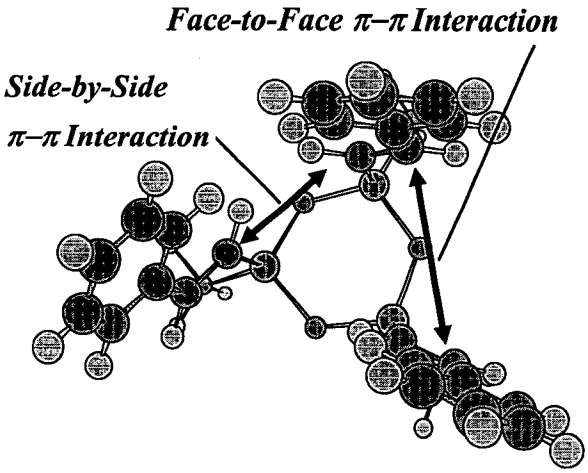
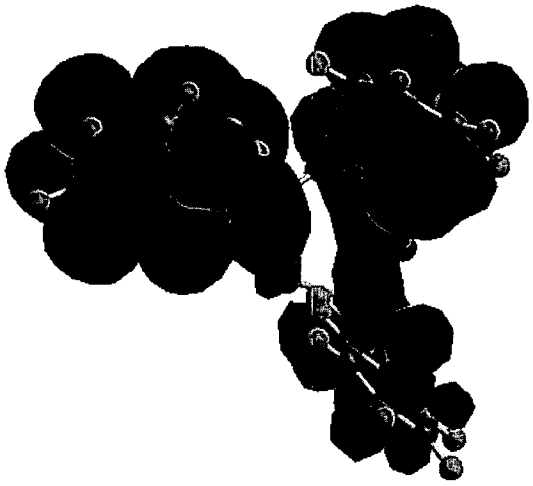
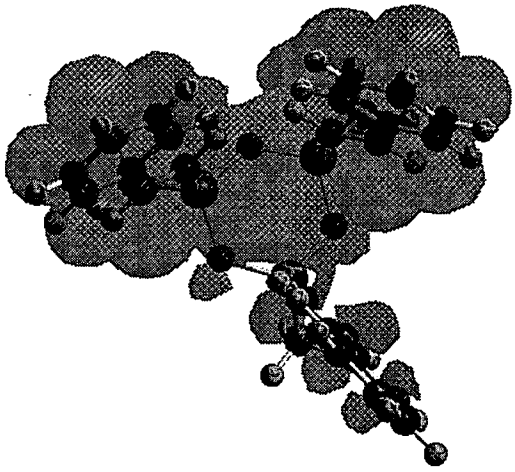
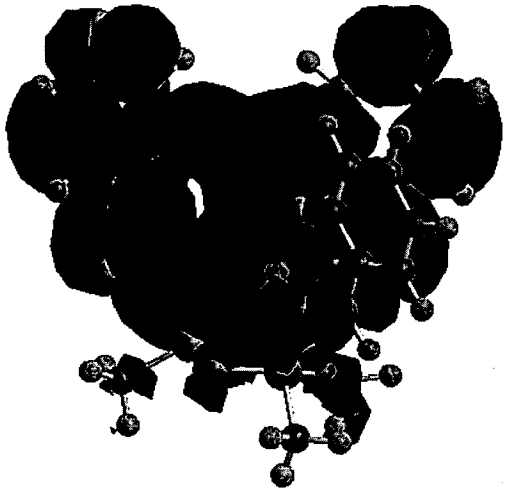


