

Novel effective racemoselective method for the synthesis of *ansa*-zirconocenes and its use for the preparation of C₂-symmetric complexes based on 2-methyl-4-aryltetrahydro(s)indacene as catalysts for isotactic propylene polymerization and ethylene-propylene copolymerization

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SUPPORTING INFORMATION

Crystal structure determination.

The single orange crystals of **12** were obtained by slow evaporation of a saturated solution of the complex in CH₂Cl₂.

Table S1. Crystallographic data and the parameters of data collection, structure solution and refinement for complexes **12** and **16**.

Empirical formula	C ₄₀ H ₃₈ Cl ₂ Si ₁ Zr ₁ (12)	C ₄₅ H ₅₀ Cl ₃ N ₁ Si ₁ Zr ₁ (16)
Formula weight	708.91	830.52
Crystal size/mm	0.40 × 0.30 × 0.20	0.25 × 0.20 × 0.08
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>
Unit cell dimensions: <i>a</i> /Å	12.2934(7)	18.1387(9)
<i>b</i> /Å	32.9760(19)	9.1186(5)
<i>c</i> /Å	17.3876(10)	24.6022(12)
β/°	107.690(1)	95.529(1)

Volume/Å ³	6715.4(7)	4050.3(4)
Z	8	4
Density (calculated)/g·cm ⁻³	1.402	1.362
Absorption coefficient/mm ⁻¹	0.550	0.532
F(000)	2928	1728
θ range/°	1.74 to 27.00	1.46 to 26.00
Reflections collected	49666	27160
Independent reflections	14580 [$R_{\text{int}} = 0.0546$]	7933 [$R_{\text{int}} = 0.0736$]
Data/restraints/parameters	14580 / 0 / 810	7933 / 0 / 467
Reflections with $I > 2\sigma(I)$	10917	5695
Goodness-of-fit on F^2	1.018	1.076
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0403$ $wR_2 = 0.0876$	$R_1 = 0.0531$ $wR_2 = 0.1383$
R indices (all data)	$R_1 = 0.0619$ $wR_2 = 0.0949$	$R_1 = 0.0816$ $wR_2 = 0.1497$
Largest diff. peak/hole (e·Å ⁻³)	0.409 / -0.360	0.661 / -1.145

Table S2. Atomic coordinates (Å × 10⁴) and equivalent isotropic displacement parameters (Å² × 10³) for **12**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U (eq)
Zr (1)	1558 (1)	2546 (1)	1966 (1)	17 (1)
Zr (2)	3167 (1)	10006 (1)	2631 (1)	18 (1)
Cl (11)	-438 (1)	2668 (1)	1260 (1)	26 (1)
Cl (12)	1858 (1)	3037 (1)	3046 (1)	27 (1)
Cl (21)	5170 (1)	9886 (1)	3313 (1)	27 (1)
Cl (22)	2885 (1)	9482 (1)	1607 (1)	30 (1)
Si (1)	3370 (1)	1905 (1)	1576 (1)	23 (1)
Si (2)	1312 (1)	10658 (1)	2949 (1)	24 (1)
C (11)	2951 (2)	2439 (1)	1236 (2)	21 (1)
C (12)	1923 (2)	2563 (1)	623 (2)	21 (1)
C (13)	1694 (2)	2970 (1)	737 (2)	20 (1)
C (14)	2565 (2)	3129 (1)	1402 (2)	20 (1)
C (15)	2752 (2)	3528 (1)	1751 (2)	21 (1)
C (16)	3699 (2)	3580 (1)	2404 (2)	24 (1)

C (17)	4075 (2)	3951 (1)	2927 (2)	30 (1)
C (18)	4882 (3)	3775 (1)	3715 (2)	40 (1)
C (19)	5432 (3)	3408 (1)	3429 (2)	36 (1)
C (20)	4488 (2)	3254 (1)	2714 (2)	25 (1)
C (21)	4337 (2)	2877 (1)	2388 (2)	24 (1)
C (22)	3358 (2)	2802 (1)	1718 (2)	21 (1)
C (23)	1926 (2)	3861 (1)	1415 (2)	21 (1)
C (24)	761 (2)	3810 (1)	1259 (2)	25 (1)
C (25)	4 (2)	4124 (1)	951 (2)	32 (1)
C (26)	403 (3)	4496 (1)	791 (2)	37 (1)
C (27)	1557 (3)	4552 (1)	943 (2)	38 (1)
C (28)	2316 (2)	4237 (1)	1248 (2)	30 (1)
C (29)	1181 (2)	2311 (1)	-63 (2)	25 (1)
C (30)	4917 (2)	1855 (1)	2132 (2)	36 (1)
C (31)	2382 (2)	1856 (1)	2212 (2)	20 (1)
C (32)	2555 (2)	2032 (1)	3001 (2)	21 (1)
C (33)	1505 (2)	2085 (1)	3140 (2)	20 (1)
C (34)	623 (2)	1926 (1)	2481 (2)	18 (1)
C (35)	-578 (2)	1896 (1)	2342 (2)	21 (1)
C (36)	-1206 (2)	1727 (1)	1631 (2)	25 (1)
C (37)	-2475 (2)	1652 (1)	1327 (2)	35 (1)
C (38A)	-2592 (5)	1325 (2)	673 (4)	42 (2)
C (38B)	-2713 (7)	1569 (3)	469 (5)	40 (2)
C (39)	-1606 (2)	1390 (1)	353 (2)	37 (1)
C (40)	-687 (2)	1574 (1)	1055 (2)	25 (1)
C (41)	461 (2)	1597 (1)	1174 (2)	22 (1)
C (42)	1161 (2)	1782 (1)	1902 (2)	20 (1)
C (43)	-1119 (2)	2052 (1)	2946 (2)	24 (1)
C (44)	-1807 (3)	2396 (1)	2771 (2)	38 (1)
C (45)	-2331 (3)	2546 (1)	3310 (2)	45 (1)
C (46)	-2178 (3)	2351 (1)	4039 (2)	41 (1)
C (47)	-1503 (3)	2010 (1)	4224 (2)	37 (1)
C (48)	-972 (2)	1864 (1)	3677 (2)	28 (1)
C (49)	3673 (2)	2134 (1)	3628 (2)	28 (1)
C (50)	3079 (3)	1536 (1)	723 (2)	33 (1)
C (51)	1782 (2)	10141 (1)	3358 (2)	21 (1)
C (52)	2824 (2)	10047 (1)	3984 (2)	22 (1)
C (53)	3094 (2)	9638 (1)	3930 (2)	22 (1)
C (54)	2233 (2)	9450 (1)	3300 (2)	20 (1)
C (55)	2083 (2)	9038 (1)	3030 (2)	21 (1)
C (56)	1115 (2)	8954 (1)	2404 (2)	23 (1)
C (57)	748 (2)	8557 (1)	1961 (2)	31 (1)
C (58)	-140 (3)	8693 (1)	1173 (2)	35 (1)
C (59)	-691 (2)	9068 (1)	1409 (2)	32 (1)
C (60)	278 (2)	9262 (1)	2056 (2)	23 (1)
C (61)	417 (2)	9650 (1)	2307 (2)	22 (1)
C (62)	1408 (2)	9760 (1)	2941 (2)	20 (1)
C (63)	2927 (2)	8722 (1)	3438 (2)	23 (1)
C (64)	4101 (2)	8783 (1)	3607 (2)	29 (1)
C (65)	4867 (3)	8488 (1)	4007 (2)	33 (1)
C (66)	4490 (3)	8129 (1)	4237 (2)	34 (1)
C (67)	3332 (3)	8065 (1)	4075 (2)	35 (1)
C (68)	2558 (2)	8360 (1)	3681 (2)	30 (1)
C (69)	3546 (2)	10320 (1)	4635 (2)	28 (1)
C (70)	-231 (2)	10687 (1)	2381 (2)	36 (1)
C (71)	2301 (2)	10690 (1)	2307 (2)	22 (1)
C (72)	2156 (2)	10492 (1)	1547 (2)	24 (1)
C (73)	3221 (2)	10436 (1)	1423 (2)	22 (1)
C (74)	4085 (2)	10615 (1)	2072 (2)	21 (1)
C (75)	5294 (2)	10641 (1)	2232 (2)	21 (1)
C (76)	5892 (2)	10829 (1)	2941 (2)	23 (1)
C (77)	7161 (2)	10903 (1)	3282 (2)	32 (1)
C (78)	7311 (2)	10981 (1)	4179 (2)	37 (1)
C (79)	6215 (2)	11193 (1)	4184 (2)	32 (1)
C (80)	5335 (2)	10999 (1)	3477 (2)	24 (1)
C (81)	4185 (2)	10973 (1)	3336 (2)	24 (1)
C (82)	3518 (2)	10772 (1)	2622 (2)	21 (1)

C (83)	5863 (2)	10446 (1)	1683 (2)	24 (1)
C (84)	5601 (3)	10551 (1)	876 (2)	41 (1)
C (85)	6150 (3)	10361 (1)	383 (2)	55 (1)
C (86)	6962 (3)	10072 (1)	688 (2)	47 (1)
C (87)	7208 (2)	9953 (1)	1485 (2)	36 (1)
C (88)	6667 (2)	10140 (1)	1975 (2)	29 (1)
C (89)	1045 (2)	10367 (1)	925 (2)	32 (1)
C (90)	1548 (3)	11048 (1)	3761 (2)	36 (1)

Table S3. Bond lengths [Å] for **12**.

Zr (1)–Cl (11)	2.4205 (7)
Zr (1)–Cl (12)	2.4213 (7)
Zr (1)–C (11)	2.448 (3)
Zr (1)–C (31)	2.475 (2)
Zr (1)–C (32)	2.506 (2)
Zr (1)–C (12)	2.509 (2)
Zr (1)–C (22)	2.525 (3)
Zr (1)–C (33)	2.562 (2)
Zr (1)–C (42)	2.563 (2)
Zr (1)–C (13)	2.600 (2)
Zr (1)–C (14)	2.632 (2)
Zr (1)–C (34)	2.633 (2)
Zr (2)–Cl (21)	2.4199 (7)
Zr (2)–Cl (22)	2.4287 (7)
Zr (2)–C (51)	2.449 (3)
Zr (2)–C (71)	2.483 (2)
Zr (2)–C (72)	2.497 (2)
Zr (2)–C (52)	2.516 (3)
Zr (2)–C (62)	2.516 (2)
Zr (2)–C (73)	2.551 (2)
Zr (2)–C (82)	2.563 (2)
Zr (2)–C (53)	2.590 (2)
Zr (2)–C (54)	2.617 (2)
Zr (2)–C (74)	2.630 (2)
Si (1)–C (30)	1.861 (3)
Si (1)–C (50)	1.867 (3)
Si (1)–C (11)	1.878 (2)
Si (1)–C (31)	1.881 (3)
Si (2)–C (70)	1.856 (3)
Si (2)–C (90)	1.865 (3)
Si (2)–C (51)	1.872 (3)
Si (2)–C (71)	1.886 (3)
C (11)–C (12)	1.443 (4)
C (11)–C (22)	1.460 (3)
C (12)–C (13)	1.398 (3)
C (12)–C (29)	1.511 (3)
C (13)–C (14)	1.416 (3)
C (13)–H (13)	0.9500
C (14)–C (15)	1.436 (3)
C (14)–C (22)	1.447 (3)
C (15)–C (16)	1.368 (4)
C (15)–C (23)	1.490 (3)
C (16)–C (20)	1.437 (4)
C (16)–C (17)	1.513 (3)
C (17)–C (18)	1.541 (4)
C (17)–H (17A)	0.9900
C (17)–H (17B)	0.9900
C (18)–C (19)	1.538 (4)
C (18)–H (18A)	0.9900
C (18)–H (18B)	0.9900
C (19)–C (20)	1.508 (4)

C (19) -H (19A)	0.9900
C (19) -H (19B)	0.9900
C (20) -C (21)	1.357 (4)
C (21) -C (22)	1.419 (3)
C (21) -H (21)	0.9500
C (23) -C (24)	1.385 (4)
C (23) -C (28)	1.392 (3)
C (24) -C (25)	1.387 (4)
C (24) -H (24)	0.9500
C (25) -C (26)	1.379 (4)
C (25) -H (25)	0.9500
C (26) -C (27)	1.375 (4)
C (26) -H (26)	0.9500
C (27) -C (28)	1.388 (4)
C (27) -H (27)	0.9500
C (28) -H (28)	0.9500
C (29) -H (29A)	0.9800
C (29) -H (29B)	0.9800
C (29) -H (29C)	0.9800
C (30) -H (30A)	0.9800
C (30) -H (30B)	0.9800
C (30) -H (30C)	0.9800
C (31) -C (32)	1.444 (3)
C (31) -C (42)	1.453 (3)
C (32) -C (33)	1.395 (4)
C (32) -C (49)	1.510 (3)
C (33) -C (34)	1.418 (3)
C (33) -H (33)	0.9500
C (34) -C (35)	1.425 (3)
C (34) -C (42)	1.443 (3)
C (35) -C (36)	1.362 (4)
C (35) -C (43)	1.493 (4)
C (36) -C (40)	1.433 (4)
C (36) -C (37)	1.509 (4)
C (37) -C (38B)	1.456 (8)
C (37) -C (38A)	1.539 (7)
C (37) -H (37C)	0.9900
C (37) -H (37D)	0.9900
C (37) -H (37A)	0.9598
C (37) -H (37B)	0.9601
C (38A) -C (39)	1.495 (7)
C (38A) -H (38A)	0.9900
C (38A) -H (38B)	0.9900
C (38B) -C (39)	1.552 (9)
C (38B) -H (38C)	0.9900
C (38B) -H (38D)	0.9900
C (39) -C (40)	1.515 (4)
C (39) -H (39C)	0.9900
C (39) -H (39D)	0.9900
C (39) -H (39A)	0.9602
C (39) -H (39B)	0.9600
C (40) -C (41)	1.365 (4)
C (41) -C (42)	1.433 (3)
C (41) -H (41)	0.9500
C (43) -C (48)	1.377 (4)
C (43) -C (44)	1.393 (4)
C (44) -C (45)	1.381 (4)
C (44) -H (44)	0.9500
C (45) -C (46)	1.382 (5)
C (45) -H (45)	0.9500
C (46) -C (47)	1.377 (4)
C (46) -H (46)	0.9500
C (47) -C (48)	1.392 (4)
C (47) -H (47)	0.9500
C (48) -H (48)	0.9500
C (49) -H (49A)	0.9800
C (49) -H (49B)	0.9800

C (49) -H (49C)	0.9800
C (50) -H (50A)	0.9800
C (50) -H (50B)	0.9800
C (50) -H (50C)	0.9800
C (51) -C (52)	1.440 (4)
C (51) -C (62)	1.452 (3)
C (52) -C (53)	1.399 (3)
C (52) -C (69)	1.507 (3)
C (53) -C (54)	1.415 (3)
C (53) -H (53)	0.9500
C (54) -C (55)	1.432 (3)
C (54) -C (62)	1.443 (3)
C (55) -C (56)	1.374 (4)
C (55) -C (63)	1.488 (3)
C (56) -C (60)	1.442 (4)
C (56) -C (57)	1.516 (3)
C (57) -C (58)	1.537 (4)
C (57) -H (57A)	0.9900
C (57) -H (57B)	0.9900
C (58) -C (59)	1.526 (4)
C (58) -H (58A)	0.9900
C (58) -H (58B)	0.9900
C (59) -C (60)	1.509 (4)
C (59) -H (59A)	0.9900
C (59) -H (59B)	0.9900
C (60) -C (61)	1.347 (3)
C (61) -C (62)	1.419 (3)
C (61) -H (61)	0.9500
C (63) -C (68)	1.390 (4)
C (63) -C (64)	1.397 (4)
C (64) -C (65)	1.385 (4)
C (64) -H (64)	0.9500
C (65) -C (66)	1.374 (4)
C (65) -H (65)	0.9500
C (66) -C (67)	1.381 (4)
C (66) -H (66)	0.9500
C (67) -C (68)	1.387 (4)
C (67) -H (67)	0.9500
C (68) -H (68)	0.9500
C (69) -H (69A)	0.9800
C (69) -H (69B)	0.9800
C (69) -H (69C)	0.9800
C (70) -H (70A)	0.9800
C (70) -H (70B)	0.9800
C (70) -H (70C)	0.9800
C (71) -C (72)	1.436 (4)
C (71) -C (82)	1.454 (4)
C (72) -C (73)	1.403 (4)
C (72) -C (89)	1.519 (4)
C (73) -C (74)	1.422 (3)
C (73) -H (73)	0.9500
C (74) -C (75)	1.429 (4)
C (74) -C (82)	1.439 (3)
C (75) -C (76)	1.376 (4)
C (75) -C (83)	1.492 (4)
C (76) -C (80)	1.428 (4)
C (76) -C (77)	1.511 (4)
C (77) -C (78)	1.534 (4)
C (77) -H (77A)	0.9900
C (77) -H (77B)	0.9900
C (78) -C (79)	1.520 (4)
C (78) -H (78A)	0.9900
C (78) -H (78B)	0.9900
C (79) -C (80)	1.511 (4)
C (79) -H (79A)	0.9900
C (79) -H (79B)	0.9900
C (80) -C (81)	1.362 (4)

C (81)–C (82)	1.427 (3)
C (81)–H (81)	0.9500
C (83)–C (84)	1.384 (4)
C (83)–C (88)	1.394 (4)
C (84)–C (85)	1.391 (4)
C (84)–H (84)	0.9500
C (85)–C (86)	1.365 (5)
C (85)–H (85)	0.9500
C (86)–C (87)	1.382 (5)
C (86)–H (86)	0.9500
C (87)–C (88)	1.377 (4)
C (87)–H (87)	0.9500
C (88)–H (88)	0.9500
C (89)–H (89A)	0.9800
C (89)–H (89B)	0.9800
C (89)–H (89C)	0.9800
C (90)–H (90A)	0.9800
C (90)–H (90B)	0.9800
C (90)–H (90C)	0.9800

Table S4. Bond angles [deg] for **12**.

