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SUPPORTING INFORMATION

Title: New Anellated 4*H*-1,4,2-Diazaphospholes

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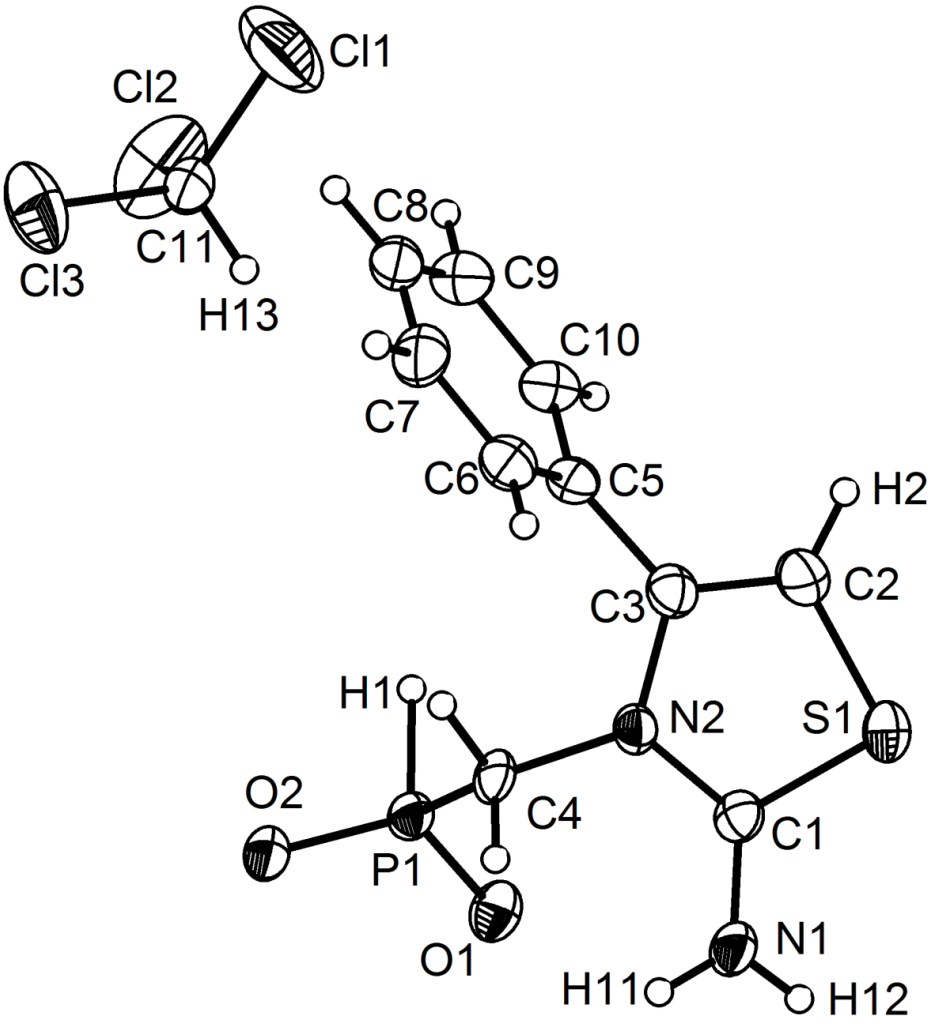

Figure 1: Molecular structure of compound **9**. Thermal ellipsoids are drawn at 50 % probability level.

Table 1: Atom distances in the crystal structure of compound **9**.

Atom distances in Å			
S1−C1	1.729(4)	C2−C3	1.334(6)
S1−C2	1.733(4)	C3−C5	1.477(6)
P1−O1	1.484(3)	C5−C10	1.379(6)
P1−O2	1.495(3)	C5−C6	1.399(6)
P1−C4	1.831(4)	C6−C7	1.373(7)
P1−H1	1.38(4)	C7−C8	1.372(8)
N1−C1	1.310(6)	C8−C9	1.386(7)
N2−C4	1.473(5)	C9−C10	1.393(6)
N2−C3	1.416(5)	Cl1−C11	1.732(4)
N2−C1	1.348(5)	Cl2−C11	1.747(4)
N1−H12	0.86(3)	Cl3−C11	1.729(4)
N1−H11	0.88(3)	C11−H13	0.93(4)

Table 2: Bond angles in the crystal structure of compound **9**.

