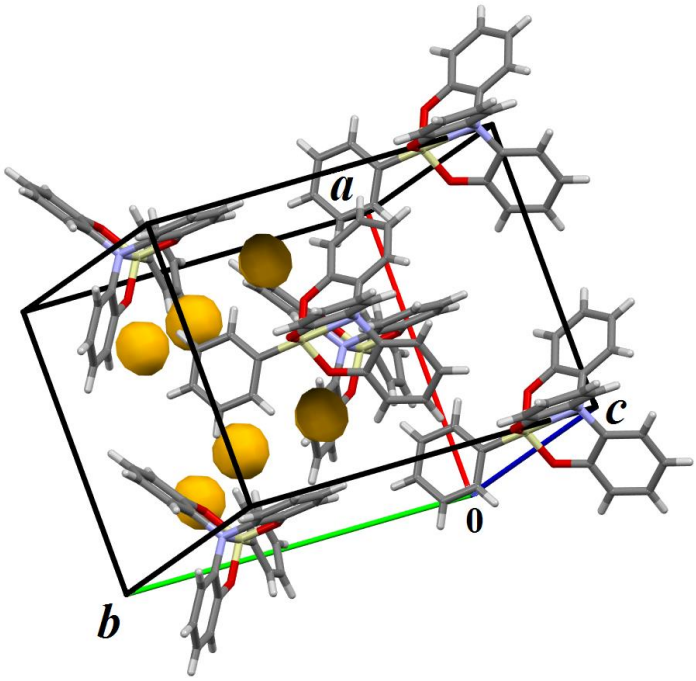

Figure S1. The voids in the molecular packing of **2a.**

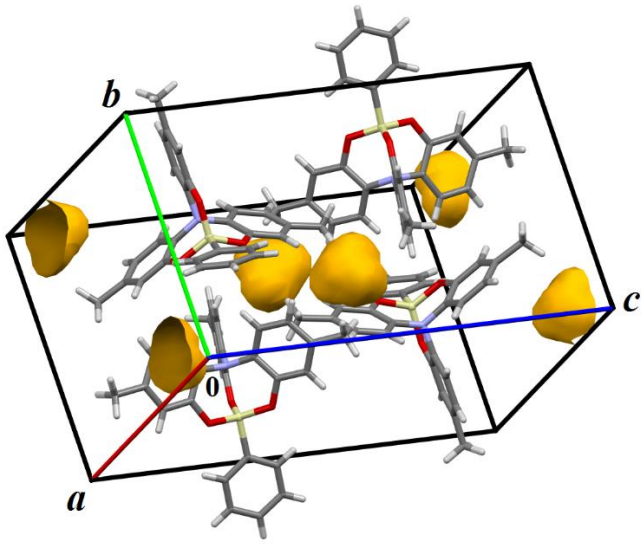

Figure S2. The voids in the molecular packing of **2b.**

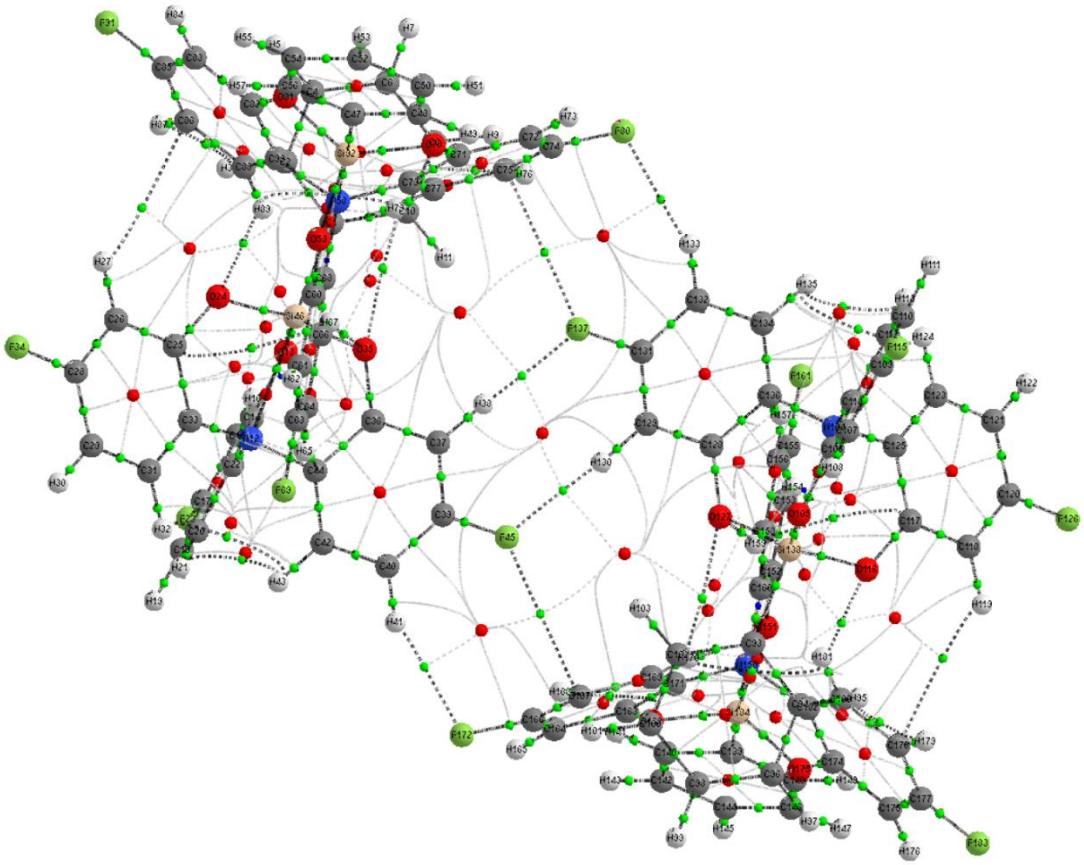

Figure S3. Crystal cell graph for **2c** from AIM analysis. Small green spheres represent bond