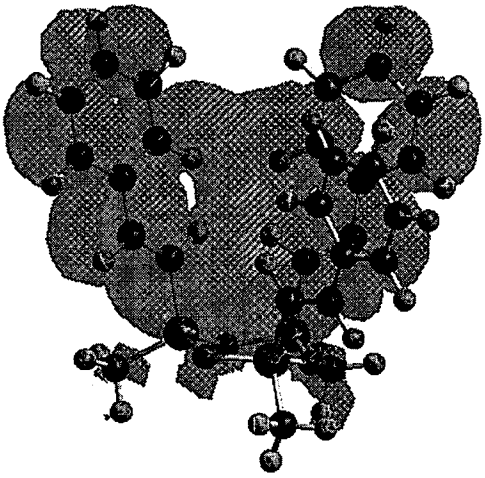


LUMO +1



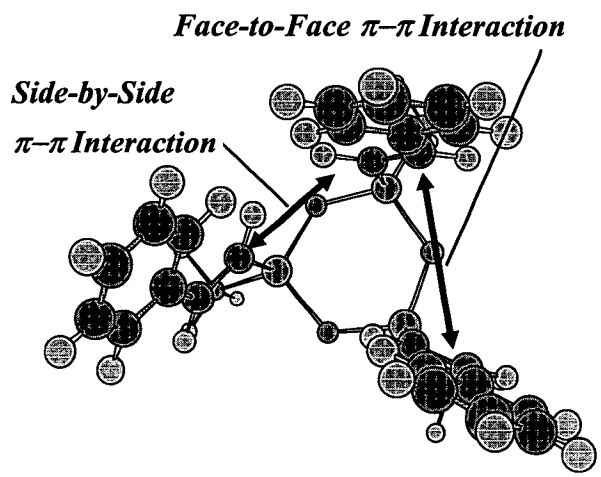
LUMO (top view)



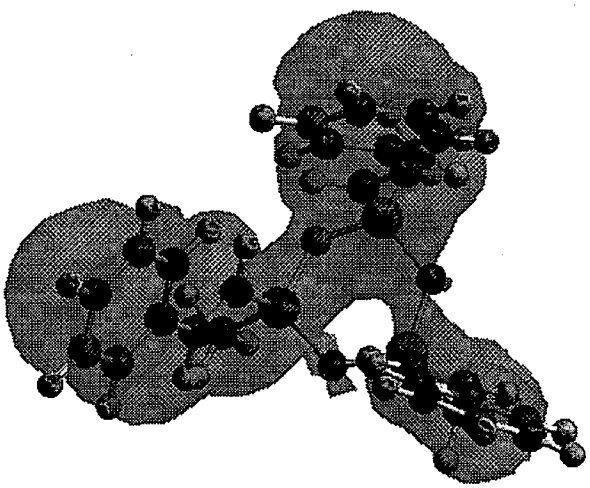


LUMO (side view)

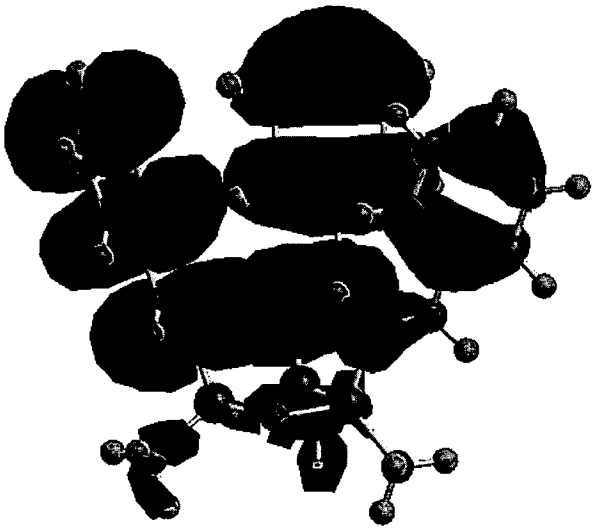
Figure 1. MO presentations of **4**-*cis* calculated using HF/LAND2DZ basis set.

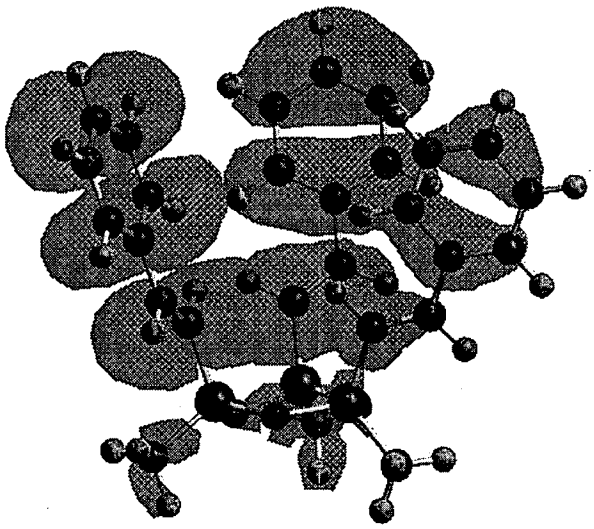


HOMO



HOMO –2 (top view)





HOMO –2 (side view)

Figure 1 (continued). MO presentations of **4-*cis*** calculated on HF/LAND2DZ basis set.

