



STRUCTURAL
CHEMISTRY

Volume 74 (2018)

Supporting information for article:

Different coordination modes of *trans*-2-[(2-methoxyphenyl)imino]-methyl}phenoxide in rare-earth complexes: influence of the metal cation radius and the number of ligands on steric congestion and ligand coordination modes

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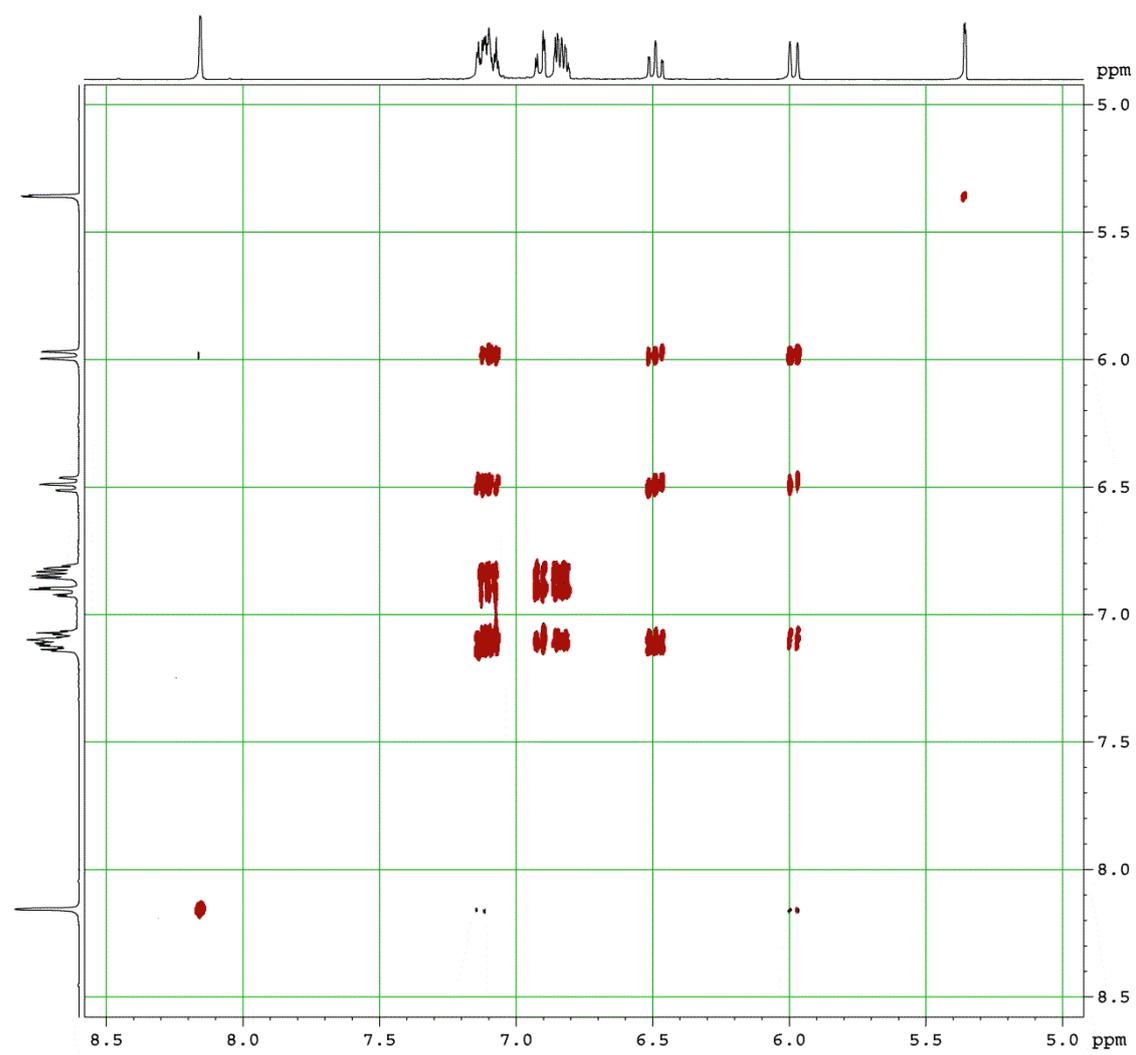


Figure S1 The ¹H-¹H COSY spectrum of Y(CH₃O-C₆H₄N=CH-C₆H₄-O)₃, (**3**), in CD₂Cl₂ at 300MHz and 299K.

