Supporting information

Supramolecular motifs formed by CH_3/Cl-substituted arene groups: evidence for structural differences in thiophosphoramides and similarities in their complexes

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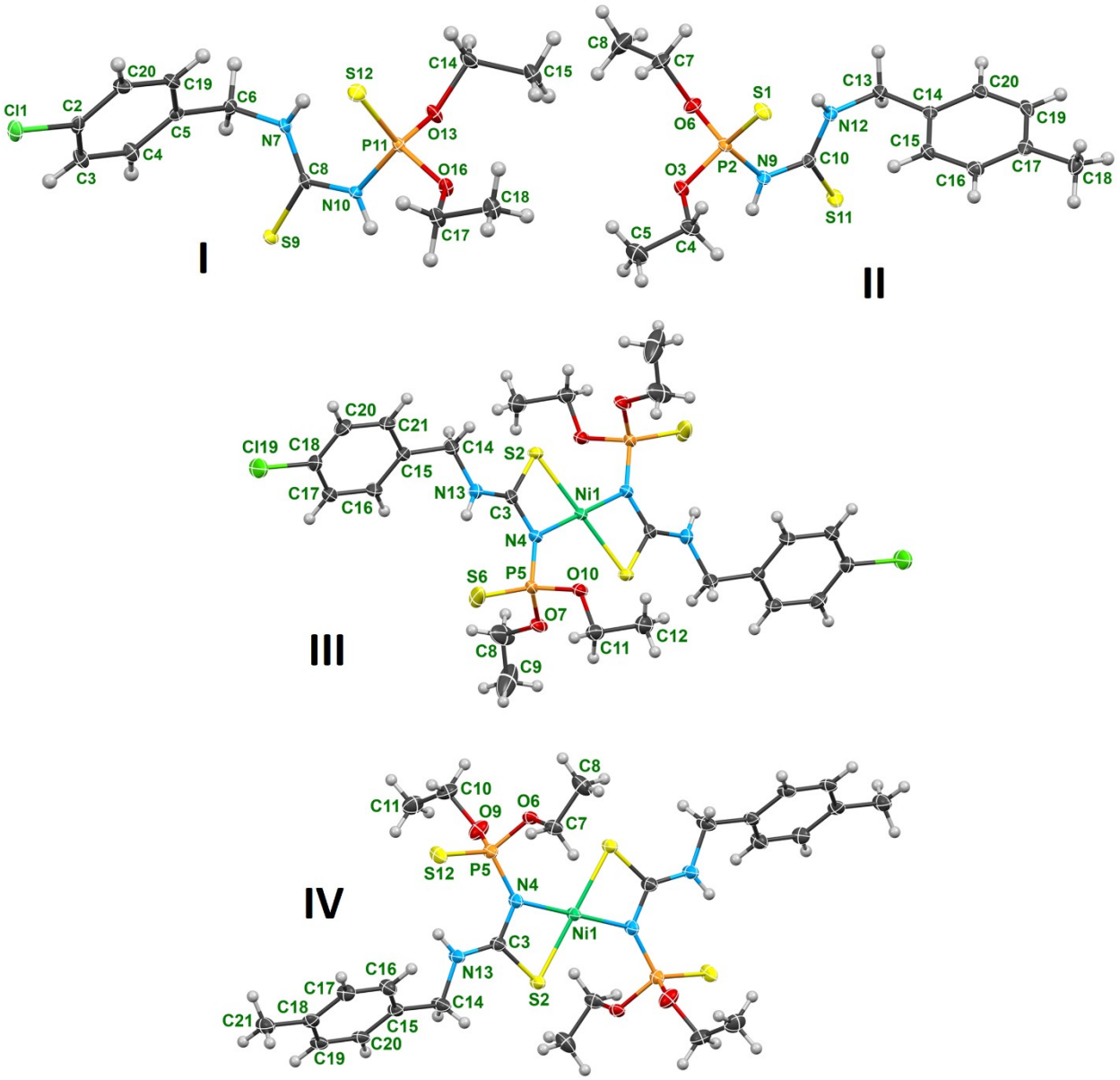

Fig. S1 The molecular structure and atom-labeling scheme for structures (**I**–**IV**). Displacement ellipsoids are drawn at the 50% probability level.