Cl (11)–Zr (1)–Cl (12)	100.06 (2)
Cl (11)–Zr (1)–C (11)	121.49 (6)
Cl (12)–Zr (1)–C (11)	122.26 (6)
Cl (11)–Zr (1)–C (31)	122.57 (6)
Cl (12)–Zr (1)–C (31)	121.52 (6)
C (11)–Zr (1)–C (31)	69.03 (8)
Cl (11)–Zr (1)–C (32)	132.49 (6)
Cl (12)–Zr (1)–C (32)	88.25 (6)
C (11)–Zr (1)–C (32)	90.44 (8)
C (31)–Zr (1)–C (32)	33.71 (8)
Cl (11)–Zr (1)–C (12)	88.01 (6)
Cl (12)–Zr (1)–C (12)	132.80 (6)
C (11)–Zr (1)–C (12)	33.81 (8)
C (31)–Zr (1)–C (12)	90.06 (8)
C (32)–Zr (1)–C (12)	119.75 (8)
Cl (11)–Zr (1)–C (22)	131.65 (6)
Cl (12)–Zr (1)–C (22)	88.57 (6)
C (11)–Zr (1)–C (22)	34.10 (8)
C (31)–Zr (1)–C (22)	90.12 (8)
C (32)–Zr (1)–C (22)	94.91 (8)
C (12)–Zr (1)–C (22)	54.52 (8)
Cl (11)–Zr (1)–C (33)	103.58 (6)
Cl (12)–Zr (1)–C (33)	79.24 (6)
C (11)–Zr (1)–C (33)	121.22 (8)
C (31)–Zr (1)–C (33)	54.88 (8)
C (32)–Zr (1)–C (33)	31.92 (8)
C (12)–Zr (1)–C (33)	144.04 (8)
C (22)–Zr (1)–C (33)	124.74 (8)
Cl (11)–Zr (1)–C (42)	89.43 (6)
Cl (12)–Zr (1)–C (42)	132.30 (6)
C (11)–Zr (1)–C (42)	89.37 (8)
C (31)–Zr (1)–C (42)	33.48 (8)
C (32)–Zr (1)–C (42)	53.89 (8)
C (12)–Zr (1)–C (42)	93.81 (8)
C (22)–Zr (1)–C (42)	119.06 (8)
C (33)–Zr (1)–C (42)	53.17 (8)
Cl (11)–Zr (1)–C (13)	78.65 (6)

Cl(12)-Zr(1)-C(13)	104.23(6)
C(11)-Zr(1)-C(13)	54.67(8)
C(31)-Zr(1)-C(13)	120.71(8)
C(32)-Zr(1)-C(13)	144.51(8)
C(12)-Zr(1)-C(13)	31.70(7)
C(22)-Zr(1)-C(13)	53.25(8)
C(33)-Zr(1)-C(13)	175.59(8)
C(42)-Zr(1)-C(13)	123.46(8)
Cl(11)-Zr(1)-C(14)	102.09(6)
Cl(12)-Zr(1)-C(14)	79.80(6)
C(11)-Zr(1)-C(14)	55.28(8)
C(31)-Zr(1)-C(14)	121.47(8)
C(32)-Zr(1)-C(14)	125.41(8)
C(12)-Zr(1)-C(14)	53.13(8)
C(22)-Zr(1)-C(14)	32.52(7)
C(33)-Zr(1)-C(14)	149.21(8)
C(42)-Zr(1)-C(14)	143.80(8)
C(13)-Zr(1)-C(14)	31.41(7)
Cl(11)-Zr(1)-C(34)	79.66(6)
Cl(12)-Zr(1)-C(34)	103.57(6)
C(11)-Zr(1)-C(34)	120.69(8)
C(31)-Zr(1)-C(34)	54.90(8)
C(32)-Zr(1)-C(34)	53.04(8)
C(12)-Zr(1)-C(34)	123.60(8)
C(22)-Zr(1)-C(34)	144.42(8)
C(33)-Zr(1)-C(34)	31.64(7)
C(42)-Zr(1)-C(34)	32.21(8)
C(13)-Zr(1)-C(34)	147.18(8)
C(14)-Zr(1)-C(34)	175.95(8)
Cl(21)-Zr(2)-Cl(22)	98.02(3)
Cl(21)-Zr(2)-C(51)	122.70(6)
Cl(22)-Zr(2)-C(51)	122.70(6)
Cl(21)-Zr(2)-C(71)	124.23(6)
Cl(22)-Zr(2)-C(71)	121.58(6)
C(51)-Zr(2)-C(71)	68.64(8)
Cl(21)-Zr(2)-C(72)	132.39(6)
Cl(22)-Zr(2)-C(72)	88.60(6)
C(51)-Zr(2)-C(72)	90.51(9)
C(71)-Zr(2)-C(72)	33.50(8)
Cl(21)-Zr(2)-C(52)	89.15(6)
Cl(22)-Zr(2)-C(52)	134.13(6)
C(51)-Zr(2)-C(52)	33.68(8)
C(71)-Zr(2)-C(52)	88.93(8)
C(72)-Zr(2)-C(52)	119.00(9)
Cl(21)-Zr(2)-C(62)	130.92(6)
Cl(22)-Zr(2)-C(62)	89.27(6)
C(51)-Zr(2)-C(62)	33.97(8)
C(71)-Zr(2)-C(62)	90.25(8)
C(72)-Zr(2)-C(62)	96.05(8)
C(52)-Zr(2)-C(62)	54.43(8)
Cl(21)-Zr(2)-C(73)	102.54(6)
Cl(22)-Zr(2)-C(73)	79.93(6)
C(51)-Zr(2)-C(73)	121.39(8)
C(71)-Zr(2)-C(73)	54.97(8)
C(72)-Zr(2)-C(73)	32.25(8)
C(52)-Zr(2)-C(73)	142.53(8)
C(62)-Zr(2)-C(73)	126.49(8)
Cl(21)-Zr(2)-C(82)	90.96(6)
Cl(22)-Zr(2)-C(82)	133.07(6)
C(51)-Zr(2)-C(82)	88.29(8)
C(71)-Zr(2)-C(82)	33.44(8)
C(72)-Zr(2)-C(82)	53.81(8)
C(52)-Zr(2)-C(82)	91.70(8)
C(62)-Zr(2)-C(82)	118.46(8)
C(73)-Zr(2)-C(82)	53.19(8)
Cl(21)-Zr(2)-C(53)	78.18(6)
Cl(22)-Zr(2)-C(53)	105.73(6)

C (51)-Zr (2)-C (53)	54.62 (8)
C (71)-Zr (2)-C (53)	119.81 (8)
C (72)-Zr (2)-C (53)	144.84 (9)
C (52)-Zr (2)-C (53)	31.75 (7)
C (62)-Zr (2)-C (53)	53.31 (8)
C (73)-Zr (2)-C (53)	174.20 (8)
C (82)-Zr (2)-C (53)	121.19 (8)
Cl (21)-Zr (2)-C (54)	100.70 (6)
Cl (22)-Zr (2)-C (54)	80.97 (6)
C (51)-Zr (2)-C (54)	55.24 (8)
C (71)-Zr (2)-C (54)	121.44 (8)
C (72)-Zr (2)-C (54)	126.87 (8)
C (52)-Zr (2)-C (54)	53.23 (8)
C (62)-Zr (2)-C (54)	32.57 (7)
C (73)-Zr (2)-C (54)	151.65 (8)
C (82)-Zr (2)-C (54)	142.30 (8)
C (53)-Zr (2)-C (54)	31.54 (8)
Cl (21)-Zr (2)-C (74)	79.59 (6)
Cl (22)-Zr (2)-C (74)	104.69 (6)
C (51)-Zr (2)-C (74)	119.77 (8)
C (71)-Zr (2)-C (74)	54.95 (8)
C (72)-Zr (2)-C (74)	53.33 (8)
C (52)-Zr (2)-C (74)	121.14 (8)
C (62)-Zr (2)-C (74)	144.94 (8)
C (73)-Zr (2)-C (74)	31.81 (8)
C (82)-Zr (2)-C (74)	32.15 (8)
C (53)-Zr (2)-C (74)	144.34 (8)
C (54)-Zr (2)-C (74)	174.27 (8)
C (30)-Si (1)-C (50)	105.94 (14)
C (30)-Si (1)-C (11)	112.62 (12)
C (50)-Si (1)-C (11)	113.08 (12)
C (30)-Si (1)-C (31)	115.31 (13)
C (50)-Si (1)-C (31)	114.19 (12)
C (11)-Si (1)-C (31)	95.82 (11)
C (70)-Si (2)-C (90)	105.45 (14)
C (70)-Si (2)-C (51)	113.29 (12)
C (90)-Si (2)-C (51)	112.41 (13)
C (70)-Si (2)-C (71)	114.91 (13)
C (90)-Si (2)-C (71)	115.44 (13)
C (51)-Si (2)-C (71)	95.50 (11)
C (12)-C (11)-C (22)	105.2 (2)
C (12)-C (11)-Si (1)	126.38 (19)
C (22)-C (11)-Si (1)	125.05 (19)
C (12)-C (11)-Zr (1)	75.42 (14)
C (22)-C (11)-Zr (1)	75.82 (15)
Si (1)-C (11)-Zr (1)	98.07 (10)
C (13)-C (12)-C (11)	109.7 (2)
C (13)-C (12)-C (29)	122.7 (2)
C (11)-C (12)-C (29)	127.6 (2)
C (13)-C (12)-Zr (1)	77.75 (15)
C (11)-C (12)-Zr (1)	70.77 (14)
C (29)-C (12)-Zr (1)	119.09 (16)
C (12)-C (13)-C (14)	109.7 (2)
C (12)-C (13)-Zr (1)	70.56 (14)
C (14)-C (13)-Zr (1)	75.51 (14)
C (12)-C (13)-H (13)	125.1
C (14)-C (13)-H (13)	125.1
Zr (1)-C (13)-H (13)	120.4
C (13)-C (14)-C (15)	132.0 (2)
C (13)-C (14)-C (22)	106.7 (2)
C (15)-C (14)-C (22)	121.3 (2)
C (13)-C (14)-Zr (1)	73.09 (14)
C (15)-C (14)-Zr (1)	122.92 (17)
C (22)-C (14)-Zr (1)	69.67 (14)
C (16)-C (15)-C (14)	116.9 (2)
C (16)-C (15)-C (23)	122.7 (2)
C (14)-C (15)-C (23)	120.5 (2)

C (15) -C (16) -C (20)	121.7 (2)
C (15) -C (16) -C (17)	128.9 (2)
C (20) -C (16) -C (17)	109.4 (2)
C (16) -C (17) -C (18)	103.0 (2)
C (16) -C (17) -H (17A)	111.2
C (18) -C (17) -H (17A)	111.2
C (16) -C (17) -H (17B)	111.2
C (18) -C (17) -H (17B)	111.2
H (17A) -C (17) -H (17B)	109.1
C (19) -C (18) -C (17)	103.7 (2)
C (19) -C (18) -H (18A)	111.0
C (17) -C (18) -H (18A)	111.0
C (19) -C (18) -H (18B)	111.0
C (17) -C (18) -H (18B)	111.0
H (18A) -C (18) -H (18B)	109.0
C (20) -C (19) -C (18)	103.1 (2)
C (20) -C (19) -H (19A)	111.1
C (18) -C (19) -H (19A)	111.1
C (20) -C (19) -H (19B)	111.1
C (18) -C (19) -H (19B)	111.1
H (19A) -C (19) -H (19B)	109.1
C (21) -C (20) -C (16)	122.5 (2)
C (21) -C (20) -C (19)	128.8 (2)
C (16) -C (20) -C (19)	108.7 (2)
C (20) -C (21) -C (22)	118.5 (2)
C (20) -C (21) -H (21)	120.7
C (22) -C (21) -H (21)	120.7
C (21) -C (22) -C (14)	119.1 (2)
C (21) -C (22) -C (11)	132.2 (2)
C (14) -C (22) -C (11)	108.7 (2)
C (21) -C (22) -Zr (1)	119.04 (18)
C (14) -C (22) -Zr (1)	77.81 (14)
C (11) -C (22) -Zr (1)	70.09 (14)
C (24) -C (23) -C (28)	118.0 (2)
C (24) -C (23) -C (15)	121.9 (2)
C (28) -C (23) -C (15)	120.1 (2)
C (23) -C (24) -C (25)	121.1 (3)
C (23) -C (24) -H (24)	119.5
C (25) -C (24) -H (24)	119.5
C (26) -C (25) -C (24)	120.3 (3)
C (26) -C (25) -H (25)	119.8
C (24) -C (25) -H (25)	119.8
C (27) -C (26) -C (25)	119.3 (3)
C (27) -C (26) -H (26)	120.4
C (25) -C (26) -H (26)	120.4
C (26) -C (27) -C (28)	120.5 (3)
C (26) -C (27) -H (27)	119.7
C (28) -C (27) -H (27)	119.7
C (27) -C (28) -C (23)	120.8 (3)
C (27) -C (28) -H (28)	119.6
C (23) -C (28) -H (28)	119.6
C (12) -C (29) -H (29A)	109.5
C (12) -C (29) -H (29B)	109.5
H (29A) -C (29) -H (29B)	109.5
C (12) -C (29) -H (29C)	109.5
H (29A) -C (29) -H (29C)	109.5
H (29B) -C (29) -H (29C)	109.5
Si (1) -C (30) -H (30A)	109.5
Si (1) -C (30) -H (30B)	109.5
H (30A) -C (30) -H (30B)	109.5
Si (1) -C (30) -H (30C)	109.5
H (30A) -C (30) -H (30C)	109.5
H (30B) -C (30) -H (30C)	109.5
C (32) -C (31) -C (42)	104.9 (2)
C (32) -C (31) -Si (1)	126.09 (19)
C (42) -C (31) -Si (1)	125.08 (18)
C (32) -C (31) -Zr (1)	74.32 (13)

C (42) -C (31) -Zr (1)	76.58 (13)
Si (1) -C (31) -Zr (1)	97.08 (10)
C (33) -C (32) -C (31)	109.8 (2)
C (33) -C (32) -C (49)	122.3 (2)
C (31) -C (32) -C (49)	127.9 (2)
C (33) -C (32) -Zr (1)	76.27 (14)
C (31) -C (32) -Zr (1)	71.97 (13)
C (49) -C (32) -Zr (1)	120.43 (16)
C (32) -C (33) -C (34)	109.5 (2)
C (32) -C (33) -Zr (1)	71.81 (14)
C (34) -C (33) -Zr (1)	76.94 (14)
C (32) -C (33) -H (33)	125.2
C (34) -C (33) -H (33)	125.2
Zr (1) -C (33) -H (33)	117.8
C (33) -C (34) -C (35)	131.4 (2)
C (33) -C (34) -C (42)	106.6 (2)
C (35) -C (34) -C (42)	122.0 (2)
C (33) -C (34) -Zr (1)	71.42 (13)
C (35) -C (34) -Zr (1)	122.24 (16)
C (42) -C (34) -Zr (1)	71.20 (13)
C (36) -C (35) -C (34)	117.0 (2)
C (36) -C (35) -C (43)	121.9 (2)
C (34) -C (35) -C (43)	121.1 (2)
C (35) -C (36) -C (40)	122.0 (2)
C (35) -C (36) -C (37)	128.7 (3)
C (40) -C (36) -C (37)	109.2 (2)
C (38B) -C (37) -C (36)	104.8 (4)
C (36) -C (37) -C (38A)	103.2 (3)
C (38B) -C (37) -H (37C)	110.8
C (36) -C (37) -H (37C)	110.8
C (38A) -C (37) -H (37C)	80.6
C (38B) -C (37) -H (37D)	110.8
C (36) -C (37) -H (37D)	110.8
C (38A) -C (37) -H (37D)	137.6
H (37C) -C (37) -H (37D)	108.9
C (36) -C (37) -H (37A)	111.2
C (38A) -C (37) -H (37A)	110.8
C (36) -C (37) -H (37B)	110.9
C (38A) -C (37) -H (37B)	111.5
H (37A) -C (37) -H (37B)	109.1
C (39) -C (38A) -C (37)	105.7 (4)
C (39) -C (38A) -H (38A)	110.6
C (37) -C (38A) -H (38A)	110.6
C (39) -C (38A) -H (38B)	110.6
C (37) -C (38A) -H (38B)	110.6
H (38A) -C (38A) -H (38B)	108.7
C (37) -C (38B) -C (39)	107.1 (5)
C (37) -C (38B) -H (38C)	110.3
C (39) -C (38B) -H (38C)	110.3
C (37) -C (38B) -H (38D)	110.3
C (39) -C (38B) -H (38D)	110.3
H (38C) -C (38B) -H (38D)	108.6
C (38A) -C (39) -C (40)	104.3 (3)
C (40) -C (39) -C (38B)	102.2 (4)
C (40) -C (39) -H (39C)	111.3
C (38B) -C (39) -H (39C)	111.3
C (40) -C (39) -H (39D)	111.3
C (38B) -C (39) -H (39D)	111.3
H (39C) -C (39) -H (39D)	109.2
C (38A) -C (39) -H (39A)	110.4
C (40) -C (39) -H (39A)	110.8
C (38A) -C (39) -H (39B)	111.4
C (40) -C (39) -H (39B)	110.9
H (39A) -C (39) -H (39B)	109.0
C (41) -C (40) -C (36)	122.2 (2)
C (41) -C (40) -C (39)	129.0 (3)
C (36) -C (40) -C (39)	108.8 (2)