critical points *bcp*(3, -1), red spheres are ring critical points *rcp*(3, 1).

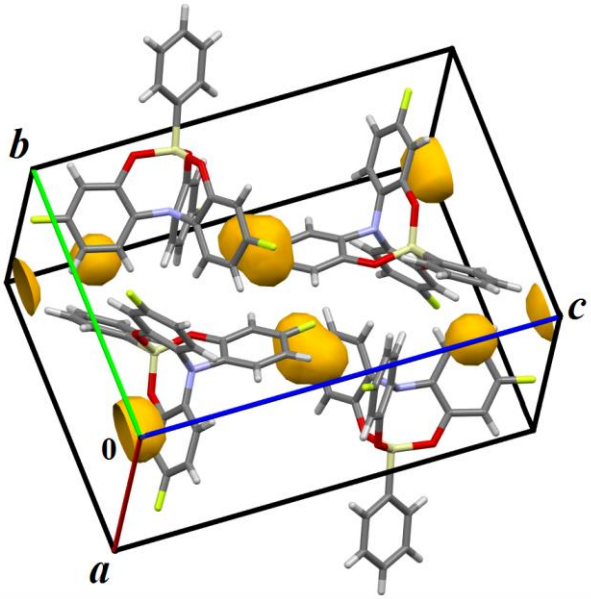

Figure S4. The voids in the molecular packing of **2c.**

Table S1. XRD Experimental and B3PW91/6-311++G(d,p) calculated (*italics*) selected geometric parameters of molecules **2a-c** (bond lengths in Å, angles in °).