Table S1 Selected geometric parameters of structure **I** (Å, °)

Cl1—C2	1.7495 (14)	C8—N10	1.3772 (18)
C2—C3	1.382 (2)	N10—P11	1.6731 (12)
C2—C20	1.388 (2)	P11—S12	1.9306 (5)
C3—C4	1.391 (2)	P11—O13	1.5676 (10)
C4—C5	1.389 (2)	P11—O16	1.5671 (10)
C5—C6	1.5141 (19)	O13—C14	1.4647 (17)
C5—C19	1.393 (2)	C14—C15	1.499 (2)
C6—N7	1.4650 (17)	O16—C17	1.4686 (16)
N7—C8	1.3341 (18)	C17—C18	1.498 (2)
C8—S9	1.6839 (14)	C19—C20	1.386 (2)
Cl1—C2—C3	119.53 (11)	C8—N10—P11	129.28 (10)
Cl1—C2—C20	118.98 (12)	N10—P11—S12	114.70 (4)
C3—C2—C20	121.48 (13)	N10—P11—O13	101.81 (6)
C2—C3—C4	118.78 (13)	S12—P11—O13	115.90 (5)
C3—C4—C5	121.07 (14)	N10—P11—O16	102.34 (6)
C4—C5—C6	120.86 (13)	S12—P11—O16	116.58 (4)
C4—C5—C19	118.81 (13)	O13—P11—O16	103.48 (6)
C6—C5—C19	120.32 (12)	P11—O13—C14	123.23 (9)
C5—C6—N7	112.67 (11)	O13—C14—C15	111.20 (12)
C6—N7—C8	123.97 (12)	P11—O16—C17	123.71 (9)
N7—C8—S9	123.07 (10)	O16—C17—C18	108.43 (11)
N7—C8—N10	117.15 (12)	C5—C19—C20	121.03 (13)
S9—C8—N10	119.78 (11)	C2—C20—C19	118.83 (14)

Table S2 Selected geometric parameters of structure **II** (Å, °)

S1—P2	1.9276 (6)	C10—N12	1.337 (2)
P2—O3	1.5682 (13)	N12—C13	1.450 (2)
P2—O6	1.5700 (13)	C13—C14	1.515 (2)
P2—N9	1.6714 (15)	C14—C15	1.387 (3)
O3—C4	1.470 (2)	C14—C20	1.397 (2)
C4—C5	1.496 (3)	C15—C16	1.390 (3)
O6—C7	1.461 (2)	C16—C17	1.391 (3)
C7—C8	1.496 (3)	C17—C18	1.506 (3)
N9—C10	1.376 (2)	C17—C19	1.393 (3)
C10—S11	1.6807 (18)	C19—C20	1.386 (3)
S1—P2—O3	116.52 (5)	S11—C10—N12	123.11 (14)
S1—P2—O6	116.08 (5)	C10—N12—C13	123.59 (15)
O3—P2—O6	102.54 (7)	N12—C13—C14	113.68 (15)
S1—P2—N9	115.87 (6)	C13—C14—C15	122.83 (16)
O3—P2—N9	102.11 (7)	C13—C14—C20	118.93 (16)
O6—P2—N9	101.44 (7)	C15—C14—C20	118.24 (16)
P2—O3—C4	121.85 (11)	C14—C15—C16	120.64 (17)
O3—C4—C5	106.86 (16)	C15—C16—C17	121.42 (18)
P2—O6—C7	121.92 (12)	C16—C17—C18	121.37 (19)
O6—C7—C8	107.73 (16)	C16—C17—C19	117.71 (17)
P2—N9—C10	129.50 (13)	C18—C17—C19	120.90 (18)
N9—C10—S11	119.95 (13)	C17—C19—C20	121.12 (17)
N9—C10—N12	116.95 (16)	C14—C20—C19	120.85 (17)

Table S3 Hydrogen-bond geometry of structure **II** (Å, °)

D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
C4—H42···O6^{i}	0.97	2.54	3.476 (3)	161

Symmetry code: (*i*) *x*+1, *y*, *z*.