C (40) -C (41) -C (42)	118.3 (2)
C (40) -C (41) -H (41)	120.9
C (42) -C (41) -H (41)	120.9
C (41) -C (42) -C (34)	118.5 (2)
C (41) -C (42) -C (31)	132.4 (2)
C (34) -C (42) -C (31)	109.1 (2)
C (41) -C (42) -Zr (1)	120.89 (16)
C (34) -C (42) -Zr (1)	76.59 (13)
C (31) -C (42) -Zr (1)	69.94 (13)
C (48) -C (43) -C (44)	118.0 (3)
C (48) -C (43) -C (35)	122.2 (2)
C (44) -C (43) -C (35)	119.8 (2)
C (45) -C (44) -C (43)	121.4 (3)
C (45) -C (44) -H (44)	119.3
C (43) -C (44) -H (44)	119.3
C (44) -C (45) -C (46)	119.7 (3)
C (44) -C (45) -H (45)	120.2
C (46) -C (45) -H (45)	120.2
C (47) -C (46) -C (45)	119.9 (3)
C (47) -C (46) -H (46)	120.0
C (45) -C (46) -H (46)	120.0
C (46) -C (47) -C (48)	119.9 (3)
C (46) -C (47) -H (47)	120.1
C (48) -C (47) -H (47)	120.1
C (43) -C (48) -C (47)	121.2 (3)
C (43) -C (48) -H (48)	119.4
C (47) -C (48) -H (48)	119.4
C (32) -C (49) -H (49A)	109.5
C (32) -C (49) -H (49B)	109.5
H (49A) -C (49) -H (49B)	109.5
C (32) -C (49) -H (49C)	109.5
H (49A) -C (49) -H (49C)	109.5
H (49B) -C (49) -H (49C)	109.5
Si (1) -C (50) -H (50A)	109.5
Si (1) -C (50) -H (50B)	109.5
H (50A) -C (50) -H (50B)	109.5
Si (1) -C (50) -H (50C)	109.5
H (50A) -C (50) -H (50C)	109.5
H (50B) -C (50) -H (50C)	109.5
C (52) -C (51) -C (62)	105.5 (2)
C (52) -C (51) -Si (2)	125.67 (18)
C (62) -C (51) -Si (2)	125.69 (19)
C (52) -C (51) -Zr (2)	75.71 (15)
C (62) -C (51) -Zr (2)	75.55 (14)
Si (2) -C (51) -Zr (2)	98.68 (11)
C (53) -C (52) -C (51)	109.3 (2)
C (53) -C (52) -C (69)	121.9 (2)
C (51) -C (52) -C (69)	128.7 (2)
C (53) -C (52) -Zr (2)	77.05 (15)
C (51) -C (52) -Zr (2)	70.62 (14)
C (69) -C (52) -Zr (2)	120.47 (17)
C (52) -C (53) -C (54)	109.7 (2)
C (52) -C (53) -Zr (2)	71.20 (14)
C (54) -C (53) -Zr (2)	75.28 (14)
C (52) -C (53) -H (53)	125.1
C (54) -C (53) -H (53)	125.1
Zr (2) -C (53) -H (53)	120.1
C (53) -C (54) -C (55)	131.5 (2)
C (53) -C (54) -C (62)	106.6 (2)
C (55) -C (54) -C (62)	121.9 (2)
C (53) -C (54) -Zr (2)	73.18 (14)
C (55) -C (54) -Zr (2)	123.36 (18)
C (62) -C (54) -Zr (2)	69.87 (14)
C (56) -C (55) -C (54)	116.4 (2)
C (56) -C (55) -C (63)	123.2 (2)
C (54) -C (55) -C (63)	120.3 (2)
C (55) -C (56) -C (60)	121.8 (2)

C (55) -C (56) -C (57)	128.9 (2)
C (60) -C (56) -C (57)	109.3 (2)
C (56) -C (57) -C (58)	102.8 (2)
C (56) -C (57) -H (57A)	111.2
C (58) -C (57) -H (57A)	111.2
C (56) -C (57) -H (57B)	111.2
C (58) -C (57) -H (57B)	111.2
H (57A) -C (57) -H (57B)	109.1
C (59) -C (58) -C (57)	104.5 (2)
C (59) -C (58) -H (58A)	110.9
C (57) -C (58) -H (58A)	110.9
C (59) -C (58) -H (58B)	110.9
C (57) -C (58) -H (58B)	110.9
H (58A) -C (58) -H (58B)	108.9
C (60) -C (59) -C (58)	103.3 (2)
C (60) -C (59) -H (59A)	111.1
C (58) -C (59) -H (59A)	111.1
C (60) -C (59) -H (59B)	111.1
C (58) -C (59) -H (59B)	111.1
H (59A) -C (59) -H (59B)	109.1
C (61) -C (60) -C (56)	122.0 (2)
C (61) -C (60) -C (59)	129.6 (2)
C (56) -C (60) -C (59)	108.4 (2)
C (60) -C (61) -C (62)	119.2 (2)
C (60) -C (61) -H (61)	120.4
C (62) -C (61) -H (61)	120.4
C (61) -C (62) -C (54)	118.7 (2)
C (61) -C (62) -C (51)	132.5 (2)
C (54) -C (62) -C (51)	108.8 (2)
C (61) -C (62) -Zr (2)	120.44 (17)
C (54) -C (62) -Zr (2)	77.57 (14)
C (51) -C (62) -Zr (2)	70.48 (14)
C (68) -C (63) -C (64)	118.1 (2)
C (68) -C (63) -C (55)	120.0 (2)
C (64) -C (63) -C (55)	121.9 (2)
C (65) -C (64) -C (63)	120.5 (3)
C (65) -C (64) -H (64)	119.8
C (63) -C (64) -H (64)	119.8
C (66) -C (65) -C (64)	120.9 (3)
C (66) -C (65) -H (65)	119.6
C (64) -C (65) -H (65)	119.6
C (65) -C (66) -C (67)	119.4 (3)
C (65) -C (66) -H (66)	120.3
C (67) -C (66) -H (66)	120.3
C (66) -C (67) -C (68)	120.3 (3)
C (66) -C (67) -H (67)	119.9
C (68) -C (67) -H (67)	119.9
C (67) -C (68) -C (63)	121.0 (3)
C (67) -C (68) -H (68)	119.5
C (63) -C (68) -H (68)	119.5
C (52) -C (69) -H (69A)	109.5
C (52) -C (69) -H (69B)	109.5
H (69A) -C (69) -H (69B)	109.5
C (52) -C (69) -H (69C)	109.5
H (69A) -C (69) -H (69C)	109.5
H (69B) -C (69) -H (69C)	109.5
Si (2) -C (70) -H (70A)	109.5
Si (2) -C (70) -H (70B)	109.5
H (70A) -C (70) -H (70B)	109.5
Si (2) -C (70) -H (70C)	109.5
H (70A) -C (70) -H (70C)	109.5
H (70B) -C (70) -H (70C)	109.5
C (72) -C (71) -C (82)	104.9 (2)
C (72) -C (71) -Si (2)	126.6 (2)
C (82) -C (71) -Si (2)	124.24 (19)
C (72) -C (71) -Zr (2)	73.78 (14)
C (82) -C (71) -Zr (2)	76.30 (13)

Si(2)-C(71)-Zr(2)	97.14(10)
C(73)-C(72)-C(71)	109.9(2)
C(73)-C(72)-C(89)	122.3(2)
C(71)-C(72)-C(89)	127.8(2)
C(73)-C(72)-Zr(2)	75.99(14)
C(71)-C(72)-Zr(2)	72.72(14)
C(89)-C(72)-Zr(2)	119.77(17)
C(72)-C(73)-C(74)	109.3(2)
C(72)-C(73)-Zr(2)	71.76(15)
C(74)-C(73)-Zr(2)	77.15(14)
C(72)-C(73)-H(73)	125.4
C(74)-C(73)-H(73)	125.4
Zr(2)-C(73)-H(73)	117.6
C(73)-C(74)-C(75)	131.4(2)
C(73)-C(74)-C(82)	106.3(2)
C(75)-C(74)-C(82)	122.3(2)
C(73)-C(74)-Zr(2)	71.04(14)
C(75)-C(74)-Zr(2)	120.76(16)
C(82)-C(74)-Zr(2)	71.37(14)
C(76)-C(75)-C(74)	116.3(2)
C(76)-C(75)-C(83)	122.8(2)
C(74)-C(75)-C(83)	120.8(2)
C(75)-C(76)-C(80)	121.9(2)
C(75)-C(76)-C(77)	129.2(2)
C(80)-C(76)-C(77)	108.9(2)
C(76)-C(77)-C(78)	102.5(2)
C(76)-C(77)-H(77A)	111.3
C(78)-C(77)-H(77A)	111.3
C(76)-C(77)-H(77B)	111.3
C(78)-C(77)-H(77B)	111.3
H(77A)-C(77)-H(77B)	109.2
C(79)-C(78)-C(77)	104.5(2)
C(79)-C(78)-H(78A)	110.9
C(77)-C(78)-H(78A)	110.9
C(79)-C(78)-H(78B)	110.9
C(77)-C(78)-H(78B)	110.9
H(78A)-C(78)-H(78B)	108.9
C(80)-C(79)-C(78)	102.5(2)
C(80)-C(79)-H(79A)	111.3
C(78)-C(79)-H(79A)	111.3
C(80)-C(79)-H(79B)	111.3
C(78)-C(79)-H(79B)	111.3
H(79A)-C(79)-H(79B)	109.2
C(81)-C(80)-C(76)	122.4(2)
C(81)-C(80)-C(79)	128.3(3)
C(76)-C(80)-C(79)	109.3(2)
C(80)-C(81)-C(82)	118.4(2)
C(80)-C(81)-H(81)	120.8
C(82)-C(81)-H(81)	120.8
C(81)-C(82)-C(74)	118.6(2)
C(81)-C(82)-C(71)	131.9(2)
C(74)-C(82)-C(71)	109.5(2)
C(81)-C(82)-Zr(2)	120.39(17)
C(74)-C(82)-Zr(2)	76.48(14)
C(71)-C(82)-Zr(2)	70.27(13)
C(84)-C(83)-C(88)	118.1(3)
C(84)-C(83)-C(75)	122.1(3)
C(88)-C(83)-C(75)	119.8(2)
C(83)-C(84)-C(85)	120.3(3)
C(83)-C(84)-H(84)	119.8
C(85)-C(84)-H(84)	119.8
C(86)-C(85)-C(84)	120.6(3)
C(86)-C(85)-H(85)	119.7
C(84)-C(85)-H(85)	119.7
C(85)-C(86)-C(87)	119.9(3)
C(85)-C(86)-H(86)	120.0
C(87)-C(86)-H(86)	120.0

C (88) -C (87) -C (86)	119.6 (3)
C (88) -C (87) -H (87)	120.2
C (86) -C (87) -H (87)	120.2
C (87) -C (88) -C (83)	121.4 (3)
C (87) -C (88) -H (88)	119.3
C (83) -C (88) -H (88)	119.3
C (72) -C (89) -H (89A)	109.5
C (72) -C (89) -H (89B)	109.5
H (89A) -C (89) -H (89B)	109.5
C (72) -C (89) -H (89C)	109.5
H (89A) -C (89) -H (89C)	109.5
H (89B) -C (89) -H (89C)	109.5
Si (2) -C (90) -H (90A)	109.5
Si (2) -C (90) -H (90B)	109.5
H (90A) -C (90) -H (90B)	109.5
Si (2) -C (90) -H (90C)	109.5
H (90A) -C (90) -H (90C)	109.5
H (90B) -C (90) -H (90C)	109.5

Table S5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **12**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
Zr (1)	18 (1)	15 (1)	19 (1)	1 (1)	8 (1)	1 (1)
Zr (2)	18 (1)	16 (1)	21 (1)	1 (1)	8 (1)	2 (1)
Cl (11)	20 (1)	28 (1)	32 (1)	8 (1)	9 (1)	4 (1)
Cl (12)	38 (1)	20 (1)	26 (1)	-4 (1)	16 (1)	-2 (1)
Cl (21)	19 (1)	31 (1)	33 (1)	9 (1)	9 (1)	5 (1)
Cl (22)	40 (1)	24 (1)	31 (1)	-6 (1)	18 (1)	-3 (1)
Si (1)	23 (1)	18 (1)	31 (1)	1 (1)	14 (1)	3 (1)
Si (2)	23 (1)	18 (1)	35 (1)	3 (1)	15 (1)	5 (1)
C (11)	22 (1)	19 (1)	26 (1)	3 (1)	13 (1)	2 (1)
C (12)	25 (2)	21 (1)	20 (1)	1 (1)	15 (1)	-2 (1)
C (13)	22 (1)	20 (1)	20 (1)	4 (1)	8 (1)	-1 (1)
C (14)	22 (1)	17 (1)	24 (1)	3 (1)	12 (1)	-1 (1)
C (15)	20 (1)	18 (1)	27 (1)	4 (1)	12 (1)	-2 (1)
C (16)	24 (2)	21 (1)	28 (2)	2 (1)	11 (1)	-4 (1)
C (17)	33 (2)	22 (1)	34 (2)	-4 (1)	8 (1)	-3 (1)
C (18)	45 (2)	32 (2)	34 (2)	-3 (1)	0 (2)	-5 (1)
C (19)	32 (2)	29 (2)	40 (2)	2 (1)	-1 (1)	-2 (1)
C (20)	24 (2)	25 (1)	27 (2)	2 (1)	9 (1)	-4 (1)
C (21)	19 (1)	24 (1)	31 (2)	6 (1)	10 (1)	3 (1)
C (22)	23 (2)	16 (1)	28 (1)	2 (1)	13 (1)	-1 (1)
C (23)	24 (2)	19 (1)	21 (1)	-1 (1)	10 (1)	1 (1)
C (24)	27 (2)	23 (1)	29 (2)	1 (1)	13 (1)	0 (1)
C (25)	27 (2)	37 (2)	33 (2)	2 (1)	12 (1)	7 (1)
C (26)	39 (2)	36 (2)	37 (2)	10 (1)	13 (2)	16 (1)
C (27)	49 (2)	22 (2)	43 (2)	7 (1)	13 (2)	1 (1)
C (28)	30 (2)	22 (1)	37 (2)	2 (1)	10 (1)	-4 (1)
C (29)	37 (2)	21 (1)	20 (1)	1 (1)	13 (1)	0 (1)
C (30)	24 (2)	30 (2)	58 (2)	11 (1)	19 (2)	9 (1)
C (31)	19 (1)	17 (1)	23 (1)	3 (1)	6 (1)	2 (1)
C (32)	25 (2)	14 (1)	23 (1)	2 (1)	7 (1)	2 (1)
C (33)	27 (2)	16 (1)	18 (1)	2 (1)	9 (1)	0 (1)
C (34)	22 (1)	13 (1)	22 (1)	3 (1)	12 (1)	2 (1)
C (35)	23 (2)	16 (1)	27 (1)	3 (1)	11 (1)	0 (1)
C (36)	22 (2)	23 (1)	30 (2)	2 (1)	10 (1)	-2 (1)
C (37)	23 (2)	45 (2)	36 (2)	-4 (1)	8 (1)	-6 (1)