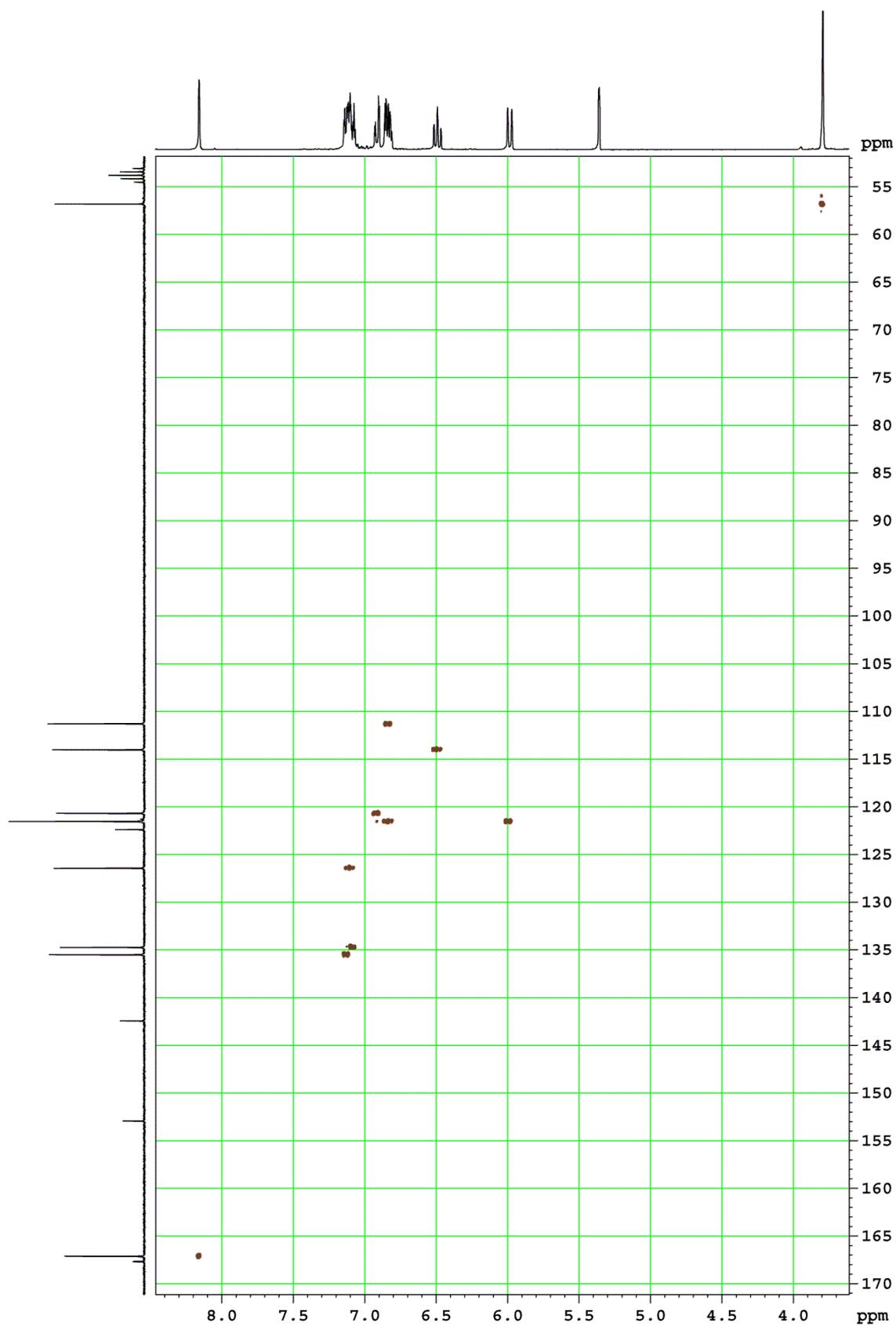


Figure S2 The ^1H - ^{13}C HSQC spectrum of $\text{Y}(\text{CH}_3\text{O}-\text{C}_6\text{H}_4\text{N}=\text{CH}-\text{C}_6\text{H}_4-\text{O})_3$, (**3**) in CD_2Cl_2 at 299K.