Table S4 Selected geometric parameters of structure **III** (Å, °)

Ni1—C3^{i}	2.503 (3)	P5—O10	1.573 (2)
Ni1—N4^{i}	1.906 (2)	O7—C8	1.457 (4)
Ni1—S2^{i}	2.2274 (7)	C8—C9	1.423 (7)
Ni1—P5^{i}	3.2190 (7)	O10—C11	1.452 (4)
Ni1—S2	2.2274 (7)	C11—C12	1.498 (5)
Ni1—C3	2.503 (3)	N13—C14	1.460 (4)
Ni1—N4	1.906 (2)	C14—C15	1.510 (4)
Ni1—P5	3.2190 (7)	C15—C16	1.391 (4)
S2—C3	1.727 (3)	C15—C21	1.392 (4)
C3—N4	1.343 (4)	C16—C17	1.392 (4)
C3—N13	1.317 (4)	C17—C18	1.375 (5)
N4—P5	1.647 (2)	C18—Cl19	1.741 (3)
P5—S6	1.9336 (11)	C18—C20	1.386 (5)
P5—O7	1.571 (2)	C20—C21	1.385 (5)
C3^{i}—Ni1—N4^{i}	31.96 (10)	Ni1—C3—N13	175.1 (2)
C3^{i}—Ni1—S2^{i}	42.32 (7)	S2—C3—N13	124.5 (2)
N4^{i}—Ni1—S2^{i}	74.27 (7)	N4—C3—N13	126.5 (3)
C3^{i}—Ni1—P5^{i}	54.97 (7)	C3—N4—Ni1	99.36 (18)
N4^{i}—Ni1—P5^{i}	23.15 (7)	C3—N4—P5	130.3 (2)
S2^{i}—Ni1—P5^{i}	97.25 (2)	Ni1—N4—P5	129.79 (14)
C3^{i}—Ni1—S2	137.68 (7)	N4—P5—Ni1	27.06 (9)
N4^{i}—Ni1—S2	105.73 (7)	N4—P5—S6	116.30 (10)
S2^{i}—Ni1—S2	179.99	Ni1—P5—S6	143.30 (4)
P5^{i}—Ni1—S2	82.75 (2)	N4—P5—O7	106.19 (13)
C3^{i}—Ni1—C3	180.00	Ni1—P5—O7	87.43 (9)
N4^{i}—Ni1—C3	148.04 (10)	S6—P5—O7	114.85 (10)
S2^{i}—Ni1—C3	137.68 (7)	N4—P5—O10	101.61 (12)
P5^{i}—Ni1—C3	125.03 (7)	Ni1—P5—O10	86.33 (8)
S2—Ni1—C3	42.32 (7)	S6—P5—O10	115.35 (10)
C3^{i}—Ni1—N4	148.04 (10)	O7—P5—O10	100.56 (11)
N4^{i}—Ni1—N4	179.99	P5—O7—C8	120.8 (3)
S2^{i}—Ni1—N4	105.73 (7)	O7—C8—C9	110.1 (3)

P5^{i}—Ni1—N4	156.85 (7)	P5—O10—C11	121.39 (18)
S2—Ni1—N4	74.27 (7)	O10—C11—C12	107.2 (3)
C3^{i}—Ni1—P5	125.03 (7)	C3—N13—C14	123.4 (3)
N4^{i}—Ni1—P5	156.85 (7)	N13—C14—C15	111.4 (3)
S2^{i}—Ni1—P5	82.75 (2)	C14—C15—C16	121.8 (3)
P5^{i}—Ni1—P5	180.00	C14—C15—C21	119.1 (3)
S2—Ni1—P5	97.25 (2)	C16—C15—C21	119.1 (3)
C3—Ni1—N4	31.96 (10)	C15—C16—C17	120.6 (3)
C3—Ni1—P5	54.97 (7)	C16—C17—C18	119.0 (3)
N4—Ni1—P5	23.15 (7)	C17—C18—Cl19	119.2 (3)
Ni1—S2—C3	77.41 (10)	C17—C18—C20	121.8 (3)
Ni1—C3—S2	60.27 (9)	Cl19—C18—C20	119.0 (2)
Ni1—C3—N4	48.68 (14)	C18—C20—C21	118.7 (3)
S2—C3—N4	108.9 (2)	C15—C21—C20	120.8 (3)

Symmetry code: (*i*) −*x*, −*y*+2, −*z*+1.