Bond angles in °			
C1−S1−C2	90.10(19)	C7−C8−C9	119.5(5)
O1−P1−O2	119.34(15)	C8−C9−C10	119.7(4)
O1−P1−C4	110.06(17)	C5−C10−C9	120.7(4)
O2−P1−C4	107.19(17)	S1−C2−H2	124.00
C4−P1−H1	101.0(16)	C3−C2−H2	124.00
O1−P1−H1	109.2(16)	P1−C4−H41	109.00
O2−P1−H1	108.5(16)	P1−C4−H42	109.00
C1−N2−C3	113.4(3)	N2−C4−H41	109.00
C1−N2−C4	121.9(3)	N2−C4−H42	109.00
C3−N2−C4	124.0(3)	H41−C4−H42	108.00
H11−N1−H12	115(3)	C5−C6−H6	120.00
C1−N1−H11	124(2)	C7−C6−H6	120.00
C1−N1−H12	120(2)	C6−C7−H7	119.00
S1−C1−N1	122.8(3)	C8−C7−H7	119.00
N1−C1−N2	125.6(4)	C7−C8−H8	120.00
S1−C1−N2	111.6(3)	C9−C8−H8	120.00
S1−C2−C3	113.0(3)	C8−C9−H9	120.00
C2−C3−C5	126.5(4)	C10−C9−H9	120.00
N2−C3−C2	111.9(4)	C5−C10−H10	120.00
N2−C3−C5	121.6(3)	C9−C10−H10	120.00
P1−C4−N2	112.2(3)	Cl1−C11−Cl2	111.0(2)
C3−C5−C6	121.1(4)	Cl1−C11−Cl3	112.1(2)
C3−C5−C10	120.0(4)	Cl2−C11−Cl3	110.2(2)
C6−C5−C10	118.9(4)	Cl1−C11−H13	110(3)
C5−C6−C7	120.1(4)	Cl2−C11−H13	108(3)
C6−C7−C8	121.2(4)	Cl3−C11−H13	105(3)

Table 3: Torsion angles in the crystal structure of compound **9**.

Torsion angles in °			
C2−S1−C1−N1	-177.9(4)	S1−C2−C3−N2	0.3(4)
C2−S1−C1−N2	0.7(3)	S1−C2−C3−C5	179.6(3)
C1−S1−C2−C3	-0.6(3)	N2−C3−C5−C6	58.9(5)
O1−P1−C4−N2	52.7(3)	N2−C3−C5−C10	-125.2(4)
O2−P1−C4−N2	-176.1(2)	C2−C3−C5−C6	-120.3(5)
C3−N2−C1−S1	-0.7(4)	C2−C3−C5−C10	55.6(6)
C3−N2−C1−N1	177.9(4)	C3−C5−C6−C7	177.3(4)
C4−N2−C1−S1	170.6(3)	C10−C5−C6−C7	1.3(6)
C4−N2−C1−N1	-10.9(6)	C3−C5−C10−C9	-177.2(4)
C1−N2−C3−C2	0.2(5)	C6−C5−C10−C9	-1.2(7)
C1−N2−C3−C5	-179.1(4)	C5−C6−C7−C8	-0.5(7)
C4−N2−C3−C2	-170.8(3)	C6−C7−C8−C9	-0.5(7)
C4−N2−C3−C5	9.9(6)	C7−C8−C9−C10	0.6(7)
C1−N2−C4−P1	-80.3(4)	C8−C9−C10−C5	0.2(7)
C3−N2−C4−P1	90.0(4)		