X-ray crystalographic data for *cis*-1,3,5-trimethyl-1,3,5-tri-(*E*)-styrylcyclotetrasiloxane (4-*cis*):

Table 1. Crystal data and structure refinement for **4-*cis*.**

Identification code	**4-*cis***	
Empirical formula	$C_{27}H_{30}O_3Si_3$	
Formula weight	486.78	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.9650(7) Å	α= 88.446(7) °.
	b = 11.1266(8) Å	β= 79.827(7) °.
	c = 12.3097(11) Å	γ = 81.088(6) °.
Volume	1327.18(18) $Å^3$	
Z	2	
Density (calculated)	1.218 mg/m^3	
Absorption coefficient	1.849 mm^{-1}	
F(000)	516	
Crystal size	0.45 x 0.25 x 0.2 mm^3	
Theta range for data collection	4.02 to 75.18 °.	
Index ranges	0<=h<=12, -13<=k<=13, -14<=l<=15	
Reflections collected	5479	
Independent reflections	5249 [R(int) = 0.0326]	
Completeness to theta = 75.18°	95.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	5249 / 0 / 337
Goodness-of-fit on F^2	1.071
Final R indices [I>2sigma(I)]	R1 = 0.0586, wR2 = 0.1314
R indices (all data)	R1 = 0.0680, wR2 = 0.1376
Extinction coefficient	0.0259(10)
Largest diff. peak and hole	0.358 and -0.350 e $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4-*cis***. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	0.91436(9)	0.30103(8)	0.75337(7)	0.0747(2)
C(1)	1.0154(4)	0.4258(4)	0.7233(3)	0.1016(11)
C(11)	1.0355(6)	0.1572(5)	0.7281(4)	0.0784(17)
C(12)	1.0159(5)	0.0678(5)	0.6689(4)	0.0726(15)
C(11a)	0.9710(20)	0.1421(17)	0.6973(16)	0.071(5)
C(12a)	1.0910(20)	0.0765(14)	0.7024(13)	0.061(5)
C(13)	1.1047(3)	-0.0545(3)	0.6557(3)	0.0773(8)
C(14)	1.0486(3)	-0.1405(3)	0.6107(3)	0.0851(9)
C(15)	1.1146(4)	-0.2580(3)	0.5968(3)	0.0908(9)
C(16)	1.2404(4)	-0.2912(3)	0.6262(3)	0.0929(10)
C(17)	1.3010(4)	-0.2068(4)	0.6704(3)	0.0929(10)
C(18)	1.2323(4)	-0.0880(3)	0.6859(3)	0.0875(9)
O(2)	0.8420(2)	0.2996(2)	0.88447(17)	0.0801(6)
Si(3)	0.69518(9)	0.26542(7)	0.94349(7)	0.0691(2)
C(3)	0.6210(4)	0.3682(3)	0.10593(3)	0.0860(9)
C(31)	0.7028(8)	0.1047(5)	0.9906(4)	0.0722(15)
C(32)	0.8146(7)	0.0214(5)	0.9640(4)	0.0662(16)
C(31a)	0.783(4)	0.104(3)	0.951(2)	0.078(9)
C(32a)	0.733(3)	0.032(3)	1.0070(3)	0.080(9)
C(33)	0.8240(3)	-0.1112(3)	0.9802(2)	0.0718(7)
C(34)	0.7239(3)	-0.1701(3)	1.0435(3)	0.0810(8)
C(35)	0.7400(3)	-0.2968(3)	1.0455(3)	0.0862(9)
C(36)	0.8546(3)	-0.3624(3)	0.9861(3)	0.0838(9)
C(37)	0.9540(3)	-0.3053(3)	0.9251(3)	0.0844(9)