C (38A)	29 (3)	54 (4)	39 (4)	-13 (3)	4 (3)	-16 (3)
C (38B)	22 (4)	64 (6)	32 (5)	-2 (4)	4 (3)	-7 (4)
C (39)	34 (2)	45 (2)	30 (2)	-10 (1)	9 (1)	-9 (1)
C (40)	27 (2)	24 (1)	25 (2)	-1 (1)	8 (1)	-5 (1)
C (41)	28 (2)	18 (1)	21 (1)	-1 (1)	11 (1)	0 (1)
C (42)	22 (1)	15 (1)	23 (1)	1 (1)	9 (1)	2 (1)
C (43)	21 (2)	22 (1)	31 (2)	-5 (1)	12 (1)	-5 (1)
C (44)	42 (2)	33 (2)	48 (2)	8 (1)	27 (2)	8 (1)
C (45)	45 (2)	36 (2)	65 (2)	1 (2)	35 (2)	10 (2)
C (46)	41 (2)	42 (2)	53 (2)	-19 (2)	34 (2)	-11 (2)
C (47)	44 (2)	43 (2)	27 (2)	-8 (1)	17 (2)	-10 (2)
C (48)	29 (2)	28 (1)	27 (2)	-4 (1)	10 (1)	-3 (1)
C (49)	25 (2)	28 (2)	26 (2)	2 (1)	3 (1)	1 (1)
C (50)	43 (2)	24 (1)	39 (2)	0 (1)	23 (2)	5 (1)
C (51)	20 (1)	19 (1)	29 (2)	1 (1)	13 (1)	0 (1)
C (52)	27 (2)	22 (1)	22 (1)	3 (1)	14 (1)	1 (1)
C (53)	22 (2)	23 (1)	24 (1)	4 (1)	10 (1)	2 (1)
C (54)	20 (1)	19 (1)	23 (1)	5 (1)	11 (1)	0 (1)
C (55)	23 (2)	18 (1)	28 (2)	2 (1)	14 (1)	-1 (1)
C (56)	23 (2)	21 (1)	31 (2)	1 (1)	15 (1)	-3 (1)
C (57)	36 (2)	23 (1)	35 (2)	-5 (1)	13 (1)	-4 (1)
C (58)	39 (2)	35 (2)	31 (2)	-7 (1)	12 (1)	-5 (1)
C (59)	28 (2)	32 (2)	32 (2)	0 (1)	4 (1)	-3 (1)
C (60)	20 (1)	27 (1)	25 (1)	0 (1)	10 (1)	-4 (1)
C (61)	18 (1)	22 (1)	28 (2)	6 (1)	10 (1)	5 (1)
C (62)	22 (1)	17 (1)	26 (1)	5 (1)	14 (1)	1 (1)
C (63)	28 (2)	21 (1)	22 (1)	-1 (1)	11 (1)	1 (1)
C (64)	32 (2)	26 (1)	34 (2)	4 (1)	17 (1)	4 (1)
C (65)	30 (2)	41 (2)	30 (2)	2 (1)	14 (1)	10 (1)
C (66)	47 (2)	29 (2)	27 (2)	4 (1)	10 (1)	18 (1)
C (67)	51 (2)	18 (1)	35 (2)	1 (1)	11 (2)	2 (1)
C (68)	31 (2)	25 (1)	32 (2)	0 (1)	7 (1)	-3 (1)
C (69)	33 (2)	27 (1)	24 (1)	-4 (1)	11 (1)	-1 (1)
C (70)	28 (2)	32 (2)	53 (2)	9 (1)	17 (2)	7 (1)
C (71)	22 (1)	14 (1)	29 (2)	5 (1)	10 (1)	5 (1)
C (72)	24 (2)	22 (1)	26 (2)	7 (1)	8 (1)	1 (1)
C (73)	26 (2)	19 (1)	22 (1)	3 (1)	8 (1)	0 (1)
C (74)	27 (2)	14 (1)	23 (1)	5 (1)	11 (1)	1 (1)
C (75)	24 (2)	17 (1)	26 (1)	4 (1)	12 (1)	1 (1)
C (76)	24 (2)	19 (1)	29 (2)	1 (1)	13 (1)	-3 (1)
C (77)	25 (2)	35 (2)	37 (2)	-6 (1)	10 (1)	-5 (1)
C (78)	32 (2)	38 (2)	36 (2)	-4 (1)	4 (1)	-6 (1)
C (79)	39 (2)	29 (2)	30 (2)	-8 (1)	14 (1)	-8 (1)
C (80)	28 (2)	20 (1)	27 (2)	0 (1)	11 (1)	-3 (1)
C (81)	31 (2)	17 (1)	28 (2)	1 (1)	15 (1)	2 (1)
C (82)	24 (2)	17 (1)	25 (1)	3 (1)	12 (1)	1 (1)
C (83)	23 (2)	26 (1)	27 (2)	-2 (1)	12 (1)	-6 (1)
C (84)	48 (2)	45 (2)	35 (2)	11 (1)	21 (2)	12 (2)
C (85)	65 (3)	77 (3)	33 (2)	3 (2)	28 (2)	13 (2)
C (86)	47 (2)	59 (2)	45 (2)	-17 (2)	26 (2)	4 (2)
C (87)	25 (2)	34 (2)	51 (2)	-9 (1)	15 (2)	3 (1)
C (88)	28 (2)	28 (2)	35 (2)	0 (1)	14 (1)	1 (1)
C (89)	27 (2)	38 (2)	30 (2)	6 (1)	6 (1)	1 (1)
C (90)	43 (2)	25 (2)	50 (2)	4 (1)	29 (2)	6 (1)

Table S6. Hydrogen coordinates ($\text{\AA} \times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **12**.

	x	y	z	U (eq)
H (13)	1052	3117	417	24
H (17A)	3416	4090	3025	36

H (17B)	4482	4145	2676	36
H (18A)	5467	3975	3995	47
H (18B)	4451	3688	4084	47
H (19A)	6105	3492	3268	44
H (19B)	5668	3199	3857	44
H (21)	4873	2667	2604	29
H (24)	475	3555	1366	30
H (25)	-792	4083	848	38
H (26)	-115	4711	579	44
H (27)	1838	4808	837	46
H (28)	3111	4279	1345	35
H (29A)	1637	2214	-401	38
H (29B)	546	2476	-389	38
H (29C)	879	2078	157	38
H (30A)	5366	1984	1820	54
H (30B)	5119	1568	2211	54
H (30C)	5080	1989	2659	54
H (33)	1398	2209	3605	24
H (37C)	-2687	1417	1606	42
H (37D)	-2903	1893	1413	42
H (37A)	-2881	1893	1099	42
H (37B)	-2754	1556	1754	42
H (38A)	-2563	1051	908	50
H (38B)	-3324	1357	238	50
H (38C)	-2931	1822	153	48
H (38D)	-3349	1372	285	48
H (39C)	-1601	1090	384	44
H (39D)	-1514	1474	-171	44
H (39A)	-1814	1573	-99	44
H (39B)	-1352	1139	186	44
H (41)	788	1492	785	26
H (44)	-1918	2531	2270	46
H (45)	-2794	2782	3181	54
H (46)	-2537	2453	4412	49
H (47)	-1401	1874	4723	44
H (48)	-499	1630	3812	33
H (49A)	4089	1884	3833	41
H (49B)	3524	2282	4074	41
H (49C)	4134	2304	3383	41
H (50A)	3639	1574	431	49
H (50B)	2309	1582	354	49
H (50C)	3136	1259	935	49
H (53)	3756	9507	4267	27
H (57A)	404	8373	2273	37
H (57B)	1401	8419	1852	37
H (58A)	232	8760	758	42
H (58B)	-715	8478	961	42
H (59A)	-985	9253	943	38
H (59B)	-1324	8993	1622	38
H (61)	-142	9849	2062	27
H (64)	4377	9027	3445	35
H (65)	5663	8534	4126	39
H (66)	5020	7926	4504	41
H (67)	3064	7818	4235	42
H (68)	1763	8313	3575	35
H (69A)	3052	10477	4873	42
H (69B)	3983	10506	4402	42
H (69C)	4073	10156	5055	42
H (70A)	-675	10562	2700	55
H (70B)	-376	10542	1867	55
H (70C)	-457	10971	2276	55
H (73)	3346	10300	976	27
H (77A)	7399	11142	3027	38
H (77B)	7605	10664	3209	38
H (78A)	7407	10722	4482	44
H (78B)	7983	11155	4421	44
H (79A)	6041	11143	4695	38

H (79B)	6263	11489	4105	38
H (81)	3836	11087	3704	29
H (84)	5043	10753	658	49
H (85)	5957	10433	-171	67
H (86)	7358	9953	353	57
H (87)	7748	9744	1693	43
H (88)	6846	10060	2524	35
H (89A)	597	10609	704	49
H (89B)	607	10193	1182	49
H (89C)	1213	10217	488	49
H (90A)	1067	10986	4103	54
H (90B)	1349	11316	3517	54
H (90C)	2353	11046	4089	54

Table S7. Torsion angles [deg] for **12**.

C (30)-Si (1)-C (11)-C (12)	162.3 (2)
C (50)-Si (1)-C (11)-C (12)	42.3 (3)
C (31)-Si (1)-C (11)-C (12)	-77.1 (2)
C (30)-Si (1)-C (11)-C (22)	-41.6 (3)
C (50)-Si (1)-C (11)-C (22)	-161.6 (2)
C (31)-Si (1)-C (11)-C (22)	79.0 (2)
C (30)-Si (1)-C (11)-Zr (1)	-119.86 (13)
C (50)-Si (1)-C (11)-Zr (1)	120.08 (12)
C (31)-Si (1)-C (11)-Zr (1)	0.67 (11)
Cl (11)-Zr (1)-C (11)-C (12)	8.86 (16)
Cl (12)-Zr (1)-C (11)-C (12)	-120.10 (13)
C (31)-Zr (1)-C (11)-C (12)	125.05 (15)
C (32)-Zr (1)-C (11)-C (12)	151.69 (14)
C (22)-Zr (1)-C (11)-C (12)	-110.2 (2)
C (33)-Zr (1)-C (11)-C (12)	142.76 (13)
C (42)-Zr (1)-C (11)-C (12)	97.81 (14)
C (13)-Zr (1)-C (11)-C (12)	-35.32 (13)
C (14)-Zr (1)-C (11)-C (12)	-73.91 (14)
C (34)-Zr (1)-C (11)-C (12)	105.69 (14)
Cl (11)-Zr (1)-C (11)-C (22)	119.04 (13)
Cl (12)-Zr (1)-C (11)-C (22)	-9.92 (16)
C (31)-Zr (1)-C (11)-C (22)	-124.77 (16)
C (32)-Zr (1)-C (11)-C (22)	-98.13 (15)
C (12)-Zr (1)-C (11)-C (22)	110.2 (2)
C (33)-Zr (1)-C (11)-C (22)	-107.06 (15)
C (42)-Zr (1)-C (11)-C (22)	-152.01 (15)
C (13)-Zr (1)-C (11)-C (22)	74.86 (15)
C (14)-Zr (1)-C (11)-C (22)	36.27 (13)
C (34)-Zr (1)-C (11)-C (22)	-144.13 (13)
Cl (11)-Zr (1)-C (11)-Si (1)	-116.73 (8)
Cl (12)-Zr (1)-C (11)-Si (1)	114.30 (8)
C (31)-Zr (1)-C (11)-Si (1)	-0.54 (9)
C (32)-Zr (1)-C (11)-Si (1)	26.09 (11)
C (12)-Zr (1)-C (11)-Si (1)	-125.60 (19)
C (22)-Zr (1)-C (11)-Si (1)	124.22 (19)
C (33)-Zr (1)-C (11)-Si (1)	17.16 (14)
C (42)-Zr (1)-C (11)-Si (1)	-27.79 (11)
C (13)-Zr (1)-C (11)-Si (1)	-160.92 (15)
C (14)-Zr (1)-C (11)-Si (1)	160.49 (15)
C (34)-Zr (1)-C (11)-Si (1)	-19.91 (14)
C (22)-C (11)-C (12)-C (13)	-1.9 (3)
Si (1)-C (11)-C (12)-C (13)	158.0 (2)
Zr (1)-C (11)-C (12)-C (13)	68.69 (18)
C (22)-C (11)-C (12)-C (29)	177.0 (2)
Si (1)-C (11)-C (12)-C (29)	-23.1 (4)
Zr (1)-C (11)-C (12)-C (29)	-112.4 (3)

C(22)-C(11)-C(12)-Zr(1)	-70.55(17)
Si(1)-C(11)-C(12)-Zr(1)	89.34(19)
Cl(11)-Zr(1)-C(12)-C(13)	71.42(14)
Cl(12)-Zr(1)-C(12)-C(13)	-30.47(18)
C(11)-Zr(1)-C(12)-C(13)	-116.1(2)
C(31)-Zr(1)-C(12)-C(13)	-165.99(15)
C(32)-Zr(1)-C(12)-C(13)	-149.24(14)
C(22)-Zr(1)-C(12)-C(13)	-75.88(16)
C(33)-Zr(1)-C(12)-C(13)	-177.95(14)
C(42)-Zr(1)-C(12)-C(13)	160.72(15)
C(14)-Zr(1)-C(12)-C(13)	-35.32(14)
C(34)-Zr(1)-C(12)-C(13)	147.61(14)
Cl(11)-Zr(1)-C(12)-C(11)	-172.45(13)
Cl(12)-Zr(1)-C(12)-C(11)	85.66(15)
C(31)-Zr(1)-C(12)-C(11)	-49.86(14)
C(32)-Zr(1)-C(12)-C(11)	-33.11(16)
C(22)-Zr(1)-C(12)-C(11)	40.25(13)
C(33)-Zr(1)-C(12)-C(11)	-61.8(2)
C(42)-Zr(1)-C(12)-C(11)	-83.15(14)
C(13)-Zr(1)-C(12)-C(11)	116.1(2)
C(14)-Zr(1)-C(12)-C(11)	80.81(15)
C(34)-Zr(1)-C(12)-C(11)	-96.26(15)
Cl(11)-Zr(1)-C(12)-C(29)	-49.40(18)
Cl(12)-Zr(1)-C(12)-C(29)	-151.29(15)
C(11)-Zr(1)-C(12)-C(29)	123.0(3)
C(31)-Zr(1)-C(12)-C(29)	73.19(19)
C(32)-Zr(1)-C(12)-C(29)	89.9(2)
C(22)-Zr(1)-C(12)-C(29)	163.3(2)
C(33)-Zr(1)-C(12)-C(29)	61.2(2)
C(42)-Zr(1)-C(12)-C(29)	39.90(19)
C(13)-Zr(1)-C(12)-C(29)	-120.8(3)
C(14)-Zr(1)-C(12)-C(29)	-156.1(2)
C(34)-Zr(1)-C(12)-C(29)	26.8(2)
C(11)-C(12)-C(13)-C(14)	1.7(3)
C(29)-C(12)-C(13)-C(14)	-177.2(2)
Zr(1)-C(12)-C(13)-C(14)	65.89(18)
C(11)-C(12)-C(13)-Zr(1)	-64.18(18)
C(29)-C(12)-C(13)-Zr(1)	116.9(2)
Cl(11)-Zr(1)-C(13)-C(12)	-104.93(15)
Cl(12)-Zr(1)-C(13)-C(12)	157.43(14)
C(11)-Zr(1)-C(13)-C(12)	37.75(15)
C(31)-Zr(1)-C(13)-C(12)	16.36(18)
C(32)-Zr(1)-C(13)-C(12)	49.9(2)
C(22)-Zr(1)-C(13)-C(12)	80.23(16)
C(42)-Zr(1)-C(13)-C(12)	-23.26(18)
C(14)-Zr(1)-C(13)-C(12)	117.4(2)
C(34)-Zr(1)-C(13)-C(12)	-55.4(2)
Cl(11)-Zr(1)-C(13)-C(14)	137.63(15)
Cl(12)-Zr(1)-C(13)-C(14)	39.99(15)
C(11)-Zr(1)-C(13)-C(14)	-79.69(16)
C(31)-Zr(1)-C(13)-C(14)	-101.08(15)
C(32)-Zr(1)-C(13)-C(14)	-67.6(2)
C(12)-Zr(1)-C(13)-C(14)	-117.4(2)
C(22)-Zr(1)-C(13)-C(14)	-37.21(14)
C(42)-Zr(1)-C(13)-C(14)	-140.70(14)
C(34)-Zr(1)-C(13)-C(14)	-172.86(14)
C(12)-C(13)-C(14)-C(15)	177.9(3)
Zr(1)-C(13)-C(14)-C(15)	-119.4(3)
C(12)-C(13)-C(14)-C(22)	-0.8(3)
Zr(1)-C(13)-C(14)-C(22)	61.93(17)
C(12)-C(13)-C(14)-Zr(1)	-62.75(18)
Cl(11)-Zr(1)-C(14)-C(13)	-42.51(15)
Cl(12)-Zr(1)-C(14)-C(13)	-140.73(15)
C(11)-Zr(1)-C(14)-C(13)	77.59(16)
C(31)-Zr(1)-C(14)-C(13)	98.43(16)
C(32)-Zr(1)-C(14)-C(13)	138.83(15)
C(12)-Zr(1)-C(14)-C(13)	35.65(14)