Table S5 Selected geometric parameters of structure **IV** (Å, °)

Ni1—C3^{i}	2.502 (3)	P5—S12	1.9370 (9)
Ni1—N4^{i}	1.911 (2)	O6—C7	1.468 (3)
Ni1—S2^{i}	2.2262 (6)	C7—C8	1.491 (4)
Ni1—P5^{i}	3.2506 (6)	O9—C10	1.452 (3)
Ni1—S2	2.2262 (6)	C10—C11	1.492 (5)
Ni1—C3	2.502 (3)	N13—C14	1.465 (4)
Ni1—N4	1.911 (2)	C14—C15	1.511 (4)
Ni1—P5	3.2506 (6)	C15—C16	1.399 (4)
S2—C3	1.729 (3)	C15—C20	1.386 (4)
C3—N4	1.348 (4)	C16—C17	1.382 (4)
C3—N13	1.316 (4)	C17—C18	1.392 (4)
N4—P5	1.646 (2)	C18—C19	1.392 (4)
P5—O6	1.5724 (19)	C18—C21	1.507 (4)
P5—O9	1.576 (2)	C19—C20	1.387 (4)
C3^{i}—Ni1—N4^{i}	32.15 (9)	Ni1—C3—N13	175.4 (2)
C3^{i}—Ni1—S2^{i}	42.41 (6)	S2—C3—N13	124.0 (2)

N4^{i}—Ni1—S2^{i}	74.56 (7)	N4—C3—N13	126.8 (2)
C3^{i}—Ni1—P5^{i}	54.13 (6)	C3—N4—Ni1	98.87 (16)
N4^{i}—Ni1—P5^{i}	22.12 (7)	C3—N4—P5	128.61 (19)
S2^{i}—Ni1—P5^{i}	96.499 (19)	Ni1—N4—P5	131.96 (13)
C3^{i}—Ni1—S2	137.59 (6)	N4—P5—Ni1	25.92 (8)
N4^{i}—Ni1—S2	105.44 (7)	N4—P5—O6	105.85 (11)
S2^{i}—Ni1—S2	179.99	Ni1—P5—O6	85.18 (7)
P5^{i}—Ni1—S2	83.501 (19)	N4—P5—O9	102.68 (11)
C3^{i}—Ni1—C3	180.00	Ni1—P5—O9	91.73 (7)
N4^{i}—Ni1—C3	147.85 (9)	O6—P5—O9	100.80 (11)
S2^{i}—Ni1—C3	137.59 (6)	N4—P5—S12	116.36 (8)
P5^{i}—Ni1—C3	125.87 (6)	Ni1—P5—S12	141.21 (4)
S2—Ni1—C3	42.41 (6)	O6—P5—S12	113.91 (8)
C3^{i}—Ni1—N4	147.85 (9)	O9—P5—S12	115.43 (9)
N4^{i}—Ni1—N4	179.99	P5—O6—C7	118.87 (15)
S2^{i}—Ni1—N4	105.44 (7)	O6—C7—C8	107.4 (2)
P5^{i}—Ni1—N4	157.88 (7)	P5—O9—C10	123.07 (18)
S2—Ni1—N4	74.56 (7)	O9—C10—C11	107.7 (2)
C3^{i}—Ni1—P5	125.87 (6)	C3—N13—C14	122.7 (2)
N4^{i}—Ni1—P5	157.88 (7)	N13—C14—C15	111.3 (2)
S2^{i}—Ni1—P5	83.501 (19)	C14—C15—C16	122.0 (3)
P5^{i}—Ni1—P5	180.00	C14—C15—C20	119.6 (2)
S2—Ni1—P5	96.499 (19)	C16—C15—C20	118.4 (2)
C3—Ni1—N4	32.15 (9)	C15—C16—C17	120.4 (3)
C3—Ni1—P5	54.13 (6)	C16—C17—C18	121.5 (3)
N4—Ni1—P5	22.12 (7)	C17—C18—C19	117.7 (2)
Ni1—S2—C3	77.35 (9)	C17—C18—C21	121.0 (3)
Ni1—C3—S2	60.24 (8)	C19—C18—C21	121.2 (3)
Ni1—C3—N4	48.98 (12)	C18—C19—C20	121.1 (3)
S2—C3—N4	109.22 (19)	C19—C20—C15	120.8 (2)