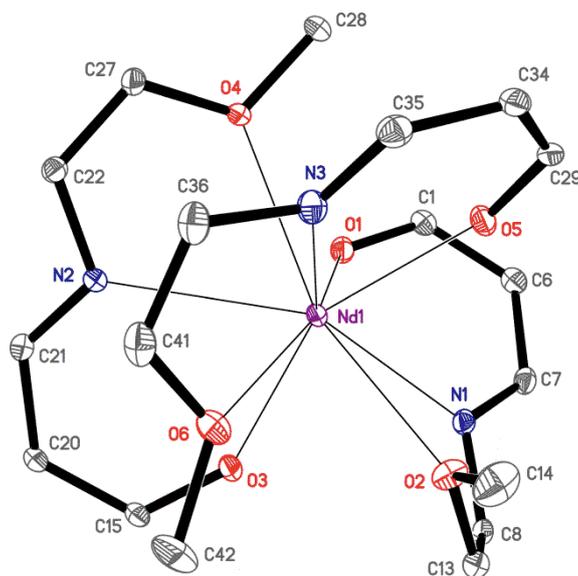


Figure S3 The environment about the Nd atom in $\text{Nd}(\text{CH}_3\text{O}-\text{C}_6\text{H}_4\text{N}=\text{CH}-\text{C}_6\text{H}_4-\text{O})_3$, (**2**). Displacement ellipsoids are drawn at the 30% probability level and all H atoms and four C atoms of each Ph-group are omitted for clarity. The Schiff-base ligand is $\kappa^3\text{O},\text{O}',\text{N}$ coordinated to the metal cation.

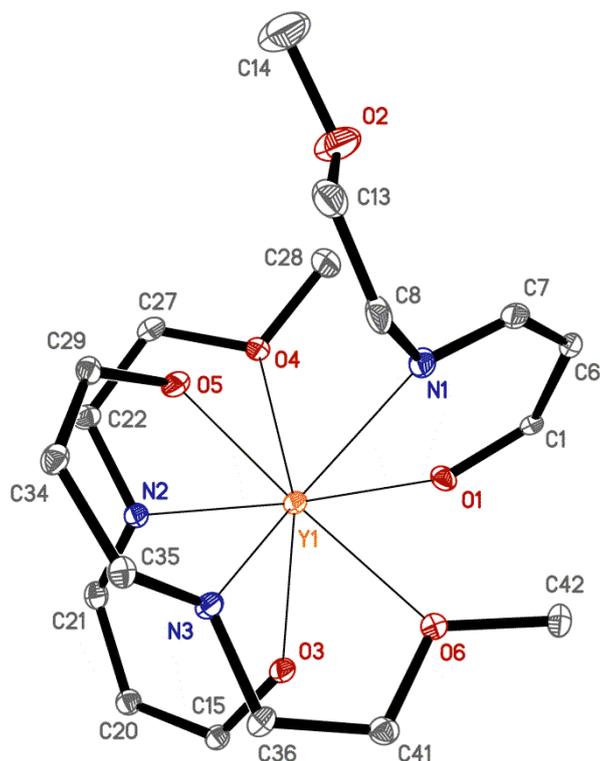


Figure S4 The environment about the Y atom in $\text{Y}(\text{CH}_3\text{O}-\text{C}_6\text{H}_4\text{N}=\text{CH}-\text{C}_6\text{H}_4-\text{O})_3$, (**3**). Displacement ellipsoids are drawn at the 30% probability level and all H atoms and four C atoms of each Ph-group are omitted for clarity. Two Schiff-base ligands exhibit $\kappa^3\text{O},\text{O}',\text{N}$ -coordination mode, one ligand is $\kappa^2\text{O},\text{N}$ -coordinated. Only one molecule is shown.