C (22)-Zr (1)-C (14)-C (13)	115.7 (2)
C (33)-Zr (1)-C (14)-C (13)	171.54 (16)
C (42)-Zr (1)-C (14)-C (13)	63.5 (2)
Cl (11)-Zr (1)-C (14)-C (15)	87.0 (2)
Cl (12)-Zr (1)-C (14)-C (15)	-11.26 (19)
C (11)-Zr (1)-C (14)-C (15)	-152.9 (2)
C (31)-Zr (1)-C (14)-C (15)	-132.10 (19)
C (32)-Zr (1)-C (14)-C (15)	-91.7 (2)
C (12)-Zr (1)-C (14)-C (15)	165.1 (2)
C (22)-Zr (1)-C (14)-C (15)	-114.9 (3)
C (33)-Zr (1)-C (14)-C (15)	-59.0 (3)
C (42)-Zr (1)-C (14)-C (15)	-167.05 (17)
C (13)-Zr (1)-C (14)-C (15)	129.5 (3)
Cl (11)-Zr (1)-C (14)-C (22)	-158.18 (13)
Cl (12)-Zr (1)-C (14)-C (22)	103.60 (14)
C (11)-Zr (1)-C (14)-C (22)	-38.08 (15)
C (31)-Zr (1)-C (14)-C (22)	-17.24 (18)
C (32)-Zr (1)-C (14)-C (22)	23.16 (18)
C (12)-Zr (1)-C (14)-C (22)	-80.02 (16)
C (33)-Zr (1)-C (14)-C (22)	55.9 (2)
C (42)-Zr (1)-C (14)-C (22)	-52.2 (2)
C (13)-Zr (1)-C (14)-C (22)	-115.7 (2)
C (13)-C (14)-C (15)-C (16)	-179.9 (3)
C (22)-C (14)-C (15)-C (16)	-1.3 (4)
Zr (1)-C (14)-C (15)-C (16)	83.5 (3)
C (13)-C (14)-C (15)-C (23)	1.3 (4)
C (22)-C (14)-C (15)-C (23)	179.8 (2)
Zr (1)-C (14)-C (15)-C (23)	-95.4 (3)
C (14)-C (15)-C (16)-C (20)	1.6 (4)
C (23)-C (15)-C (16)-C (20)	-179.6 (2)
C (14)-C (15)-C (16)-C (17)	-175.6 (3)
C (23)-C (15)-C (16)-C (17)	3.2 (4)
C (15)-C (16)-C (17)-C (18)	158.4 (3)
C (20)-C (16)-C (17)-C (18)	-19.0 (3)
C (16)-C (17)-C (18)-C (19)	32.4 (3)
C (17)-C (18)-C (19)-C (20)	-33.9 (3)
C (15)-C (16)-C (20)-C (21)	-0.8 (4)
C (17)-C (16)-C (20)-C (21)	176.8 (3)
C (15)-C (16)-C (20)-C (19)	180.0 (3)
C (17)-C (16)-C (20)-C (19)	-2.4 (3)
C (18)-C (19)-C (20)-C (21)	-156.3 (3)
C (18)-C (19)-C (20)-C (16)	22.8 (3)
C (16)-C (20)-C (21)-C (22)	-0.3 (4)
C (19)-C (20)-C (21)-C (22)	178.8 (3)
C (20)-C (21)-C (22)-C (14)	0.5 (4)
C (20)-C (21)-C (22)-C (11)	179.9 (3)
C (20)-C (21)-C (22)-Zr (1)	-91.4 (3)
C (13)-C (14)-C (22)-C (21)	179.2 (2)
C (15)-C (14)-C (22)-C (21)	0.3 (4)
Zr (1)-C (14)-C (22)-C (21)	-116.6 (2)
C (13)-C (14)-C (22)-C (11)	-0.4 (3)
C (15)-C (14)-C (22)-C (11)	-179.2 (2)
Zr (1)-C (14)-C (22)-C (11)	63.84 (17)
C (13)-C (14)-C (22)-Zr (1)	-64.20 (18)
C (15)-C (14)-C (22)-Zr (1)	116.9 (2)
C (12)-C (11)-C (22)-C (21)	-178.1 (3)
Si (1)-C (11)-C (22)-C (21)	21.6 (4)
Zr (1)-C (11)-C (22)-C (21)	111.6 (3)
C (12)-C (11)-C (22)-C (14)	1.3 (3)
Si (1)-C (11)-C (22)-C (14)	-158.90 (19)
Zr (1)-C (11)-C (22)-C (14)	-68.93 (18)
C (12)-C (11)-C (22)-Zr (1)	70.27 (17)
Si (1)-C (11)-C (22)-Zr (1)	-89.97 (19)
Cl (11)-Zr (1)-C (22)-C (21)	145.80 (16)
Cl (12)-Zr (1)-C (22)-C (21)	43.58 (18)
C (11)-Zr (1)-C (22)-C (21)	-128.0 (3)
C (31)-Zr (1)-C (22)-C (21)	-77.94 (19)

C (32)-Zr (1)-C (22)-C (21)	-44.53 (19)
C (12)-Zr (1)-C (22)-C (21)	-167.9 (2)
C (33)-Zr (1)-C (22)-C (21)	-32.3 (2)
C (42)-Zr (1)-C (22)-C (21)	-95.6 (2)
C (13)-Zr (1)-C (22)-C (21)	152.6 (2)
C (14)-Zr (1)-C (22)-C (21)	116.7 (3)
C (34)-Zr (1)-C (22)-C (21)	-68.0 (2)
Cl (11)-Zr (1)-C (22)-C (14)	29.10 (17)
Cl (12)-Zr (1)-C (22)-C (14)	-73.12 (14)
C (11)-Zr (1)-C (22)-C (14)	115.3 (2)
C (31)-Zr (1)-C (22)-C (14)	165.36 (15)
C (32)-Zr (1)-C (22)-C (14)	-161.23 (15)
C (12)-Zr (1)-C (22)-C (14)	75.37 (15)
C (33)-Zr (1)-C (22)-C (14)	-148.96 (14)
C (42)-Zr (1)-C (22)-C (14)	147.74 (14)
C (13)-Zr (1)-C (22)-C (14)	35.88 (14)
C (34)-Zr (1)-C (22)-C (14)	175.26 (14)
Cl (11)-Zr (1)-C (22)-C (11)	-86.16 (15)
Cl (12)-Zr (1)-C (22)-C (11)	171.62 (14)
C (31)-Zr (1)-C (22)-C (11)	50.09 (15)
C (32)-Zr (1)-C (22)-C (11)	83.50 (15)
C (12)-Zr (1)-C (22)-C (11)	-39.89 (14)
C (33)-Zr (1)-C (22)-C (11)	95.78 (16)
C (42)-Zr (1)-C (22)-C (11)	32.47 (17)
C (13)-Zr (1)-C (22)-C (11)	-79.38 (15)
C (14)-Zr (1)-C (22)-C (11)	-115.3 (2)
C (34)-Zr (1)-C (22)-C (11)	60.0 (2)
C (16)-C (15)-C (23)-C (24)	-130.2 (3)
C (14)-C (15)-C (23)-C (24)	48.6 (4)
C (16)-C (15)-C (23)-C (28)	49.7 (4)
C (14)-C (15)-C (23)-C (28)	-131.5 (3)
C (28)-C (23)-C (24)-C (25)	-0.3 (4)
C (15)-C (23)-C (24)-C (25)	179.7 (2)
C (23)-C (24)-C (25)-C (26)	0.0 (4)
C (24)-C (25)-C (26)-C (27)	-0.1 (5)
C (25)-C (26)-C (27)-C (28)	0.4 (5)
C (26)-C (27)-C (28)-C (23)	-0.6 (5)
C (24)-C (23)-C (28)-C (27)	0.6 (4)
C (15)-C (23)-C (28)-C (27)	-179.4 (3)
C (30)-Si (1)-C (31)-C (32)	42.0 (2)
C (50)-Si (1)-C (31)-C (32)	165.1 (2)
C (11)-Si (1)-C (31)-C (32)	-76.4 (2)
C (30)-Si (1)-C (31)-C (42)	-163.7 (2)
C (50)-Si (1)-C (31)-C (42)	-40.6 (2)
C (11)-Si (1)-C (31)-C (42)	77.9 (2)
C (30)-Si (1)-C (31)-Zr (1)	117.75 (12)
C (50)-Si (1)-C (31)-Zr (1)	-119.20 (12)
C (11)-Si (1)-C (31)-Zr (1)	-0.66 (11)
Cl (11)-Zr (1)-C (31)-C (32)	-119.12 (13)
Cl (12)-Zr (1)-C (31)-C (32)	10.29 (17)
C (11)-Zr (1)-C (31)-C (32)	126.11 (16)
C (12)-Zr (1)-C (31)-C (32)	153.21 (15)
C (22)-Zr (1)-C (31)-C (32)	98.69 (15)
C (33)-Zr (1)-C (31)-C (32)	-35.35 (14)
C (42)-Zr (1)-C (31)-C (32)	-110.0 (2)
C (13)-Zr (1)-C (31)-C (32)	144.70 (14)
C (14)-Zr (1)-C (31)-C (32)	107.86 (15)
C (34)-Zr (1)-C (31)-C (32)	-74.29 (15)
Cl (11)-Zr (1)-C (31)-C (42)	-9.14 (16)
Cl (12)-Zr (1)-C (31)-C (42)	120.27 (13)
C (11)-Zr (1)-C (31)-C (42)	-123.92 (16)
C (32)-Zr (1)-C (31)-C (42)	110.0 (2)
C (12)-Zr (1)-C (31)-C (42)	-96.82 (15)
C (22)-Zr (1)-C (31)-C (42)	-151.33 (15)
C (33)-Zr (1)-C (31)-C (42)	74.62 (15)
C (13)-Zr (1)-C (31)-C (42)	-105.33 (15)
C (14)-Zr (1)-C (31)-C (42)	-142.17 (14)

C (34)-Zr (1)-C (31)-C (42)	35.69 (13)
Cl (11)-Zr (1)-C (31)-Si (1)	115.31 (8)
Cl (12)-Zr (1)-C (31)-Si (1)	-115.28 (8)
C (11)-Zr (1)-C (31)-Si (1)	0.54 (9)
C (32)-Zr (1)-C (31)-Si (1)	-125.57 (19)
C (12)-Zr (1)-C (31)-Si (1)	27.64 (10)
C (22)-Zr (1)-C (31)-Si (1)	-26.88 (10)
C (33)-Zr (1)-C (31)-Si (1)	-160.92 (14)
C (42)-Zr (1)-C (31)-Si (1)	124.46 (18)
C (13)-Zr (1)-C (31)-Si (1)	19.13 (13)
C (14)-Zr (1)-C (31)-Si (1)	-17.71 (13)
C (34)-Zr (1)-C (31)-Si (1)	160.14 (14)
C (42)-C (31)-C (32)-C (33)	-3.6 (3)
Si (1)-C (31)-C (32)-C (33)	154.87 (18)
Zr (1)-C (31)-C (32)-C (33)	67.52 (17)
C (42)-C (31)-C (32)-C (49)	174.0 (2)
Si (1)-C (31)-C (32)-C (49)	-27.6 (4)
Zr (1)-C (31)-C (32)-C (49)	-114.9 (2)
C (42)-C (31)-C (32)-Zr (1)	-71.09 (15)
Si (1)-C (31)-C (32)-Zr (1)	87.35 (18)
Cl (11)-Zr (1)-C (32)-C (33)	-29.77 (17)
Cl (12)-Zr (1)-C (32)-C (33)	72.29 (14)
C (11)-Zr (1)-C (32)-C (33)	-165.45 (15)
C (31)-Zr (1)-C (32)-C (33)	-116.5 (2)
C (12)-Zr (1)-C (32)-C (33)	-147.76 (14)
C (22)-Zr (1)-C (32)-C (33)	160.70 (15)
C (42)-Zr (1)-C (32)-C (33)	-76.56 (15)
C (13)-Zr (1)-C (32)-C (33)	-175.33 (14)
C (14)-Zr (1)-C (32)-C (33)	148.45 (14)
C (34)-Zr (1)-C (32)-C (33)	-36.18 (14)
Cl (11)-Zr (1)-C (32)-C (31)	86.71 (16)
Cl (12)-Zr (1)-C (32)-C (31)	-171.23 (14)
C (11)-Zr (1)-C (32)-C (31)	-48.97 (15)
C (12)-Zr (1)-C (32)-C (31)	-31.28 (17)
C (22)-Zr (1)-C (32)-C (31)	-82.82 (15)
C (33)-Zr (1)-C (32)-C (31)	116.5 (2)
C (42)-Zr (1)-C (32)-C (31)	39.92 (14)
C (13)-Zr (1)-C (32)-C (31)	-58.9 (2)
C (14)-Zr (1)-C (32)-C (31)	-95.07 (16)
C (34)-Zr (1)-C (32)-C (31)	80.29 (15)
Cl (11)-Zr (1)-C (32)-C (49)	-149.39 (17)
Cl (12)-Zr (1)-C (32)-C (49)	-47.3 (2)
C (11)-Zr (1)-C (32)-C (49)	74.9 (2)
C (31)-Zr (1)-C (32)-C (49)	123.9 (3)
C (12)-Zr (1)-C (32)-C (49)	92.6 (2)
C (22)-Zr (1)-C (32)-C (49)	41.1 (2)
C (33)-Zr (1)-C (32)-C (49)	-119.6 (3)
C (42)-Zr (1)-C (32)-C (49)	163.8 (2)
C (13)-Zr (1)-C (32)-C (49)	65.1 (2)
C (14)-Zr (1)-C (32)-C (49)	28.8 (2)
C (34)-Zr (1)-C (32)-C (49)	-155.8 (2)
C (31)-C (32)-C (33)-C (34)	3.6 (3)
C (49)-C (32)-C (33)-C (34)	-174.1 (2)
Zr (1)-C (32)-C (33)-C (34)	68.35 (17)
C (31)-C (32)-C (33)-Zr (1)	-64.76 (17)
C (49)-C (32)-C (33)-Zr (1)	117.5 (2)
Cl (11)-Zr (1)-C (33)-C (32)	157.87 (13)
Cl (12)-Zr (1)-C (33)-C (32)	-104.26 (14)
C (11)-Zr (1)-C (33)-C (32)	17.08 (18)
C (31)-Zr (1)-C (33)-C (32)	37.39 (14)
C (12)-Zr (1)-C (33)-C (32)	52.1 (2)
C (22)-Zr (1)-C (33)-C (32)	-23.62 (18)
C (42)-Zr (1)-C (33)-C (32)	79.04 (16)
C (14)-Zr (1)-C (33)-C (32)	-56.4 (2)
C (34)-Zr (1)-C (33)-C (32)	115.9 (2)
Cl (11)-Zr (1)-C (33)-C (34)	41.93 (15)
Cl (12)-Zr (1)-C (33)-C (34)	139.80 (14)

C (11) -Zr (1) -C (33) -C (34)	-98.86 (16)
C (31) -Zr (1) -C (33) -C (34)	-78.55 (15)
C (32) -Zr (1) -C (33) -C (34)	-115.9 (2)
C (12) -Zr (1) -C (33) -C (34)	-63.9 (2)
C (22) -Zr (1) -C (33) -C (34)	-139.57 (14)
C (42) -Zr (1) -C (33) -C (34)	-36.91 (14)
C (14) -Zr (1) -C (33) -C (34)	-172.36 (15)
C (32) -C (33) -C (34) -C (35)	178.0 (2)
Zr (1) -C (33) -C (34) -C (35)	-117.0 (3)
C (32) -C (33) -C (34) -C (42)	-2.1 (3)
Zr (1) -C (33) -C (34) -C (42)	62.96 (16)
C (32) -C (33) -C (34) -Zr (1)	-65.02 (17)
Cl (11) -Zr (1) -C (34) -C (33)	-138.68 (15)
Cl (12) -Zr (1) -C (34) -C (33)	-40.71 (15)
C (11) -Zr (1) -C (34) -C (33)	100.71 (16)
C (31) -Zr (1) -C (34) -C (33)	78.47 (16)
C (32) -Zr (1) -C (34) -C (33)	36.51 (14)
C (12) -Zr (1) -C (34) -C (33)	140.74 (15)
C (22) -Zr (1) -C (34) -C (33)	66.3 (2)
C (42) -Zr (1) -C (34) -C (33)	115.6 (2)
C (13) -Zr (1) -C (34) -C (33)	172.03 (15)
Cl (11) -Zr (1) -C (34) -C (35)	-10.85 (19)
Cl (12) -Zr (1) -C (34) -C (35)	87.1 (2)
C (11) -Zr (1) -C (34) -C (35)	-131.46 (19)
C (31) -Zr (1) -C (34) -C (35)	-153.7 (2)
C (32) -Zr (1) -C (34) -C (35)	164.3 (2)
C (12) -Zr (1) -C (34) -C (35)	-91.4 (2)
C (22) -Zr (1) -C (34) -C (35)	-165.83 (18)
C (33) -Zr (1) -C (34) -C (35)	127.8 (3)
C (42) -Zr (1) -C (34) -C (35)	-116.6 (3)
C (13) -Zr (1) -C (34) -C (35)	-60.1 (3)
Cl (11) -Zr (1) -C (34) -C (42)	105.71 (14)
Cl (12) -Zr (1) -C (34) -C (42)	-156.32 (13)
C (11) -Zr (1) -C (34) -C (42)	-14.90 (17)
C (31) -Zr (1) -C (34) -C (42)	-37.14 (14)
C (32) -Zr (1) -C (34) -C (42)	-79.09 (15)
C (12) -Zr (1) -C (34) -C (42)	25.13 (17)
C (22) -Zr (1) -C (34) -C (42)	-49.3 (2)
C (33) -Zr (1) -C (34) -C (42)	-115.6 (2)
C (13) -Zr (1) -C (34) -C (42)	56.4 (2)
C (33) -C (34) -C (35) -C (36)	179.5 (2)
C (42) -C (34) -C (35) -C (36)	-0.5 (3)
Zr (1) -C (34) -C (35) -C (36)	86.4 (3)
C (33) -C (34) -C (35) -C (43)	0.7 (4)
C (42) -C (34) -C (35) -C (43)	-179.3 (2)
Zr (1) -C (34) -C (35) -C (43)	-92.4 (3)
C (34) -C (35) -C (36) -C (40)	1.9 (4)
C (43) -C (35) -C (36) -C (40)	-179.4 (2)
C (34) -C (35) -C (36) -C (37)	179.2 (2)
C (43) -C (35) -C (36) -C (37)	-2.0 (4)
C (35) -C (36) -C (37) -C (38B)	165.3 (5)
C (40) -C (36) -C (37) -C (38B)	-17.1 (5)
C (35) -C (36) -C (37) -C (38A)	-160.0 (4)
C (40) -C (36) -C (37) -C (38A)	17.6 (4)
C (38B) -C (37) -C (38A) -C (39)	68.5 (8)
C (36) -C (37) -C (38A) -C (39)	-28.4 (5)
C (36) -C (37) -C (38B) -C (39)	27.3 (6)
C (38A) -C (37) -C (38B) -C (39)	-64.5 (7)
C (37) -C (38A) -C (39) -C (40)	28.4 (5)
C (37) -C (38A) -C (39) -C (38B)	-62.2 (7)
C (37) -C (38B) -C (39) -C (38A)	70.4 (7)
C (37) -C (38B) -C (39) -C (40)	-27.1 (6)
C (35) -C (36) -C (40) -C (41)	-1.6 (4)
C (37) -C (36) -C (40) -C (41)	-179.4 (2)
C (35) -C (36) -C (40) -C (39)	177.5 (2)
C (37) -C (36) -C (40) -C (39)	-0.3 (3)
C (38A) -C (39) -C (40) -C (41)	161.3 (4)