Symmetry code: (*i*) −*x*+1, −*y*, −*z*+1.

Table S6 The scale factors of energy components

k_{ele}	k_{pol}	k_{dis}	k_{rep}
1.057	0.740	0.871	0.618

Table S7 The interaction energies for the different molecular pairs in structure **I** (energy values are in kJ/mole). *R* is the distance between molecular centroids in Å.

N	**Symmetry operation**	***R***	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
1	–*x*, –*y*, –*z*	7.36	–76.2	–14.3	–25.7	94.6	–55.1
1	–*x*, –*y*, –*z*	11.84	–4.5	–1.4	–26	19.7	–16.2
1	–*x*, –*y*, –*z*	9.93	–1.7	–1.9	–6.8	1.6	–8.2
1	–*x*, –*y*, –*z*	9.49	–5.4	–1.2	–23.7	23.1	–13
2	*x*, *y*, *z*	10.04	–12	–3.3	–27.8	26.3	–23.1
2	*x*, *y*, *z*	7.63	–11.1	–3.3	–26.4	18.3	–25.9
2	*x*, *y*, *z*	7.67	–14.3	–4.4	–50.6	39.4	–38.1
1	–*x*, –*y*, –*z*	6.79	–11.3	–2	–24.9	21.6	–21.8
1	–*x*, –*y*, –*z*	10.58	–4.2	–1	–5.8	0.6	–9.9
1	–*x*, –*y*, –*z*	10.49	–10.3	–2	–40.2	34.5	–26
1	–*x*, –*y*, –*z*	9.08	–1.4	–0.3	–3.9	0	–5.1
	$\sum \frac{1}{2} E.N$		–94.9	–23.05	–183.3	181.85	–164.75

Table S8 The interaction energies for the different molecular pairs in structure **II** (energy values are in kJ/mole). *R* is the distance between molecular centroids in Å.

N	**Symmetry operation**	***R***	$\mathbf{E_{ele}}$	$\mathbf{E_{pol}}$	$\mathbf{E_{dis}}$	$\mathbf{E_{rep}}$	$\mathbf{E_{tot}}$
1	–*x*, –*y*, –*z*	11.79	–0.8	–0.4	–10	2.7	–8.2
2	*x*, *y*, *z*	5.8	–11.6	–5.7	–52.5	35.2	–40.5
2	*x*, *y*, *z*	10.79	–9.5	–2.9	–23.1	13.3	–24
1	–*x*, –*y*, –*z*	7.59	–24.5	–3.9	–62.2	58.6	–46.7
2	*x*, *y*, *z*	12.31	2.2	–0.3	–8	0	–4.8
1	–*x*, –*y*, –*z*	9.92	0.4	–0.2	–7.7	1.9	–5.3
1	–*x*, –*y*, –*z*	6.7	–79.8	–15.9	–30.7	98.8	–61.8
1	–*x*, –*y*, –*z*	15.54	1.2	–0.2	–8.8	0	–6.6
1	–*x*, –*y*, –*z*	12.08	1.8	–0.9	–22	0	–17.9
1	–*x*, –*y*, –*z*	7.3	–17.3	–6	–27	19.5	–34.2
1	–*x*, –*y*, –*z*	9.18	–1.6	–0.6	–9.9	7	–6.4
1	–*x*, –*y*, –*z*	16.42	–0.4	0	–8.5	0	–7.9
	$\sum \frac{1}{2} E.N$		–79.4	–22.95	–177	142.75	–166.8