Supporting information

Table 1. Coordinates (x 10^4) and Equivalent isotropic heat parameters ($Å^2x10^3$) non hydrogenic atoms in structure **4e**

	X	У	z	U(eq)
8(1)	8493(1)	1145(1)	3017(1)	40(1)
N(1)	8803(1)	219(2)	3945(1)	36(1)
N(2)	9763(1)	-2696(2)	4144(1)	32(1)
N(3)	10634(1)	-2099(2)	4402(1)	41(1)
N(4)	11118(1)	-2611(2)	3854(1)	42(1)
0(1)	7502(1)	1016(2)	2640(1)	59(1)
0(2)	8900(1)	2649(2)	3185(1)	62(1)
C(1)	8323(1)	-1203(2)	4102(1)	31(1)
C(2)	7564(2)	-878(3)	4598(2)	44(1)
C(3)	7121(2)	-2357(3)	4841(2)	50(1)
C(4)	7858(2)	-3451(3)	5365(2)	58(1)
C(3)	8598(2)	-3805(3)	4861(2)	49(1)
C(6)	9051(1)	-2328(2)	4630(1)	34(1)
C(7)	9692(1)	-3588(2)	3425(1)	33(1)
C(8)	10551(1)	-3534(2)	3239(1)	32(1)
C(9)	10886(1)	-4340(2)	2539(1)	35(1)
C(10)	10275(2)	-5237(3)	1914(2)	58(1)
C(11)	10593(2)	-6029(3)	1271(2)	71(1)
C(12)	11511(2)	-5954(3)	1237(2)	62(1)
C(13)	12116(2)	-5066(3)	1844(2)	63(1)
C(14)	11812(2)	-4250(3)	2490(2)	50(1)
C(15)	9039(1)	166(2)	2283(1)	40(1)
C(16)	8534(2)	-897(3)	1692(2)	57(1)
C(17)	8947(3)	-1608(4)	1087(2)	83(1)
C(18)	9848(3)	-1257(4)	1073(2)	89(1)
C(19)	10349(3)	-223(5)	1657(2)	85(1)
C(20)	9952(2)	502(3)	2270(2)	62(1)

Table2. Bond lengths (Å) in structure **4e**

S(l)-0(2)	1.427(2)	C(5)-C(6)	1.522(3)
S(l)-0(l)	1.430(2)	C(7)-C(8)	1.360(3)
S(1)-N(1)	1.607(2)	C(8)-C(9)	1.469(3)
S(1)-C(15)	1.757(2)	C(9)-C(14)	1.380(3)
N(1)-C(1)	1.465(2)	C(9)-C(10)	1.383(3)
N(2)-C(7)	1.335(2)	C(10)-C(11)	1.378(3)
N(2)-N(3)	1.344(2)	C(11)-C(12)	1.362(4)
N(2)-C(6)	1.461(2)	C(12)-C(13)	1.359(4)
N(3)-N(4)	1.308(2)	C(13)-C(14)	1.382(3)
N(4)-C(8)	1.358(2)	C(15)-C(20)	1.375(3)
C(1)-C(6)	1.524(3)	C(15)-C(16)	1.375(3)
C(1)-C(2)	1.524(3)	C(16)-C(17)	1.377(4)
C(2)-C(3)	1.522(3)	C(17)-C(18)	1.362(5)
C(3)-C(4)	1.512(3)	C(18)-C(19)	1.352(5)
C(4)-C(5)	1.512(3)	C(19)-C(20)	1.379(4)

Table 3. Valence angles (°) in structure **4e**

0(2)-S(1)-0(1)	118.8(2)	C(5)-C(6)-C(1)	111.8(2)
0(2)-S(1)-N(1)	106.1(2)	N(2)-C(7)-C(8)	105.6(2)
0(1)-S(1)-N(1)	111.2(2)	N(4)-C(8)-C(7)	108.2(2)
0(2)-S(1)-C(15)	108.7(2)	N(4)-C(8)-C(9)	122.4(2)
0(1)-S(1)-C(15)	106.1(2)	C(7)-C(8)-C(9)	129.4(2)
N(1)-S(1)-C(15)	105.2(9)	C(14)-C(9)-C(10)	118.1(2)
C(1)-N(1)-S(1)	121.5(1)	C(14)-C(9)-C(8)	121.7(2)
C(7)-N(2)-N(3)	110.1(2)	C(10)-C(9)-C(8)	120.2(2)
C(7)-N(2)-C(6)	129.3(2)	C(11)-C(10)-C(9)	120.4(2)
N(3)-N(2)-C(6)	120.7(2)	C(12)-C(11)-C(10)	121.0(3)
N(4)-N(3)-N(2)	107.8(2)	C(13)-C(12)-C(11)	119.0(2)
N(3)-N(4)-C(8)	108.4(2)	C(12)-C(13)-C(14)	121.0(2)
N(1)-C(1)-C(6)	108.8(2)	C(9)-C(14)-C(13)	120.5(2)
N(1)-C(1)-C(2)	111.6(2)	C(20)-C(15)-C(16)	119.9(2)
C(6)-C(1)-C(2)	110.5(2)	C(20)-C(15)-S(1)	120.4(2)
C(3)-C(2)-C(1)	112.2(2)	C(16)-C(15)-S(1)	119.6(2)
C(4)-C(3)-C(2)	111.4(2)	C(15)-C(16)-C(17)	119.6(3)
C(3)-C(4)-C(5)	111.1(2)	C(18)-C(17)-C(16)	120.1(3)
C(4)-C(5)-C(6)	111.1(2)	C(19)-C(18)-C(17)	120.5(3)
N(2)-C(6)-C(5)	110.2(2)	C(18)-C(19)-C(20)	120.5(3)
N(2)-C(6)-C(1)	111.0(2)	C(15)-C(20)-C(19)	119.4(3)