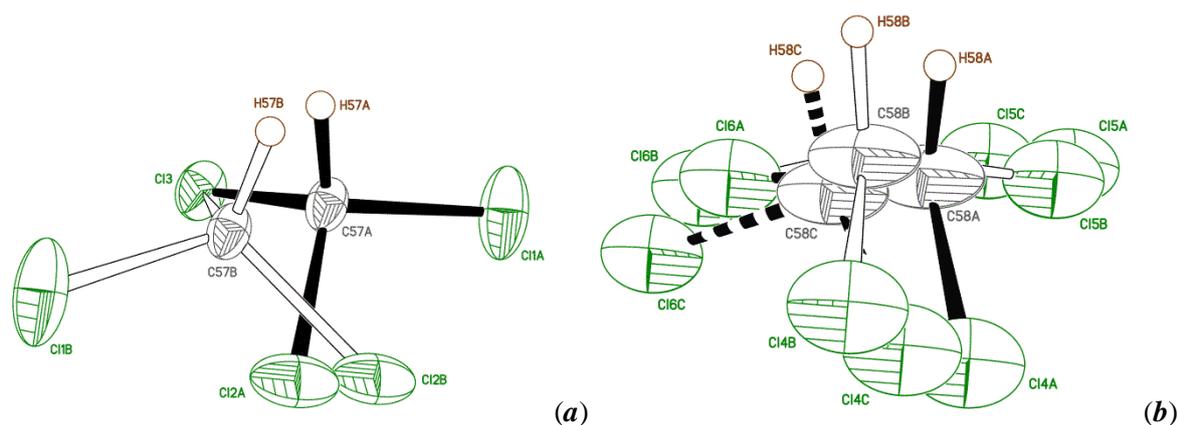


Figure S5 Disordered non-coordinating chloroform molecules in $\text{Na}[\text{Y}(\text{CH}_3\text{O}-\text{C}_6\text{H}_4\text{N}=\text{CH}-\text{C}_6\text{H}_4-\text{O})_4] \cdot (\text{CHCl}_3)_2$, **(5)** $\cdot (\text{CHCl}_3)_2$. Displacement ellipsoids are drawn at the 30% probability level. The disorder ratios are 0.773(2):0.227(2) for atoms C57A, C11A, C12A / C57B, C11B, C12B (**a**) and 0.293(3):0.497(3):0.210(3) for atoms C58A, C14A, C15A, C16A / C58B, C14B, C15B, C16B / C58C, C14C, C15C, C16C (**b**). In the second molecule for each component of disorder, C58-Cl bond distances are constrained to be 1.760(4) Å; Cl \cdots Cl distances are set to be equal within 0.004 Å.

Table S1 Selected distances (Å) in complexes $\text{La}(\text{CH}_3\text{O}-\text{C}_6\text{H}_4\text{N}=\text{CH}-\text{C}_6\text{H}_4-\text{O})_3$ or **(1)**, $\text{Nd}(\text{CH}_3\text{O}-\text{C}_6\text{H}_4\text{N}=\text{CH}-\text{C}_6\text{H}_4-\text{O})_3$ or **(2)**, and $\text{Y}(\text{CH}_3\text{O}-\text{C}_6\text{H}_4\text{N}=\text{CH}-\text{C}_6\text{H}_4-\text{O})_3$ or **(3)**.

	(1), Ln=La	(2), Ln=Nd	(3), Ln=Y, molecule 1	(3), Ln=Y, molecule 2	
Ln1—O1	2.324 (3)	2.3113 (15)	2.181 (3)	Y2—O7	2.174 (3)
Ln1—O2	2.781 (3)	2.6736 (15)	4.465 (3)	Y2—O8	4.452 (3)
Ln1—O3	2.365 (3)	2.2676 (14)	2.190 (3)	Y2—O9	2.185 (3)
Ln1—O4	2.860 (3)	2.6104 (14)	2.630 (3)	Y2—O10	2.744 (3)
Ln1—O5	2.329 (3)	2.2922 (14)	2.183 (3)	Y2—O11	2.183 (3)
Ln1—O6	2.839 (3)	2.8590 (16)	2.576 (3)	Y2—O12	2.650 (3)
Ln1—N1	2.747 (3)	2.6311 (17)	2.572 (3)	Y2—N4	2.538 (3)
Ln1—N2	2.749 (3)	2.6778 (17)	2.522 (3)	Y2—N5	2.489 (3)
Ln1—N3	2.769 (3)	2.7104 (18)	2.512 (3)	Y2—N6	2.524 (3)

C7—N1	1.288 (5)	1.281 (3)	1.294 (5)	C49—N4	1.287 (5)
C21—N2	1.290 (5)	1.296 (3)	1.298 (5)	C63—N5	1.302 (5)
C35—N3	1.292 (5)	1.295 (3)	1.296 (5)	C77—N6	1.305 (5)
N1—C8	1.427 (5)	1.421 (3)	1.454 (5)	N4—C50	1.456 (5)
N2—C22	1.436 (5)	1.431 (2)	1.426 (5)	N5—C64	1.434 (5)
N3—C36	1.433 (5)	1.426 (3)	1.425 (5)	N6—C78	1.426 (5)
C6—C7	1.432 (5)	1.452 (3)	1.442 (6)	C48—C49	1.431 (6)
C20—C21	1.444 (6)	1.450 (3)	1.433 (5)	C62—C63	1.446 (5)
C34—C35	1.443 (6)	1.440 (3)	1.441 (5)	C76—C77	1.445 (5)