C(38)	0.9393(3)	-0.1810(3)	0.9229(3)	0.0778(8)
O(4)	0.59597(19)	0.28052(17)	0.85008(15)	0.0708(5)
Si(5)	0.63134(8)	0.28735(7)	0.71525(7)	0.0675(2)
C(5)	0.5080(4)	0.4073(3)	0.6658(3)	0.0886(9)
C(51)	0.6305(3)	0.1383(3)	0.6545(2)	0.0725(7)
C(52)	0.6274(3)	0.0347(2)	0.7103(2)	0.0676(7)
C(53)	0.6485(3)	-0.0892(2)	0.6654(2)	0.0622(6)
C(54)	0.6687(3)	-0.1875(3)	0.7361(3)	0.0758(8)
C(55)	0.6978(3)	-0.3051(3)	0.6952(4)	0.0912(10)
C(56)	0.7066(4)	-0.3262(3)	0.5858(4)	0.0957(11)
C(57)	0.6847(4)	-0.2301(3)	0.5154(3)	0.0922(10)
C(58)	0.6557(3)	-0.1127(3)	0.5547(3)	0.0747(7)
O(6)	0.7880(2)	0.32002(18)	0.68356(15)	0.0750(5)

Table 3. Bond lengths [Å], bond angles [°] and torsion angles [°] for **4-*cis***.

Si(1)-O(6)	1.630(2)	Si(1)-O(2)	1.648(2)
Si(1)-C(1)	1.831(4)		
Si(1)-C(11)	1.847(6)	Si(1)-C(11a)	1.882(19)
C(11)-C(12)	1.307(11)	C(11a)-C(12a)	1.31(4)
C(12)-C(13)	1.500(6)	C(12a)-C(13)	1.559(16)
C(13)-C(14)	1.356(5)	C(13)-C(18)	1.381(5)
C(14)-C(15)	1.370(5)	C(15)-C(16)	1.360(5)
C(16)-C(17)	1.364(5)	C(17)-C(18)	1.393(5)
O(2)-Si(3)	1.610(2)	Si(3)-O(4)	1.633(2)
Si(3)-C(3)	1.828(3)		
Si(3)-C(31)	1.860(6)	Si(3)-C(31a)	1.88(4)
C(31)-C(32)	1.332(12)	C(31a)-C(32a)	1.16(7)
C(32)-C(33)	1.474(6)	C(32a)-C(33)	1.71(3)
C(33)-C(38)	1.375(4)	C(33)-C(34)	1.390(4)
C(34)-C(35)	1.393(4)	C(35)-C(36)	1.359(4)
C(36)-C(37)	1.362(4)	C(37)-C(38)	1.368(4)
O(4)-Si(5)	1.637(2)	Si(5)-O(6)	1.635(2)
Si(5)-C(5)	1.837(3)	Si(5)-C(51)	1.839(3)
C(51)-C(52)	1.327(4)	C(52)-C(53)	1.470(4)
C(53)-C(58)	1.381(4)	C(53)-C(54)	1.392(4)
C(54)-C(55)	1.383(4)	C(55)-C(56)	1.359(5)
C(56)-C(57)	1.373(5)	C(57)-C(58)	1.375(4)