Parameter	**2a**		**2b**		**2c**	
	exp.	*calc.*	exp.	*calc.*	exp.	*calc.*
Si1–O2	1.654(8)	*1.681*	1.657(2)	*1.684*	1.655(2)	*1.683*
Si1–O8	1.645(6)	*1.683*	1.663(2)	*1.682*	1.658(2)	*1.682*
Si1–O9	1.645(6)	*1.682*	1.658(2)	*1.682*	1.660(2)	*1.681*
Si1–C12	1.863(11)	*1.861*	1.850(3)	*1.863*	1.852(3)	*1.857*
O2–C3	1.342(14)	*1.353*	1.370(4)	*1.353*	1.369(4)	*1.349*
O8–C7	1.341(8)	*1.352*	1.372(4)	*1.353*	1.366(4)	*1.349*
O9–C10	1.341(8)	*1.352*	1.374(4)	*1.353*	1.365(4)	*1.349*
C3–C4	1.400(15)	*1.399*	1.387(4)	*1.398*	1.392(4)	*1.400*
C6–C7	1.390(11)	*1.399*	1.376(4)	*1.398*	1.388(4)	*1.400*
C10–C11	1.390(11)	*1.399*	1.381(4)	*1.397*	1.390(4)	*1.400*
N5–C4	1.443(13)	*1.438*	1.446(4)	*1.440*	1.444(4)	*1.437*
N5–C6	1.426(8)	*1.439*	1.451(4)	*1.438*	1.449(4)	*1.436*
N5–C11	1.426(8)	*1.438*	1.458(4)	*1.439*	1.441(4)	*1.436*
O2–Si1–O8	117.1(3)	*115.0*	116.0(1)	*115.4*	116.2(1)	*114.7*
O2–Si1–O9	117.1(3)	*116.8*	117.8(1)	*115.2*	116.3(1)	*114.6*
O8–Si1–O9	117.2(5)	*115.1*	117.5(1)	*117.1*	116.8(1)	*116.5*
O2–Si1–C12	100.3(4)	*102.1*	98.9(1)	*102.2*	102.5(1)	*103.2*
O8–Si1–C12	99.7(3)	*102.6*	101.2(1)	*101.7*	101.2(1)	*102.6*
O9–Si1–C12	99.7(3)	*102.1*	99.7(1)	*101.7*	99.5(1)	*102.5*
Si1–O2–C3	126.3(7)	*126.4*	125.7(2)	*126.1*	125.9(2)	*126.8*
Si1–O8–C7	125.3(6)	*126.2*	124.5(2)	*126.2*	126.1(2)	*127.0*
Si1–O9–C10	125.3(6)	*126.3*	124.9(2)	*126.2*	126.1(2)	*127.0*
O2–C3–C4	118.2(11)	*119.7*	118.1(3)	*119.6*	119.2(3)	*120.0*
O8–C7–C6	119.1(11)	*119.7*	119.5(3)	*119.5*	119.5(3)	*119.8*
O9–C10–C11	119.1(11)	*119.6*	119.9(3)	*119.6*	119.5(3)	*119.9*
C3–C4–N5	113.3(10)	*114.7*	113.9(3)	*114.8*	114.4(3)	*115.0*
C7–C6–N5	113.3(9)	*114.7*	114.1(3)	*114.7*	113.9(3)	*114.9*
C10–C11–N5	113.3(9)	*114.6*	112.8(3)	*114.8*	113.7(3)	*115.0*
C4–N5–C6	116.5(7)	*117.1*	114.7(2)	*117.3*	116.8(2)	*117.4*
C4–N5–C11	116.5(7)	*117.4*	116.1(2)	*117.0*	116.8(2)	*117.4*
C6–N5–C11	114.3(9)	*117.1*	117.4(2)	*117.0*	116.4(2)	*117.7*
N5–Si1–C12	179.8(4)	*179.6*	178.2(1)	*179.6*	178.0(1)	*179.5*
Si1–N5	2.329(9)	*2.463*	2.358(3)	*2.451*	2.411(3)	*2.494*
ΔN	0.300(9)	*0.357*	0.292(4)	*0.247*	0.267(4)	*0.230*
ΔSi	0.284(7)	*0.243*	0.286(3)	*0.346*	0.318(3)	*0.372*
η_e	72.4	*58.4*	72.2	*60.9*	65.8	*54.9*
Σ(O-Si-O)	351.4(3)	*346.9*	351.3(1)	*347.7*	349.3(1)	*345.8*
Σ(C-N-C)	347.4(7)	*351.6*	348.2(2)	*351.3*	350.0(2)	*352.5*
Si-O-C-C	-3.3(3)	*11.5*	-5.1(5)	*10.1*	-9.1(2)	*11.6*
	0.0(0)	*11.8*	2.0(9)	*10.4*	-7.1(6)	*11.9*