Table S2 Selected distances (Å) in $[\text{Y}_2(\text{CH}_3\text{O}-\text{C}_6\text{H}_4\text{N}=\text{CH}-\text{C}_6\text{H}_4-\text{O})_3\text{Cl}_2(\text{MeO})(\text{MeOH})]\cdot(\text{CH}_3\text{OH})\cdot(\text{THF})$ or **(4)** $\cdot(\text{MeOH})\cdot(\text{THF})$.

Y1—Cl1	2.7078 (8)	Y2—O5	2.175 (2)	C21—N2	1.296 (4)
Y2—Cl2	2.6406 (9)	Y2—O6	2.484 (2)	C35—N3	1.296 (4)
Y1—O1	2.192 (2)	Y2—O7	2.281 (2)	N1—C8	1.431(4)
Y1—O2	2.548 (2)	Y2—O8	2.352 (2)	N2—C22	1.427(4)
Y1—O3	2.335 (2)	Y1—N1	2.521 (3)	N3—C36	1.436(4)
Y1—O4	2.585 (2)	Y1—N2	2.536 (2)	C6—C7	1.431(5)
Y1—O7	2.257 (2)	Y2—N3	2.487 (3)	C20—C21	1.455(4)
Y2—O3	2.293 (2)	C7—N1	1.299 (4)	C34—C35	1.443(4)

Table S3 Selected distances (Å) in $[\text{NaY}(\text{CH}_3\text{O}-\text{C}_6\text{H}_4\text{N}=\text{CH}-\text{C}_6\text{H}_4-\text{O})_4]$ or **(5)**.

Y1—O1	2.233 (2)	Na1—O6	2.418 (3)	N1—C8	1.420(4)
Y1—O2	2.579 (3)	Na1—O7	2.301 (3)	N2—C22	1.421(4)
Y1—O3	2.179 (3)	Na1—O8	2.447 (3)	N3—C36	1.432(5)
Y1—O4	2.490 (3)	Na1—N3	2.405 (3)	N4—C50	1.417(5)

Y1—O5	2.297 (2)	Na1—N4	2.397 (3)	C6-C7	1.436(5)
Y1—O7	2.303 (2)	C7—N1	1.291 (5)	C20-C21	1.443(5)
Y1—N1	2.528 (3)	C21—N2	1.297 (4)	C34-C35	1.458(5)
Y1—N2	2.519 (3)	C35—N3	1.268 (5)	C48-C49	1.454(5)
Na1—O5	2.316 (3)	C49—N4	1.277 (4)		

Table S4 The Ph rotation angles ($^{\circ}$) with respect to $C_{\text{ipso}}\text{-CH=N-}C_{\text{ipso}}$ planes in complexes **(1)**–**(5)**.

Complex	$C_{\text{ipso}}\text{-CH=N-}C_{\text{ipso}}$	Ph atoms	Ph rotation angle	Ph atoms	Ph rotation angle
(1)	C6-C7-N1-C8	C1...C6	0.4 (4)	C8...C13	38.3 (4)
	C20-C21-N2-C22	C15...C20	4.6 (5)	C22...C27	41.4 (3)
	C34-C35-N3-C36	C29...C34	2.5 (6)	C36...C41	35.2 (3)
(2)	C6-C7-N1-C8	C1...C6	17.1 (1)	C8...C13	45.8 (2)
	C20-C21-N2-C22	C15...C20	6.7 (2)	C22...C27	28.3 (2)
	C34-C35-N3-C36	C29...C34	3.6 (3)	C36...C41	38.5 (2)
(3)	C6-C7-N1-C8	C1...C6	3.3 (5)	C8...C13 ^a	69.4 (3)
	C20-C21-N2-C22	C15...C20	6.4 (6)	C22...C27	35.0 (4)
	C34-C35-N3-C36	C29...C34	5.4 (2)	C36...C41	37.4 (3)
	C48-C49-N4-C50	C43...C48	2.1 (6)	C50...C55 ^a	73.7 (3)
	C62-C63-N5-C64	C57...C62	11.0 (8)	C64...C69	38.5 (5)
	C76-C77-N6-C78	C71...C76	4.17 (8)	C78...C83	45.3 (3)
(4)	C6-C7-N1-C8	C1...C6	11.3 (3)	C8...C13	26.7 (2)
	C20-C21-N2-C22	C15...C20	17.4 (3)	C22...C27	27.3 (2)
	C34-C35-N3-C36	C29...C34	5.9 (4)	C36...C41	34.5 (3)
(5)	C6-C7-N1-C8	C1...C6	17.77 (19)	C8...C13	29.6 (4)
	C20-C21-N2-C22	C15...C20	9.3 (5)	C22...C27	23.3 (4)
	C34-C35-N3-C36	C29...C34	7.4 (7)	C36...C41 ^b	17.8 (7)
	C48-C49-N4-C50	C43...C48	16.27 (19)	C50...C55	26.74 (18)