C (38B) -C (39) -C (40) -C (41)	-164.7 (4)
C (38A) -C (39) -C (40) -C (36)	-17.7 (4)
C (38B) -C (39) -C (40) -C (36)	16.3 (4)
C (36) -C (40) -C (41) -C (42)	-0.2 (4)
C (39) -C (40) -C (41) -C (42)	-179.1 (3)
C (40) -C (41) -C (42) -C (34)	1.5 (3)
C (40) -C (41) -C (42) -C (31)	-179.7 (2)
C (40) -C (41) -C (42) -Zr (1)	-89.4 (3)
C (33) -C (34) -C (42) -C (41)	178.8 (2)
C (35) -C (34) -C (42) -C (41)	-1.2 (3)
Zr (1) -C (34) -C (42) -C (41)	-118.1 (2)
C (33) -C (34) -C (42) -C (31)	-0.2 (3)
C (35) -C (34) -C (42) -C (31)	179.8 (2)
Zr (1) -C (34) -C (42) -C (31)	62.90 (16)
C (33) -C (34) -C (42) -Zr (1)	-63.10 (16)
C (35) -C (34) -C (42) -Zr (1)	116.9 (2)
C (32) -C (31) -C (42) -C (41)	-176.6 (3)
Si (1) -C (31) -C (42) -C (41)	24.7 (4)
Zr (1) -C (31) -C (42) -C (41)	114.0 (3)
C (32) -C (31) -C (42) -C (34)	2.3 (3)
Si (1) -C (31) -C (42) -C (34)	-156.46 (18)
Zr (1) -C (31) -C (42) -C (34)	-67.19 (17)
C (32) -C (31) -C (42) -Zr (1)	69.45 (15)
Si (1) -C (31) -C (42) -Zr (1)	-89.27 (17)
Cl (11) -Zr (1) -C (42) -C (41)	44.1 (2)
Cl (12) -Zr (1) -C (42) -C (41)	147.26 (17)
C (11) -Zr (1) -C (42) -C (41)	-77.4 (2)
C (31) -Zr (1) -C (42) -C (41)	-128.2 (3)
C (32) -Zr (1) -C (42) -C (41)	-168.4 (2)
C (12) -Zr (1) -C (42) -C (41)	-43.8 (2)
C (22) -Zr (1) -C (42) -C (41)	-94.9 (2)
C (33) -Zr (1) -C (42) -C (41)	151.6 (2)
C (13) -Zr (1) -C (42) -C (41)	-31.8 (2)
C (14) -Zr (1) -C (42) -C (41)	-65.8 (3)
C (34) -Zr (1) -C (42) -C (41)	115.4 (3)
Cl (11) -Zr (1) -C (42) -C (34)	-71.27 (13)
Cl (12) -Zr (1) -C (42) -C (34)	31.86 (17)
C (11) -Zr (1) -C (42) -C (34)	167.23 (15)
C (31) -Zr (1) -C (42) -C (34)	116.4 (2)
C (32) -Zr (1) -C (42) -C (34)	76.21 (15)
C (12) -Zr (1) -C (42) -C (34)	-159.24 (14)
C (22) -Zr (1) -C (42) -C (34)	149.71 (14)
C (33) -Zr (1) -C (42) -C (34)	36.23 (13)
C (13) -Zr (1) -C (42) -C (34)	-147.24 (13)
C (14) -Zr (1) -C (42) -C (34)	178.78 (14)
Cl (11) -Zr (1) -C (42) -C (31)	172.30 (14)
Cl (12) -Zr (1) -C (42) -C (31)	-84.56 (15)
C (11) -Zr (1) -C (42) -C (31)	50.80 (15)
C (32) -Zr (1) -C (42) -C (31)	-40.21 (14)
C (12) -Zr (1) -C (42) -C (31)	84.34 (15)
C (22) -Zr (1) -C (42) -C (31)	33.28 (17)
C (33) -Zr (1) -C (42) -C (31)	-80.19 (15)
C (13) -Zr (1) -C (42) -C (31)	96.34 (15)
C (14) -Zr (1) -C (42) -C (31)	62.4 (2)
C (34) -Zr (1) -C (42) -C (31)	-116.4 (2)
C (36) -C (35) -C (43) -C (48)	110.6 (3)
C (34) -C (35) -C (43) -C (48)	-70.7 (3)
C (36) -C (35) -C (43) -C (44)	-68.9 (3)
C (34) -C (35) -C (43) -C (44)	109.8 (3)
C (48) -C (43) -C (44) -C (45)	-0.2 (4)
C (35) -C (43) -C (44) -C (45)	179.3 (3)
C (43) -C (44) -C (45) -C (46)	-0.2 (5)
C (44) -C (45) -C (46) -C (47)	0.1 (5)
C (45) -C (46) -C (47) -C (48)	0.4 (5)
C (44) -C (43) -C (48) -C (47)	0.8 (4)
C (35) -C (43) -C (48) -C (47)	-178.7 (2)
C (46) -C (47) -C (48) -C (43)	-0.9 (4)

C(70)-Si(2)-C(51)-C(52)	-162.9(2)
C(90)-Si(2)-C(51)-C(52)	-43.5(3)
C(71)-Si(2)-C(51)-C(52)	77.0(2)
C(70)-Si(2)-C(51)-C(62)	40.1(3)
C(90)-Si(2)-C(51)-C(62)	159.5(2)
C(71)-Si(2)-C(51)-C(62)	-80.0(2)
C(70)-Si(2)-C(51)-Zr(2)	118.52(13)
C(90)-Si(2)-C(51)-Zr(2)	-122.06(12)
C(71)-Si(2)-C(51)-Zr(2)	-1.62(12)
Cl(21)-Zr(2)-C(51)-C(52)	-5.60(16)
Cl(22)-Zr(2)-C(51)-C(52)	121.93(13)
C(71)-Zr(2)-C(51)-C(52)	-123.42(16)
C(72)-Zr(2)-C(51)-C(52)	-149.41(14)
C(62)-Zr(2)-C(51)-C(52)	110.5(2)
C(73)-Zr(2)-C(51)-C(52)	-139.55(14)
C(82)-Zr(2)-C(51)-C(52)	-95.64(14)
C(53)-Zr(2)-C(51)-C(52)	35.41(13)
C(54)-Zr(2)-C(51)-C(52)	74.19(15)
C(74)-Zr(2)-C(51)-C(52)	-102.48(15)
Cl(21)-Zr(2)-C(51)-C(62)	-116.11(13)
Cl(22)-Zr(2)-C(51)-C(62)	11.42(16)
C(71)-Zr(2)-C(51)-C(62)	126.08(16)
C(72)-Zr(2)-C(51)-C(62)	100.09(15)
C(52)-Zr(2)-C(51)-C(62)	-110.5(2)
C(73)-Zr(2)-C(51)-C(62)	109.95(15)
C(82)-Zr(2)-C(51)-C(62)	153.86(15)
C(53)-Zr(2)-C(51)-C(62)	-75.09(15)
C(54)-Zr(2)-C(51)-C(62)	-36.31(13)
C(74)-Zr(2)-C(51)-C(62)	147.02(13)
Cl(21)-Zr(2)-C(51)-Si(2)	119.13(8)
Cl(22)-Zr(2)-C(51)-Si(2)	-113.34(9)
C(71)-Zr(2)-C(51)-Si(2)	1.32(9)
C(72)-Zr(2)-C(51)-Si(2)	-24.67(11)
C(52)-Zr(2)-C(51)-Si(2)	124.74(18)
C(62)-Zr(2)-C(51)-Si(2)	-124.76(19)
C(73)-Zr(2)-C(51)-Si(2)	-14.81(14)
C(82)-Zr(2)-C(51)-Si(2)	29.10(11)
C(53)-Zr(2)-C(51)-Si(2)	160.15(15)
C(54)-Zr(2)-C(51)-Si(2)	-161.07(15)
C(74)-Zr(2)-C(51)-Si(2)	22.26(14)
C(62)-C(51)-C(52)-C(53)	2.3(3)
Si(2)-C(51)-C(52)-C(53)	-158.5(2)
Zr(2)-C(51)-C(52)-C(53)	-67.98(19)
C(62)-C(51)-C(52)-C(69)	-175.7(3)
Si(2)-C(51)-C(52)-C(69)	23.5(4)
Zr(2)-C(51)-C(52)-C(69)	114.0(3)
C(62)-C(51)-C(52)-Zr(2)	70.26(17)
Si(2)-C(51)-C(52)-Zr(2)	-90.51(19)
Cl(21)-Zr(2)-C(52)-C(53)	-68.58(15)
Cl(22)-Zr(2)-C(52)-C(53)	31.79(19)
C(51)-Zr(2)-C(52)-C(53)	116.1(2)
C(71)-Zr(2)-C(52)-C(53)	167.17(16)
C(72)-Zr(2)-C(52)-C(53)	151.72(15)
C(62)-Zr(2)-C(52)-C(53)	76.10(16)
C(73)-Zr(2)-C(52)-C(53)	-178.31(15)
C(82)-Zr(2)-C(52)-C(53)	-159.51(16)
C(54)-Zr(2)-C(52)-C(53)	35.48(14)
C(74)-Zr(2)-C(52)-C(53)	-145.86(15)
Cl(21)-Zr(2)-C(52)-C(51)	175.29(13)
Cl(22)-Zr(2)-C(52)-C(51)	-84.34(15)
C(71)-Zr(2)-C(52)-C(51)	51.03(14)
C(72)-Zr(2)-C(52)-C(51)	35.58(17)
C(62)-Zr(2)-C(52)-C(51)	-40.04(13)
C(73)-Zr(2)-C(52)-C(51)	65.6(2)
C(82)-Zr(2)-C(52)-C(51)	84.35(14)
C(53)-Zr(2)-C(52)-C(51)	-116.1(2)
C(54)-Zr(2)-C(52)-C(51)	-80.66(15)

C (74) -Zr (2) -C (52) -C (51)	98.01 (15)
Cl (21) -Zr (2) -C (52) -C (69)	51.05 (19)
Cl (22) -Zr (2) -C (52) -C (69)	151.41 (16)
C (51) -Zr (2) -C (52) -C (69)	-124.2 (3)
C (71) -Zr (2) -C (52) -C (69)	-73.2 (2)
C (72) -Zr (2) -C (52) -C (69)	-88.7 (2)
C (62) -Zr (2) -C (52) -C (69)	-164.3 (2)
C (73) -Zr (2) -C (52) -C (69)	-58.7 (3)
C (82) -Zr (2) -C (52) -C (69)	-39.9 (2)
C (53) -Zr (2) -C (52) -C (69)	119.6 (3)
C (54) -Zr (2) -C (52) -C (69)	155.1 (2)
C (74) -Zr (2) -C (52) -C (69)	-26.2 (2)
C (51) -C (52) -C (53) -C (54)	-2.2 (3)
C (69) -C (52) -C (53) -C (54)	176.0 (2)
Zr (2) -C (52) -C (53) -C (54)	-65.96 (19)
C (51) -C (52) -C (53) -Zr (2)	63.81 (18)
C (69) -C (52) -C (53) -Zr (2)	-118.0 (2)
Cl (21) -Zr (2) -C (53) -C (52)	108.02 (15)
Cl (22) -Zr (2) -C (53) -C (52)	-156.87 (14)
C (51) -Zr (2) -C (53) -C (52)	-37.63 (15)
C (71) -Zr (2) -C (53) -C (52)	-14.83 (18)
C (72) -Zr (2) -C (53) -C (52)	-46.0 (2)
C (62) -Zr (2) -C (53) -C (52)	-79.95 (16)
C (82) -Zr (2) -C (53) -C (52)	24.15 (18)
C (54) -Zr (2) -C (53) -C (52)	-117.3 (2)
C (74) -Zr (2) -C (53) -C (52)	55.5 (2)
Cl (21) -Zr (2) -C (53) -C (54)	-134.70 (15)
Cl (22) -Zr (2) -C (53) -C (54)	-39.59 (15)
C (51) -Zr (2) -C (53) -C (54)	79.64 (16)
C (71) -Zr (2) -C (53) -C (54)	102.45 (16)
C (72) -Zr (2) -C (53) -C (54)	71.3 (2)
C (52) -Zr (2) -C (53) -C (54)	117.3 (2)
C (62) -Zr (2) -C (53) -C (54)	37.32 (14)
C (82) -Zr (2) -C (53) -C (54)	141.42 (14)
C (74) -Zr (2) -C (53) -C (54)	172.77 (14)
C (52) -C (53) -C (54) -C (55)	-176.7 (3)
Zr (2) -C (53) -C (54) -C (55)	120.0 (3)
C (52) -C (53) -C (54) -C (62)	1.1 (3)
Zr (2) -C (53) -C (54) -C (62)	-62.26 (17)
C (52) -C (53) -C (54) -Zr (2)	63.37 (18)
Cl (21) -Zr (2) -C (54) -C (53)	45.07 (15)
Cl (22) -Zr (2) -C (54) -C (53)	141.60 (15)
C (51) -Zr (2) -C (54) -C (53)	-77.49 (16)
C (71) -Zr (2) -C (54) -C (53)	-96.78 (16)
C (72) -Zr (2) -C (54) -C (53)	-137.03 (15)
C (52) -Zr (2) -C (54) -C (53)	-35.72 (14)
C (62) -Zr (2) -C (54) -C (53)	-115.4 (2)
C (73) -Zr (2) -C (54) -C (53)	-170.28 (16)
C (82) -Zr (2) -C (54) -C (53)	-60.7 (2)
Cl (21) -Zr (2) -C (54) -C (55)	-83.9 (2)
Cl (22) -Zr (2) -C (54) -C (55)	12.60 (19)
C (51) -Zr (2) -C (54) -C (55)	153.5 (2)
C (71) -Zr (2) -C (54) -C (55)	134.2 (2)
C (72) -Zr (2) -C (54) -C (55)	94.0 (2)
C (52) -Zr (2) -C (54) -C (55)	-164.7 (2)
C (62) -Zr (2) -C (54) -C (55)	115.6 (3)
C (73) -Zr (2) -C (54) -C (55)	60.7 (3)
C (82) -Zr (2) -C (54) -C (55)	170.28 (18)
C (53) -Zr (2) -C (54) -C (55)	-129.0 (3)
Cl (21) -Zr (2) -C (54) -C (62)	160.48 (14)
Cl (22) -Zr (2) -C (54) -C (62)	-102.99 (14)
C (51) -Zr (2) -C (54) -C (62)	37.92 (15)
C (71) -Zr (2) -C (54) -C (62)	18.64 (18)
C (72) -Zr (2) -C (54) -C (62)	-21.62 (19)
C (52) -Zr (2) -C (54) -C (62)	79.69 (16)
C (73) -Zr (2) -C (54) -C (62)	-54.9 (2)
C (82) -Zr (2) -C (54) -C (62)	54.7 (2)