	3.3(3)	*12.2*	-8.0(4)	*9.7*	-9.7(4)	*11.1*
O-C-C-N	2.0(8)	*1.4*	0.2(0)	*1.6*	-0.7(6)	*1.6*
	0.0(0)	*1.8*	-5.7(8)	*1.9*	-2.8(8)	*1.9*
	-2.0(8)	*2.0*	2.1(5)	*1.2*	0.0(8)	*1.3*
C-C-N-Si	-0.4(6)	*-8.0*	2.7(7)	*-7.5*	6.0(1)	*-8.1*
	0.0(0)	*-8.6*	5.4(9)	*-7.9*	7.3(3)	*-8.5*
	0.4(6)	*-9.0*	2.2(3)	*-6.8*	5.4(0)	*-7.5*
C-N-Si-O	-0.8(4)	*10.5*	-4.1(5)	*9.6*	-8.2(1)	*10.6*
	0.0(0)	*11.1*	-3.7(0)	*10.1*	-8.5(6)	*11.0*
	0.8(4)	*11.6*	-4.8(0)	*9.0*	-7.9(1)	*9.9*
N-Si-O-C	2.2(2)	*-12.1*	5.1(4)	*-10.9*	9.5(7)	*-12.2*
	0.0(0)	*-12.7*	1.1(7)	*-11.3*	8.7(9)	*-12.7*
	-2.2(2)	*-13.2*	6.9(2)	*-10.4*	9.6(6)	*-11.6*

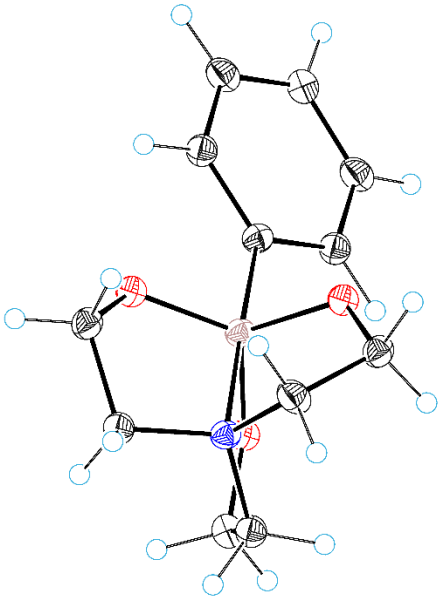

Figure S5. ORTEP drawing of phenylsilatrane (**1**) (first reported in [1]). Thermal ellipsoids are shown with 50% probability; hydrogen atoms are placed at a fixed distance using the riding model and shown as small spheres of arbitrary radii. The molecular structure of phenylsilatrane is practically the same for all three (α, β, γ) crystal modifications, only their crystal packaging being different.

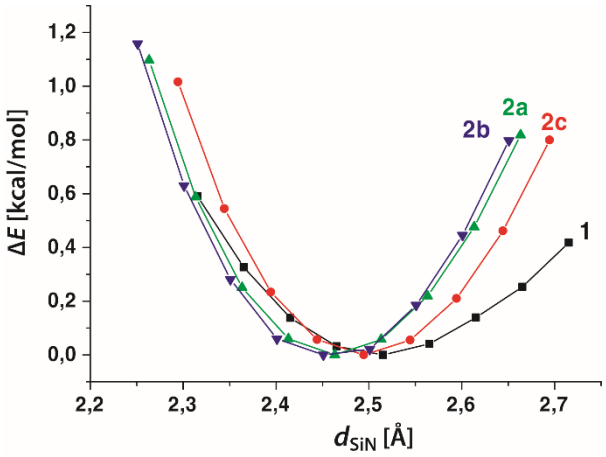

Figure S6. Potential functions of deformation of the N→Si bond in "common" silatrane Ph-Si(OCH_2CH_2)$_3$N **1** and tribenzsilatranes **2a-c**.

References

[1] L. Parkanyi, K. Simon, J. Nagy, *Acta Crystallogr. Sec. B,* **1974**, *30*, 2328.