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Electronic Supplementary Information

Detailed studies of interaction of 3-chloroaniline with O,O'-diphenylphosphorylisothiocyanate

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Table S1 Selected bond lengths (Å) and bond angles (°) for **1**

Bond lengths					
N(17)–C(18)	1.386(2)	Cl(27)–C(25)	1.739(2)	P(1)–O(3)	1.5826(14)
N(20)–C(18)	1.346(2)	P(1)–N(17)	1.6471(15)	P(1)–O(10)	1.5697(14)
N(20)–C(21)	1.426(3)	P(1)–O(2)	1.4602(14)	S(19)–C(18)	1.6617(19)
Bond angles					
N(17)–C(18)–N(20)	113.03(16)	O(10)–P(1)–N(17)	109.86(8)	P(1)–N(17)–C(18)	125.79(12)
C(18)–N(20)–C(21)	124.66(16)	O(2)–P(1)–O(3)	114.48(8)	S(19)–C(18)–N(17)	121.57(14)
O(2)–P(1)–N(17)	118.06(8)	O(2)–P(1)–O(10)	109.87(7)	S(19)–C(18)–N(20)	125.39(14)
O(3)–P(1)–N(17)	100.54(7)	O(3)–P(1)–O(10)	102.70(7)		
Torsion angles					
N(20)–C(18)–N(17)–P(1)	176.55(13)	O(2)–P(1)–N(17)–C(18)	–52.33(17)	S(19)–C(18)–N(17)–P(1)	–4.4(2)

Table S2 Selected bond lengths (Å) and bond angles (°) for **2**

Bond lengths					
N(8)–C(6)	1.443(10)	N(13)–C(12)	1.181(10)	S(11)–C(12)	1.636(8)
Cl(1)–C(2)	1.759(7)				
Bond angles					
S(11)–C(12)–N(13)	178.6(7)				

Table S3 Selected bond lengths (Å) and bond angles (°) for **3·0.5(C_6H_6)**

Bond lengths					
P(11)–O(12)	1.482(2)	P(11)–O(14)	1.619(2)	Cl(1)–C(2)	1.750(3)
P(11)–O(13)	1.492(2)	P(11)–O(21)	1.619(2)	N(8)–C(6)	1.477(3)
Bond angles					
O(12)–P(11)–O(13)	118.15(11)	O(12)–P(11)–O(21)	112.20(12)	O(13)–P(11)–O(21)	104.63(11)
O(12)–P(11)–O(14)	104.95(11)	O(13)–P(11)–O(14)	111.53(11)	O(14)–P(11)–O(21)	104.72(10)

Table S4 Selected bond lengths (Å) and bond angles (°) for **4**

Bond lengths					
Cl(1)–C(2)	1.734(3)	N(8)–C(13)	1.428(4)	N(10)–C(11)	1.469(4)
N(8)–C(6)	1.440(4)	N(10)–C(9)	1.316(4)	S(14)–C(9)	1.690(3)
N(8)–C(9)	1.363(4)				
Bond angles					
N(8)–C(9)–N(10)	117.8(3)	S(14)–C(9)–N(8)	121.3(2)	S(14)–C(9)–N(10)	120.9(2)
Torsion angles					
C(5)–C(6)–N(8)–C(9)	–93.4(4)	C(7)–C(6)–N(8)–C(9)	88.3(4)	C(7)–C(6)–N(8)–C(13)	–93.8(4)
C(5)–C(6)–N(8)–C(13)	84.5(4)				

Table S5. Hydrogen bond lengths (Å) and angles (°) for **1–4**

	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
1[a]	N(17)–H(17)···O(2)$^{\#1}$	0.88	1.91	2.7458(19)	159
	N(20)–H(20)···O(2)$^{\#1}$	0.88	2.11	2.905(2)	149
2[b]	N(8)–H(8A)···N(13)$^{\#1}$	0.91	2.00	2.904(8)	173
	N(8)–H(8B)···S(11)$^{\#2}$	0.91	2.43	3.306(6)	162
	N(8)–H(8C)···N(13)$^{\#3}$	0.91	1.95	2.832(9)	163
3·0.5(C$_6$H$_6$)[c]	N(8)–H(8A)···O(13)$^{\#1}$	0.89	1.96	2.850(3)	175
	N(8)–H(8B)···O(13)$^{\#2}$	0.89	1.92	2.785(3)	163
	N(8)–H(8C)···O(12)$^{\#2}$	0.89	1.79	2.668(3)	171
4[d]	N(10)–H(10)···S(14)$^{\#1}$	0.86	2.60	3.400(3)	156

[a] Symmetry transformations used to generate equivalent atoms: #1 x, 3/2 – y, –1/2 + z.
[b] Symmetry transformations used to generate equivalent atoms: #1 x, 1 + y, z; #2 x, 1/2 – y, 1/2 + z; #3 x, 1/2 – y, –1/2 + z.
[c] Symmetry transformations used to generate equivalent atoms: #1 1 – x, 1 – y, 1 – z; #2 1 + x, y, z.
[d] Symmetry transformations used to generate equivalent atoms: #1 1 – x, 2 – y, –z.

Table S6. π···π bond lengths (Å) and angles (°) for **1** and **3·0.5(C$_6$H$_6$)**[a]

	Cg(*I*)	Cg(*J*)	*d*[Cg(*I*)–Cg(*J*)]	*α*	*β*
1[b]	Cg(2)	Cg(2)$^{\#1}$	3.644(3)	0.0(3)	18.8
	Cg(2)	Cg(4)$^{\#1}$	3.693(5)	39.6(4)	21.4
	Cg(3)	Cg(3)$^{\#2}$	3.6611(13)	0.03(11)	16.5
	Cg(4)	Cg(2)$^{\#1}$	3.693(5)	39.6(4)	24.3
	Cg(4)	Cg(4)$^{\#1}$	3.752(6)	0.0(4)	21.9
3·0.5(C$_6$H$_6$)[c]	Cg(2)	Cg(3)$^{\#1}$	3.765(2)	3.14(14)	19.1
	Cg(3)	Cg(2)$^{\#1}$	3.765(2)	3.14(14)	20.9

[a] Cg(*I*)–Cg(*J*): distance between ring centroids; *α*: dihedral angle between planes Cg(*I*) and Cg(*J*); *β*: angle Cg(*I*) → Cg(*J*) vector and normal to plane *I*.
[b] Symmetry transformations used to generate equivalent atoms: #1 1 – x, 1 – y, 1 – z; #2 –x, 1 – y, –z. Cg(2): C(11)–C(12)–C(13)–C(14)–C(15)–C(16), Cg(3): C(21)–C(22)–C(23)–C(24)–C(25)–C(26), Cg(4): C(11B)–C(12B)–C(13B)–C(14B)–C(15B)–C(16B).
[c] Symmetry transformations used to generate equivalent atoms: #1 x, y, z. Cg(2): C(22)–C(23)–C(24)–C(25)–C(26)–C(27), Cg(3): C(2)–C(3)–C(4)–C(5)–C(6)–C(7).