C (53) -Zr (2) -C (54) -C (62)	115.4 (2)
C (53) -C (54) -C (55) -C (56)	178.0 (3)
C (62) -C (54) -C (55) -C (56)	0.5 (4)
Zr (2) -C (54) -C (55) -C (56)	-85.1 (3)
C (53) -C (54) -C (55) -C (63)	0.1 (4)
C (62) -C (54) -C (55) -C (63)	-177.4 (2)
Zr (2) -C (54) -C (55) -C (63)	96.9 (3)
C (54) -C (55) -C (56) -C (60)	-1.9 (4)
C (63) -C (55) -C (56) -C (60)	176.0 (2)
C (54) -C (55) -C (56) -C (57)	176.6 (3)
C (63) -C (55) -C (56) -C (57)	-5.5 (4)
C (55) -C (56) -C (57) -C (58)	-160.9 (3)
C (60) -C (56) -C (57) -C (58)	17.7 (3)
C (56) -C (57) -C (58) -C (59)	-31.5 (3)
C (57) -C (58) -C (59) -C (60)	33.7 (3)
C (55) -C (56) -C (60) -C (61)	2.2 (4)
C (57) -C (56) -C (60) -C (61)	-176.6 (2)
C (55) -C (56) -C (60) -C (59)	-178.0 (2)
C (57) -C (56) -C (60) -C (59)	3.3 (3)
C (58) -C (59) -C (60) -C (61)	156.7 (3)
C (58) -C (59) -C (60) -C (56)	-23.1 (3)
C (56) -C (60) -C (61) -C (62)	-0.9 (4)
C (59) -C (60) -C (61) -C (62)	179.3 (3)
C (60) -C (61) -C (62) -C (54)	-0.4 (4)
C (60) -C (61) -C (62) -C (51)	-177.6 (3)
C (60) -C (61) -C (62) -Zr (2)	91.7 (3)
C (53) -C (54) -C (62) -C (61)	-177.5 (2)
C (55) -C (54) -C (62) -C (61)	0.6 (4)
Zr (2) -C (54) -C (62) -C (61)	118.1 (2)
C (53) -C (54) -C (62) -C (51)	0.3 (3)
C (55) -C (54) -C (62) -C (51)	178.4 (2)
Zr (2) -C (54) -C (62) -C (51)	-64.12 (17)
C (53) -C (54) -C (62) -Zr (2)	64.46 (18)
C (55) -C (54) -C (62) -Zr (2)	-117.5 (2)
C (52) -C (51) -C (62) -C (61)	175.8 (3)
Si (2) -C (51) -C (62) -C (61)	-23.4 (4)
Zr (2) -C (51) -C (62) -C (61)	-113.8 (3)
C (52) -C (51) -C (62) -C (54)	-1.6 (3)
Si (2) -C (51) -C (62) -C (54)	159.17 (19)
Zr (2) -C (51) -C (62) -C (54)	68.78 (18)
C (52) -C (51) -C (62) -Zr (2)	-70.37 (17)
Si (2) -C (51) -C (62) -Zr (2)	90.39 (19)
Cl (21) -Zr (2) -C (62) -C (61)	-141.88 (16)
Cl (22) -Zr (2) -C (62) -C (61)	-41.89 (19)
C (51) -Zr (2) -C (62) -C (61)	128.5 (3)
C (71) -Zr (2) -C (62) -C (61)	79.69 (19)
C (72) -Zr (2) -C (62) -C (61)	46.6 (2)
C (52) -Zr (2) -C (62) -C (61)	168.2 (2)
C (73) -Zr (2) -C (62) -C (61)	35.0 (2)
C (82) -Zr (2) -C (62) -C (61)	98.5 (2)
C (53) -Zr (2) -C (62) -C (61)	-152.2 (2)
C (54) -Zr (2) -C (62) -C (61)	-116.1 (3)
C (74) -Zr (2) -C (62) -C (61)	73.2 (2)
Cl (21) -Zr (2) -C (62) -C (54)	-25.75 (18)
Cl (22) -Zr (2) -C (62) -C (54)	74.24 (14)
C (51) -Zr (2) -C (62) -C (54)	-115.4 (2)
C (71) -Zr (2) -C (62) -C (54)	-164.18 (15)
C (72) -Zr (2) -C (62) -C (54)	162.76 (15)
C (52) -Zr (2) -C (62) -C (54)	-75.67 (15)
C (73) -Zr (2) -C (62) -C (54)	151.12 (14)
C (82) -Zr (2) -C (62) -C (54)	-145.42 (14)
C (53) -Zr (2) -C (62) -C (54)	-36.10 (14)
C (74) -Zr (2) -C (62) -C (54)	-170.71 (14)
Cl (21) -Zr (2) -C (62) -C (51)	89.60 (14)
Cl (22) -Zr (2) -C (62) -C (51)	-170.41 (14)
C (71) -Zr (2) -C (62) -C (51)	-48.83 (15)
C (72) -Zr (2) -C (62) -C (51)	-81.89 (15)

C (52) -Zr (2) -C (62) -C (51)	39.68 (14)
C (73) -Zr (2) -C (62) -C (51)	-93.53 (16)
C (82) -Zr (2) -C (62) -C (51)	-30.06 (17)
C (53) -Zr (2) -C (62) -C (51)	79.25 (16)
C (54) -Zr (2) -C (62) -C (51)	115.4 (2)
C (74) -Zr (2) -C (62) -C (51)	-55.4 (2)
C (56) -C (55) -C (63) -C (68)	-47.3 (4)
C (54) -C (55) -C (63) -C (68)	130.5 (3)
C (56) -C (55) -C (63) -C (64)	134.3 (3)
C (54) -C (55) -C (63) -C (64)	-47.8 (4)
C (68) -C (63) -C (64) -C (65)	-0.2 (4)
C (55) -C (63) -C (64) -C (65)	178.2 (3)
C (63) -C (64) -C (65) -C (66)	1.0 (4)
C (64) -C (65) -C (66) -C (67)	-1.1 (4)
C (65) -C (66) -C (67) -C (68)	0.4 (4)
C (66) -C (67) -C (68) -C (63)	0.3 (4)
C (64) -C (63) -C (68) -C (67)	-0.4 (4)
C (55) -C (63) -C (68) -C (67)	-178.8 (3)
C (70) -Si (2) -C (71) -C (72)	-42.2 (3)
C (90) -Si (2) -C (71) -C (72)	-165.3 (2)
C (51) -Si (2) -C (71) -C (72)	76.7 (2)
C (70) -Si (2) -C (71) -C (82)	164.47 (19)
C (90) -Si (2) -C (71) -C (82)	41.4 (2)
C (51) -Si (2) -C (71) -C (82)	-76.7 (2)
C (70) -Si (2) -C (71) -Zr (2)	-117.27 (12)
C (90) -Si (2) -C (71) -Zr (2)	119.62 (12)
C (51) -Si (2) -C (71) -Zr (2)	1.59 (11)
Cl (21) -Zr (2) -C (71) -C (72)	116.72 (14)
Cl (22) -Zr (2) -C (71) -C (72)	-11.32 (17)
C (51) -Zr (2) -C (71) -C (72)	-127.46 (17)
C (52) -Zr (2) -C (71) -C (72)	-155.03 (16)
C (62) -Zr (2) -C (71) -C (72)	-100.61 (16)
C (73) -Zr (2) -C (71) -C (72)	35.70 (14)
C (82) -Zr (2) -C (71) -C (72)	110.3 (2)
C (53) -Zr (2) -C (71) -C (72)	-147.29 (15)
C (54) -Zr (2) -C (71) -C (72)	-110.52 (16)
C (74) -Zr (2) -C (71) -C (72)	74.81 (16)
Cl (21) -Zr (2) -C (71) -C (82)	6.45 (17)
Cl (22) -Zr (2) -C (71) -C (82)	-121.58 (13)
C (51) -Zr (2) -C (71) -C (82)	122.28 (16)
C (72) -Zr (2) -C (71) -C (82)	-110.3 (2)
C (52) -Zr (2) -C (71) -C (82)	94.70 (15)
C (62) -Zr (2) -C (71) -C (82)	149.12 (15)
C (73) -Zr (2) -C (71) -C (82)	-74.56 (15)
C (53) -Zr (2) -C (71) -C (82)	102.44 (15)
C (54) -Zr (2) -C (71) -C (82)	139.22 (14)
C (74) -Zr (2) -C (71) -C (82)	-35.45 (14)
Cl (21) -Zr (2) -C (71) -Si (2)	-117.13 (8)
Cl (22) -Zr (2) -C (71) -Si (2)	114.84 (9)
C (51) -Zr (2) -C (71) -Si (2)	-1.30 (9)
C (72) -Zr (2) -C (71) -Si (2)	126.2 (2)
C (52) -Zr (2) -C (71) -Si (2)	-28.88 (11)
C (62) -Zr (2) -C (71) -Si (2)	25.54 (11)
C (73) -Zr (2) -C (71) -Si (2)	161.86 (15)
C (82) -Zr (2) -C (71) -Si (2)	-123.58 (19)
C (53) -Zr (2) -C (71) -Si (2)	-21.14 (14)
C (54) -Zr (2) -C (71) -Si (2)	15.64 (14)
C (74) -Zr (2) -C (71) -Si (2)	-159.03 (14)
C (82) -C (71) -C (72) -C (73)	3.1 (3)
Si (2) -C (71) -C (72) -C (73)	-154.36 (19)
Zr (2) -C (71) -C (72) -C (73)	-67.52 (18)
C (82) -C (71) -C (72) -C (89)	-174.8 (2)
Si (2) -C (71) -C (72) -C (89)	27.8 (4)
Zr (2) -C (71) -C (72) -C (89)	114.6 (3)
C (82) -C (71) -C (72) -Zr (2)	70.57 (16)
Si (2) -C (71) -C (72) -Zr (2)	-86.84 (18)
Cl (21) -Zr (2) -C (72) -C (73)	26.40 (19)

Cl (22)-Zr (2)-C (72)-C (73)	-73.19 (14)
C (51)-Zr (2)-C (72)-C (73)	164.11 (16)
C (71)-Zr (2)-C (72)-C (73)	116.4 (2)
C (52)-Zr (2)-C (72)-C (73)	145.29 (15)
C (62)-Zr (2)-C (72)-C (73)	-162.31 (15)
C (82)-Zr (2)-C (72)-C (73)	76.61 (16)
C (53)-Zr (2)-C (72)-C (73)	170.94 (14)
C (54)-Zr (2)-C (72)-C (73)	-150.80 (14)
C (74)-Zr (2)-C (72)-C (73)	36.35 (14)
Cl (21)-Zr (2)-C (72)-C (71)	-90.04 (16)
Cl (22)-Zr (2)-C (72)-C (71)	170.37 (15)
C (51)-Zr (2)-C (72)-C (71)	47.67 (16)
C (52)-Zr (2)-C (72)-C (71)	28.85 (18)
C (62)-Zr (2)-C (72)-C (71)	81.26 (16)
C (73)-Zr (2)-C (72)-C (71)	-116.4 (2)
C (82)-Zr (2)-C (72)-C (71)	-39.83 (15)
C (53)-Zr (2)-C (72)-C (71)	54.5 (2)
C (54)-Zr (2)-C (72)-C (71)	92.76 (16)
C (74)-Zr (2)-C (72)-C (71)	-80.09 (16)
Cl (21)-Zr (2)-C (72)-C (89)	145.82 (17)
Cl (22)-Zr (2)-C (72)-C (89)	46.2 (2)
C (51)-Zr (2)-C (72)-C (89)	-76.5 (2)
C (71)-Zr (2)-C (72)-C (89)	-124.1 (3)
C (52)-Zr (2)-C (72)-C (89)	-95.3 (2)
C (62)-Zr (2)-C (72)-C (89)	-42.9 (2)
C (73)-Zr (2)-C (72)-C (89)	119.4 (3)
C (82)-Zr (2)-C (72)-C (89)	-164.0 (3)
C (53)-Zr (2)-C (72)-C (89)	-69.6 (3)
C (54)-Zr (2)-C (72)-C (89)	-31.4 (2)
C (74)-Zr (2)-C (72)-C (89)	155.8 (2)
C (71)-C (72)-C (73)-C (74)	-3.3 (3)
C (89)-C (72)-C (73)-C (74)	174.7 (2)
Zr (2)-C (72)-C (73)-C (74)	-68.70 (17)
C (71)-C (72)-C (73)-Zr (2)	65.41 (17)
C (89)-C (72)-C (73)-Zr (2)	-116.6 (2)
Cl (21)-Zr (2)-C (73)-C (72)	-160.34 (14)
Cl (22)-Zr (2)-C (73)-C (72)	103.60 (15)
C (51)-Zr (2)-C (73)-C (72)	-18.71 (18)
C (71)-Zr (2)-C (73)-C (72)	-37.13 (15)
C (52)-Zr (2)-C (73)-C (72)	-55.0 (2)
C (62)-Zr (2)-C (73)-C (72)	22.08 (19)
C (82)-Zr (2)-C (73)-C (72)	-78.68 (16)
C (54)-Zr (2)-C (73)-C (72)	55.3 (2)
C (74)-Zr (2)-C (73)-C (72)	-115.6 (2)
Cl (21)-Zr (2)-C (73)-C (74)	-44.77 (15)
Cl (22)-Zr (2)-C (73)-C (74)	-140.83 (15)
C (51)-Zr (2)-C (73)-C (74)	96.87 (16)
C (71)-Zr (2)-C (73)-C (74)	78.45 (16)
C (72)-Zr (2)-C (73)-C (74)	115.6 (2)
C (52)-Zr (2)-C (73)-C (74)	60.6 (2)
C (62)-Zr (2)-C (73)-C (74)	137.66 (14)
C (82)-Zr (2)-C (73)-C (74)	36.89 (14)
C (54)-Zr (2)-C (73)-C (74)	170.86 (16)
C (72)-C (73)-C (74)-C (75)	179.9 (2)
Zr (2)-C (73)-C (74)-C (75)	114.7 (3)
C (72)-C (73)-C (74)-C (82)	2.1 (3)
Zr (2)-C (73)-C (74)-C (82)	-63.10 (16)
C (72)-C (73)-C (74)-Zr (2)	65.17 (17)
Cl (21)-Zr (2)-C (74)-C (73)	135.66 (15)
Cl (22)-Zr (2)-C (74)-C (73)	40.01 (15)
C (51)-Zr (2)-C (74)-C (73)	-102.49 (16)
C (71)-Zr (2)-C (74)-C (73)	-78.50 (16)
C (72)-Zr (2)-C (74)-C (73)	-36.88 (15)
C (52)-Zr (2)-C (74)-C (73)	-141.73 (15)
C (62)-Zr (2)-C (74)-C (73)	-70.5 (2)
C (82)-Zr (2)-C (74)-C (73)	-115.4 (2)
C (53)-Zr (2)-C (74)-C (73)	-172.18 (15)