(a) These Ph rings in **(3)** are not involved in formation of a chelating fragment by coordination via O_{Me} atom.(b) Only major component of the Ph disorder (atoms C37A, C38A and C39A) was used in calculations in **(5)**.

Table S5 Hydrogen-bond parameters (Å, °) for complexes La(CH₃O-C₆H₄N=CH-C₆H₄-O)₃ or **(1)**, Nd(CH₃O-C₆H₄N=CH-C₆H₄-O)₃•(THF)₂ or **(2)**•(THF)₂, Y(CH₃O-C₆H₄N=CH-C₆H₄-O)₃ or **(3)**, [Y₂(CH₃O-C₆H₄N=CH-C₆H₄-O)₃Cl₂(MeO)(MeOH)]•(CH₃OH)•(THF) or **(4)**•(MeOH)•(THF), [NaY(CH₃O-C₆H₄N=CH-C₆H₄-O)₄]•(CHCl₃)₂ or **(5)**•(CHCl₃)₂.

Complex	<i>D</i> —H... <i>A</i>	<i>D</i> —H (Å)	H... <i>A</i> (Å)	<i>D</i> ... <i>A</i> (Å)	<i>D</i> —H... <i>A</i> (°)
(1)	C12—H12...O3 ⁱ	0.95	2.51	3.402 (6)	157.0
	C14—H14A...O1 ⁱ	0.98	2.32	3.295 (5)	170.5
	C28—H28B...O1	0.98	2.50	3.132 (6)	122.4
(2) •(THF) ₂	C28—H28B...O5	0.98	2.61	3.174 (3)	116.6
	C35—H35...O8A ⁱⁱ	0.95	2.54	3.413 (6)	152.9
	C40—H40...O7A ⁱⁱⁱ	0.95	2.63	3.545 (7)	160.8
(3)	C51—H51...O12	0.95	2.56	3.293 (5)	134.0
(4) •(MeOH)•(THF)	O8—H8...Cl1	0.837 (19)	2.20 (2)	3.032 (3)	174 (4)
	O9—H9A...Cl2	0.89 (2)	2.29 (2)	3.175 (4)	177 (6)
	C43—H43A...O1	0.98	2.45	3.158 (4)	128.5
	C44—H44B...O5	0.98	2.59	3.132 (4)	114.6
	C14—H14C...Cl1	0.98	2.66	3.344 (3)	127.6
	C42—H42C...Cl2	0.98	2.89	3.591 (4)	129.3
(5) •(CHCl ₃) ₂	C28—H28B...O5	0.98	2.64	3.129 (4)	111.3
	C28—H28C...O8	0.98	2.61	3.402 (5)	137.9
	C30—H30...O1	0.95	2.63	3.470 (4)	147.6
	C42—H42C...Cl4B	0.98	2.87	3.604 (7)	132.4
	C42—H42C...Cl4C	0.98	2.92	3.711 (10)	138.6
	C9—H9...Cl1B ^{iv}	0.95	2.61	3.557 (10)	175.2
	C16—H16...Cl3 ^v	0.95	2.97	3.838 (4)	152.6
	C37B—H37B...Cl4B ^{vi}	0.95	2.95	3.624 (13)	128.9
	C51—H51...Cl2B ^{vii}	0.95	2.68	3.498 (8)	144.3

Symmetry code(s): (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $-x+2, -y+1, -z+1$; (iv) $-x+1, -y+1, -z$; (v) $x-1, y-1, z$; (vi) $-x+1, -y, -z+1$; (vii) $-x+1, -y+1, -z+1$.