O(6)-Si(1)-O(2)	106.03(11)	O(6)-Si(1)-C(1)	109.56(15)
O(2)-Si(1)-C(1)	111.57(15)		
O(6)-Si(1)-C(11)	115.9(2)	O(6)-Si(1)-C(11a)	90.5(7)
O(2)-Si(1)-C(11)	106.36(17)	O(2)-Si(1)-C(11a)	111.3(6)
C(1)-Si(1)-C(11)	107.4(2)	C(1)-Si(1)-C(11a)	124.4(6)
C(12)-C(11)-Si(1)	123.7(6)	C(12a)-C(11a)-Si(1)	124.8(19)
C(11)-C(12)-C(13)	125.1(6)	C(11a)-C(12a)-C(13)	112.9(19)
C(14)-C(13)-C(12)	114.4(4)	C(14)-C(13)-C(12a)	149.7(8)
C(18)-C(13)-C(12)	127.5(4)	C(18)-C(13)-C(12a)	92.0(8)
C(14)-C(13)-C(18)	118.1(3)	C(13)-C(14)-C(15)	121.5(3)
C(16)-C(15)-C(14)	120.5(4)	C(15)-C(16)-C(17)	119.7(3)
C(16)-C(17)-C(18)	119.5(3)	C(13)-C(18)-C(17)	120.7(3)
Si(3)-O(2)-Si(1)	131.35(13)	O(2)-Si(3)-O(4)	106.62(11)
O(2)-Si(3)-C(3)	110.08(14)	O(4)-Si(3)-C(3)	110.36(14)
O(2)-Si(3)-C(31)	113.8(2)	O(2)-Si(3)-C(31a)	87.7(11)
O(4)-Si(3)-C(31)	105.75(17)	O(4)-Si(3)-C(31a)	111.0(7)
C(3)-Si(3)-C(31)	110.0(2)	C(3)-Si(3)-C(31a)	127.2(8)
C(32)-C(31)-Si(3)	122.8(6)	C(32a)-C(31a)-Si(3)	122(4)
C(31)-C(32)-C(33)	126.9(6)	C(31a)-C(32a)-C(33)	111(4)
C(38)-C(33)-C(32)	116.1(4)	C(38)-C(33)-C(32a)	147.0(14)
C(34)-C(33)-C(32)	125.6(4)	C(34)-C(33)-C(32a)	94.7(14)
C(38)-C(33)-C(34)	118.2(3)	C(33)-C(34)-C(35)	120.1(3)
C(36)-C(35)-C(34)	119.7(3)	C(35)-C(36)-C(37)	120.5(3)
C(36)-C(37)-C(38)	120.3(3)	C(37)-C(38)-C(33)	121.2(3)
Si(3)-O(4)-Si(5)	131.70(13)	O(6)-Si(5)-O(4)	106.60(10)
O(6)-Si(5)-C(5)	110.36(14)	O(4)-Si(5)-C(5)	109.38(14)
O(6)-Si(5)-C(51)	107.83(12)	O(4)-Si(5)-C(51)	110.42(12)
C(5)-Si(5)-C(51)	112.10(14)	C(52)-C(51)-Si(5)	125.1(2)
C(51)-C(52)-C(53)	127.6(3)	C(58)-C(53)-C(54)	118.2(3)
C(58)-C(53)-C(52)	122.9(3)	C(54)-C(53)-C(52)	118.8(3)
C(55)-C(54)-C(53)	120.3(3)	C(56)-C(55)-C(54)	120.6(3)
C(55)-C(56)-C(57)	119.7(3)	C(56)-C(57)-C(58)	120.5(3)
C(57)-C(58)-C(53)	120.8(3)	Si(1)-O(6)-Si(5)	130.57(13)

O(6)-Si(1)-C(11)-C(12)	-7.9(5)	O(6)-Si(1)-C(11a)-C(12a)	165.3(15)
O(2)-Si(1)-C(11)-C(12)	109.6(4)	O(2)-Si(1)-C(11a)-C(12a)	-87.3(16)
C(1)-Si(1)-C(11)-C(12)	-130.8(4)	C(1)-Si(1)-C(11a)-C(12a)	50.9(18)
C(11)-Si(1)-C(11)-C(12)	4.5(13)	C(11)-Si(1)-C(11a)-C(12a)	-3.6(9)

Si(1)-C(11)-C(12)-C(13)	-173.7(3)	Si(1)-C(11a)-C(12a)-C(13)	176.3(10)
C(11)-C(12)-C(13)-C(14)	166.4(4)	C(11a)-C(12a)-C(13)-C(14)	-2(2)
C(11)-C(12)-C(13)-C(18)	-12.1(6)	C(11a)-C(12a)-C(13)-C(18)	-175.3(13)
C(12)-C(13)-C(14)-C(15)	-177.7(3)	C(12a)-C(13)-C(14)-C(15)	-171.6(11)
C(18)-C(13)-C(14)-C(15)	1.0(5)	C(13)-C(14)-C(15)-C(16)	-1.2(5)
C(14)-C(15)-C(16)-C(17)	0.4(5)	C(15)-C(16)-C(17)-C(18)	0.7(5)
C(14)-C(13)-C(18)-C(17)	0.0(5)	C(16)-C(17)-C(18)-C(13)	-0.8(5)
C(12)-C(13)-C(18)-C(17)	178.5(3)	C(12a)-C(13)-C(18)-C(17)	176.3(6)
O(6)-Si(1)-O(2)-Si(3)	25.1(2)	C(1)-Si(1)-O(2)-Si(3)	144.3(2)
C(11)-Si(1)-O(2)-Si(3)	-98.9(3)	C(11a)-Si(1)-O(2)-Si(3)	-72.0(8)
Si(1)-O(2)-Si(3)-O(4)	-21.8(2)	Si(1)-O(2)-Si(3)-C(3)	-141.54(19)
Si(1)-O(2)-Si(3)-C(31)	94.4(2)	Si(1)-O(2)-Si(3)-C(31a)	89.5(7)
O(2)-Si(3)-C(31)-C(32)	-9.1(4)	O(2)-Si(3)-C(31a)-C(32a)	164(2)
O(4)-Si(3)-C(31)-C(32)	107.6(4)	O(4)-Si(3)-C(31a)-C(32a)	-89(2)
C(3)-Si(3)-C(31)-C(32)	-133.2(4)	C(3)-Si(3)-C(31a)-C(32a)	50(3)
C(31)-Si(3)-C(31)-C(32)	1.9(15)	C(31)-Si(3)-C(31a)-C(32a)	-5.8(15)
Si(3)-C(31)-C(32)-C(33)	-168.6(3)	Si(3)-C(31a)-C(32a)-C(33)	170.6(12)
C(31)-C(32)-C(33)-C(38)	164.6(4)	C(31a)-C(32a)-C(33)-C(38)	6(3)
C(31)-C(32)-C(33)-C(34)	-12.0(6)	C(31a)-C(32a)-C(33)-C(34)	-169(2)
C(32)-C(33)-C(34)-C(35)	174.9(3)	C(32a)-C(33)-C(34)-C(35)	175.4(8)
C(38)-C(33)-C(34)-C(35)	-1.7(4)	C(33)-C(34)-C(35)-C(36)	0.6(5)
C(34)-C(35)-C(36)-C(37)	0.3(5)	C(35)-C(36)-C(37)-C(38)	-0.1(5)
C(36)-C(37)-C(38)-C(33)	-1.0(5)	C(34)-C(33)-C(38)-C(37)	1.9(4)
C(32)-C(33)-C(38)-C(37)	-175.0(3)	C(32a)-C(33)-C(38)-C(37)	-172.8(14)
O(2)-Si(3)-O(4)-Si(5)	17.64(19)	C(3)-Si(3)-O(4)-Si(5)	137.18(18)
C(31)-Si(3)-O(4)-Si(5)	-103.9(3)	C(31)-Si(3)-O(4)-Si(5)	-76.4(12)
Si(3)-O(4)-Si(5)-O(6)	-17.92(19)	Si(3)-O(4)-Si(5)-C(5)	-137.24(18)
Si(3)-O(4)-Si(5)-C(51)	98.94(18)	O(6)-Si(5)-C(51)-C(52)	104.5(3)
O(4)-Si(5)-C(51)-C(52)	-11.6(3)	C(5)-Si(5)-C(51)-C(52)	-133.8(3)
Si(5)-C(51)-C(52)-C(53)	-169.5(2)	C(51)-C(52)-C(53)-C(58)	-9.6(5)
C(51)-C(52)-C(53)-C(54)	167.3(3)	C(58)-C(53)-C(54)-C(55)	1.2(4)
C(52)-C(53)-C(54)-C(55)	-175.8(3)	C(53)-C(54)-C(55)-C(56)	-0.2(5)
C(54)-C(55)-C(56)-C(57)	-0.9(5)	C(55)-C(56)-C(57)-C(58)	0.9(5)
C(56)-C(57)-C(58)-C(53)	0.2(5)	C(54)-C(53)-C(58)-C(57)	-1.2(4)
C(52)-C(53)-C(58)-C(57)	175.6(3)	O(2)-Si(1)-O(6)-Si(5)	-25.3(2)
C(1)-Si(1)-O(6)-Si(5)	-145.78(19)	C(11)-Si(1)-O(6)-Si(5)	92.5(2)
C(11)-Si(1)-O(6)-Si(5)	87.1(6)	O(4)-Si(5)-O(6)-Si(1)	22.5(2)
C(5)-Si(5)-O(6)-Si(1)	141.15(18)	C(51)-Si(5)-O(6)-Si(1)	-96.11(18)