Cl (21)-Zr (2)-C (74)-C (75)	8.14 (19)
Cl (22)-Zr (2)-C (74)-C (75)	-87.5 (2)
C (51)-Zr (2)-C (74)-C (75)	129.99 (19)
C (71)-Zr (2)-C (74)-C (75)	154.0 (2)
C (72)-Zr (2)-C (74)-C (75)	-164.4 (2)
C (52)-Zr (2)-C (74)-C (75)	90.7 (2)
C (62)-Zr (2)-C (74)-C (75)	161.96 (18)
C (73)-Zr (2)-C (74)-C (75)	-127.5 (3)
C (82)-Zr (2)-C (74)-C (75)	117.1 (3)
C (53)-Zr (2)-C (74)-C (75)	60.3 (3)
Cl (21)-Zr (2)-C (74)-C (82)	-108.93 (14)
Cl (22)-Zr (2)-C (74)-C (82)	155.43 (13)
C (51)-Zr (2)-C (74)-C (82)	12.93 (17)
C (71)-Zr (2)-C (74)-C (82)	36.91 (14)
C (72)-Zr (2)-C (74)-C (82)	78.53 (16)
C (52)-Zr (2)-C (74)-C (82)	-26.32 (17)
C (62)-Zr (2)-C (74)-C (82)	44.9 (2)
C (73)-Zr (2)-C (74)-C (82)	115.4 (2)
C (53)-Zr (2)-C (74)-C (82)	-56.8 (2)
C (73)-C (74)-C (75)-C (76)	-178.1 (2)
C (82)-C (74)-C (75)-C (76)	-0.6 (4)
Zr (2)-C (74)-C (75)-C (76)	-86.9 (2)
C (73)-C (74)-C (75)-C (83)	-2.5 (4)
C (82)-C (74)-C (75)-C (83)	175.0 (2)
Zr (2)-C (74)-C (75)-C (83)	88.7 (3)
C (74)-C (75)-C (76)-C (80)	-1.7 (4)
C (83)-C (75)-C (76)-C (80)	-177.2 (2)
C (74)-C (75)-C (76)-C (77)	179.9 (2)
C (83)-C (75)-C (76)-C (77)	4.4 (4)
C (75)-C (76)-C (77)-C (78)	-160.8 (3)
C (80)-C (76)-C (77)-C (78)	20.6 (3)
C (76)-C (77)-C (78)-C (79)	-33.6 (3)
C (77)-C (78)-C (79)-C (80)	33.7 (3)
C (75)-C (76)-C (80)-C (81)	2.4 (4)
C (77)-C (76)-C (80)-C (81)	-178.9 (2)
C (75)-C (76)-C (80)-C (79)	-178.3 (2)
C (77)-C (76)-C (80)-C (79)	0.4 (3)
C (78)-C (79)-C (80)-C (81)	157.8 (3)
C (78)-C (79)-C (80)-C (76)	-21.4 (3)
C (76)-C (80)-C (81)-C (82)	-0.6 (4)
C (79)-C (80)-C (81)-C (82)	-179.7 (2)
C (80)-C (81)-C (82)-C (74)	-1.7 (4)
C (80)-C (81)-C (82)-C (71)	179.0 (2)
C (80)-C (81)-C (82)-Zr (2)	89.0 (3)
C (73)-C (74)-C (82)-C (81)	-179.6 (2)
C (75)-C (74)-C (82)-C (81)	2.3 (4)
Zr (2)-C (74)-C (82)-C (81)	117.5 (2)
C (73)-C (74)-C (82)-C (71)	-0.1 (3)
C (75)-C (74)-C (82)-C (71)	-178.2 (2)
Zr (2)-C (74)-C (82)-C (71)	-63.02 (16)
C (73)-C (74)-C (82)-Zr (2)	62.88 (16)
C (75)-C (74)-C (82)-Zr (2)	-115.2 (2)
C (72)-C (71)-C (82)-C (81)	177.6 (3)
Si (2)-C (71)-C (82)-C (81)	-24.2 (4)
Zr (2)-C (71)-C (82)-C (81)	-113.6 (3)
C (72)-C (71)-C (82)-C (74)	-1.8 (3)
Si (2)-C (71)-C (82)-C (74)	156.36 (18)
Zr (2)-C (71)-C (82)-C (74)	67.01 (17)
C (72)-C (71)-C (82)-Zr (2)	-68.76 (16)
Si (2)-C (71)-C (82)-Zr (2)	89.35 (17)
Cl (21)-Zr (2)-C (82)-C (81)	-46.9 (2)
Cl (22)-Zr (2)-C (82)-C (81)	-148.85 (17)
C (51)-Zr (2)-C (82)-C (81)	75.8 (2)
C (71)-Zr (2)-C (82)-C (81)	127.7 (3)
C (72)-Zr (2)-C (82)-C (81)	167.7 (2)
C (52)-Zr (2)-C (82)-C (81)	42.3 (2)
C (62)-Zr (2)-C (82)-C (81)	92.0 (2)

C (73) -Zr (2) -C (82) -C (81)	-151.9 (2)
C (53) -Zr (2) -C (82) -C (81)	29.8 (2)
C (54) -Zr (2) -C (82) -C (81)	62.1 (3)
C (74) -Zr (2) -C (82) -C (81)	-115.4 (3)
Cl (21) -Zr (2) -C (82) -C (74)	68.51 (14)
Cl (22) -Zr (2) -C (82) -C (74)	-33.41 (17)
C (51) -Zr (2) -C (82) -C (74)	-168.80 (15)
C (71) -Zr (2) -C (82) -C (74)	-116.8 (2)
C (72) -Zr (2) -C (82) -C (74)	-76.91 (16)
C (52) -Zr (2) -C (82) -C (74)	157.69 (15)
C (62) -Zr (2) -C (82) -C (74)	-152.54 (14)
C (73) -Zr (2) -C (82) -C (74)	-36.48 (14)
C (53) -Zr (2) -C (82) -C (74)	145.25 (14)
C (54) -Zr (2) -C (82) -C (74)	177.49 (14)
Cl (21) -Zr (2) -C (82) -C (71)	-174.67 (14)
Cl (22) -Zr (2) -C (82) -C (71)	83.41 (16)
C (51) -Zr (2) -C (82) -C (71)	-51.98 (15)
C (72) -Zr (2) -C (82) -C (71)	39.91 (15)
C (52) -Zr (2) -C (82) -C (71)	-85.49 (15)
C (62) -Zr (2) -C (82) -C (71)	-35.72 (17)
C (73) -Zr (2) -C (82) -C (71)	80.34 (16)
C (53) -Zr (2) -C (82) -C (71)	-97.92 (16)
C (54) -Zr (2) -C (82) -C (71)	-65.7 (2)
C (74) -Zr (2) -C (82) -C (71)	116.8 (2)
C (76) -C (75) -C (83) -C (84)	-124.6 (3)
C (74) -C (75) -C (83) -C (84)	60.1 (4)
C (76) -C (75) -C (83) -C (88)	57.0 (4)
C (74) -C (75) -C (83) -C (88)	-118.3 (3)
C (88) -C (83) -C (84) -C (85)	-1.4 (5)
C (75) -C (83) -C (84) -C (85)	-179.9 (3)
C (83) -C (84) -C (85) -C (86)	-0.7 (6)
C (84) -C (85) -C (86) -C (87)	2.9 (6)
C (85) -C (86) -C (87) -C (88)	-2.9 (5)
C (86) -C (87) -C (88) -C (83)	0.7 (4)
C (84) -C (83) -C (88) -C (87)	1.4 (4)
C (75) -C (83) -C (88) -C (87)	179.9 (3)

Table S8. Atomic coordinates ($\text{\AA} \times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **16**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U (eq)
Zr (1)	5072 (1)	8705 (1)	8298 (1)	15 (1)
Cl (1)	6298 (1)	7682 (1)	8187 (1)	27 (1)
Si (1)	3991 (1)	8053 (1)	9289 (1)	20 (1)
N (1)	4855 (2)	9837 (3)	7587 (1)	22 (1)
C (1)	5043 (2)	11094 (4)	7243 (2)	26 (1)
C (2)	4500 (3)	12337 (5)	7294 (2)	47 (1)
C (3)	5833 (3)	11592 (6)	7401 (2)	43 (1)
C (4)	4992 (3)	10558 (6)	6651 (2)	50 (2)
C (11)	4096 (2)	7117 (4)	8623 (2)	19 (1)
C (12)	4682 (2)	6108 (4)	8515 (2)	21 (1)
C (13)	4722 (2)	6011 (4)	7953 (2)	20 (1)
C (14)	4152 (2)	6873 (4)	7677 (2)	18 (1)

C (15)	3930 (2)	7052 (4)	7111 (2)	20 (1)
C (16)	3330 (2)	7966 (4)	6976 (2)	21 (1)
C (17)	2976 (2)	8396 (5)	6414 (2)	27 (1)
C (18)	2540 (3)	9809 (5)	6531 (2)	35 (1)
C (19)	2328 (2)	9607 (5)	7112 (2)	30 (1)
C (20)	2949 (2)	8679 (4)	7385 (2)	22 (1)
C (21)	3147 (2)	8500 (4)	7929 (2)	20 (1)
C (22)	3767 (2)	7575 (4)	8094 (2)	18 (1)
C (23)	4314 (2)	6261 (4)	6695 (2)	20 (1)
C (24)	5091 (2)	6276 (5)	6706 (2)	31 (1)
C (25)	5438 (3)	5485 (6)	6326 (2)	39 (1)
C (26)	5032 (3)	4679 (6)	5931 (2)	44 (1)
C (27)	4279 (3)	4643 (5)	5912 (2)	35 (1)
C (28)	3920 (2)	5424 (4)	6294 (2)	27 (1)
C (29)	5175 (2)	5219 (4)	8910 (2)	26 (1)
C (30)	3044 (2)	8804 (5)	9339 (2)	29 (1)
C (31)	4725 (2)	9475 (4)	9231 (2)	19 (1)
C (32)	4654 (2)	10756 (4)	8889 (2)	19 (1)
C (33)	5358 (2)	11194 (4)	8759 (2)	18 (1)
C (34)	5901 (2)	10280 (4)	9037 (2)	18 (1)
C (35)	6699 (2)	10275 (4)	9054 (2)	21 (1)
C (36)	7061 (2)	9192 (4)	9351 (2)	22 (1)
C (37)	7893 (2)	8898 (5)	9437 (2)	33 (1)
C (38)	7966 (2)	7899 (6)	9940 (2)	42 (1)
C (39)	7236 (2)	7082 (5)	9932 (2)	30 (1)
C (40)	6684 (2)	8121 (4)	9647 (2)	21 (1)
C (41)	5931 (2)	8128 (4)	9650 (2)	20 (1)
C (42)	5511 (2)	9195 (4)	9327 (2)	18 (1)
C (43)	7067 (2)	11379 (5)	8731 (2)	23 (1)
C (44)	6966 (2)	12879 (5)	8803 (2)	34 (1)
C (45)	7283 (3)	13889 (6)	8475 (2)	47 (1)
C (46)	7711 (3)	13401 (6)	8072 (2)	51 (2)
C (47)	7817 (3)	11924 (7)	8001 (2)	47 (1)
C (48)	7504 (2)	10920 (5)	8327 (2)	34 (1)
C (49)	3955 (2)	11596 (4)	8717 (2)	26 (1)
C (50)	4175 (2)	6804 (5)	9888 (2)	28 (1)
C (10)	988 (4)	6193 (9)	456 (3)	97 (3)
Cl (2)	1554 (1)	6316 (3)	-54 (1)	130 (1)
Cl (3)	95 (1)	6872 (3)	275 (1)	113 (1)

Table S9. Bond lengths [Å] for **16**.

Zr (1) -N (1)	2.036 (3)
Zr (1) -Cl (1)	2.4503 (10)
Zr (1) -C (11)	2.478 (4)
Zr (1) -C (32)	2.529 (4)
Zr (1) -C (31)	2.538 (4)
Zr (1) -C (12)	2.542 (4)
Zr (1) -C (33)	2.568 (4)
Zr (1) -C (22)	2.586 (4)
Zr (1) -C (42)	2.619 (4)
Zr (1) -C (13)	2.656 (4)
Zr (1) -C (34)	2.665 (4)
Zr (1) -C (14)	2.724 (4)
Si (1) -C (30)	1.865 (4)
Si (1) -C (50)	1.867 (4)
Si (1) -C (31)	1.873 (4)
Si (1) -C (11)	1.874 (4)
N (1) -C (1)	1.484 (5)
N (1) -H (1)	0.8800

C (1) -C (3)	1.517 (6)
C (1) -C (2)	1.515 (6)
C (1) -C (4)	1.531 (6)
C (2) -H (2A)	0.9800
C (2) -H (2B)	0.9800
C (2) -H (2C)	0.9800
C (3) -H (3A)	0.9800
C (3) -H (3B)	0.9800
C (3) -H (3C)	0.9800
C (4) -H (4A)	0.9800
C (4) -H (4B)	0.9800
C (4) -H (4C)	0.9800
C (11) -C (22)	1.440 (6)
C (11) -C (12)	1.450 (5)
C (12) -C (13)	1.394 (6)
C (12) -C (29)	1.496 (5)
C (13) -C (14)	1.419 (5)
C (13) -H (13)	0.9500
C (14) -C (15)	1.421 (6)
C (14) -C (22)	1.445 (5)
C (15) -C (16)	1.385 (5)
C (15) -C (23)	1.480 (5)
C (16) -C (20)	1.431 (5)
C (16) -C (17)	1.519 (6)
C (17) -C (18)	1.553 (6)
C (17) -H (17A)	0.9900
C (17) -H (17B)	0.9900
C (18) -C (19)	1.528 (6)
C (18) -H (18A)	0.9900
C (18) -H (18B)	0.9900
C (19) -C (20)	1.513 (5)
C (19) -H (19A)	0.9900
C (19) -H (19B)	0.9900
C (20) -C (21)	1.360 (6)
C (21) -C (22)	1.433 (5)
C (21) -H (21)	0.9500
C (23) -C (28)	1.389 (6)
C (23) -C (24)	1.406 (5)
C (24) -C (25)	1.382 (6)
C (24) -H (24)	0.9500
C (25) -C (26)	1.374 (7)
C (25) -H (25)	0.9500
C (26) -C (27)	1.363 (6)
C (26) -H (26)	0.9500
C (27) -C (28)	1.391 (6)
C (27) -H (27)	0.9500
C (28) -H (28)	0.9500
C (29) -H (29A)	0.9800
C (29) -H (29B)	0.9800
C (29) -H (29C)	0.9800
C (30) -H (30A)	0.9800
C (30) -H (30B)	0.9800
C (30) -H (30C)	0.9800
C (31) -C (32)	1.439 (5)
C (31) -C (42)	1.445 (5)
C (32) -C (33)	1.403 (5)
C (32) -C (49)	1.508 (5)
C (33) -C (34)	1.414 (5)
C (33) -H (33)	0.9500
C (34) -C (42)	1.444 (5)
C (34) -C (35)	1.445 (5)
C (35) -C (36)	1.359 (6)
C (35) -C (43)	1.480 (5)
C (36) -C (40)	1.431 (6)
C (36) -C (37)	1.528 (5)
C (37) -C (38)	1.533 (6)
C (37) -H (37A)	0.9900

C (37) -H (37B)	0.9900
C (38) -C (39)	1.519 (6)
C (38) -H (38A)	0.9900
C (38) -H (38B)	0.9900
C (39) -C (40)	1.502 (6)
C (39) -H (39A)	0.9900
C (39) -H (39B)	0.9900
C (40) -C (41)	1.367 (5)
C (41) -C (42)	1.429 (6)
C (41) -H (41)	0.9500
C (43) -C (44)	1.394 (6)
C (43) -C (48)	1.395 (6)
C (44) -C (45)	1.387 (6)
C (44) -H (44)	0.9500
C (45) -C (46)	1.389 (8)
C (45) -H (45)	0.9500
C (46) -C (47)	1.374 (8)
C (46) -H (46)	0.9500
C (47) -C (48)	1.375 (7)
C (47) -H (47)	0.9500
C (48) -H (48)	0.9500
C (49) -H (49A)	0.9800
C (49) -H (49B)	0.9800
C (49) -H (49C)	0.9800
C (50) -H (50A)	0.9800
C (50) -H (50B)	0.9800
C (50) -H (50C)	0.9800
C (10) -Cl (2)	1.702 (8)
C (10) -Cl (3)	1.751 (8)
C (10) -H (10A)	0.9900
C (10) -H (10B)	0.9900

Table S10. Bond angles [deg] for **16**.

N (1) -Zr (1) -Cl (1)	101.53 (10)
N (1) -Zr (1) -C (11)	119.25 (13)
Cl (1) -Zr (1) -C (11)	119.80 (9)
N (1) -Zr (1) -C (32)	94.31 (13)
Cl (1) -Zr (1) -C (32)	132.12 (9)
C (11) -Zr (1) -C (32)	89.07 (13)
N (1) -Zr (1) -C (31)	126.36 (13)
Cl (1) -Zr (1) -C (31)	120.82 (9)
C (11) -Zr (1) -C (31)	67.84 (13)
C (32) -Zr (1) -C (31)	32.99 (12)
N (1) -Zr (1) -C (12)	128.16 (13)
Cl (1) -Zr (1) -C (12)	86.67 (9)
C (11) -Zr (1) -C (12)	33.54 (12)
C (32) -Zr (1) -C (12)	117.60 (13)
C (31) -Zr (1) -C (12)	88.26 (13)
N (1) -Zr (1) -C (33)	86.89 (13)
Cl (1) -Zr (1) -C (33)	103.82 (9)
C (11) -Zr (1) -C (33)	119.60 (12)
C (32) -Zr (1) -C (33)	31.94 (12)
C (31) -Zr (1) -C (33)	54.03 (12)
C (12) -Zr (1) -C (33)	141.14 (13)
N (1) -Zr (1) -C (22)	86.45 (13)
Cl (1) -Zr (1) -C (22)	130.52 (9)
C (11) -Zr (1) -C (22)	32.97 (13)
C (32) -Zr (1) -C (22)	95.00 (12)
C (31) -Zr (1) -C (22)	89.09 (12)
C (12) -Zr (1) -C (22)	53.26 (12)

C(33)-Zr(1)-C(22)	125.47(12)
N(1)-Zr(1)-C(42)	139.42(13)
Cl(1)-Zr(1)-C(42)	88.73(9)
C(11)-Zr(1)-C(42)	87.02(12)
C(32)-Zr(1)-C(42)	52.98(12)
C(31)-Zr(1)-C(42)	32.49(12)
C(12)-Zr(1)-C(42)	91.20(13)
C(33)-Zr(1)-C(42)	52.55(12)
C(22)-Zr(1)-C(42)	116.31(12)
N(1)-Zr(1)-C(13)	100.03(13)
Cl(1)-Zr(1)-C(13)	78.65(9)
C(11)-Zr(1)-C(13)	53.61(12)
C(32)-Zr(1)-C(13)	142.39(13)
C(31)-Zr(1)-C(13)	118.21(12)
C(12)-Zr(1)-C(13)	31.01(13)
C(33)-Zr(1)-C(13)	172.11(12)
C(22)-Zr(1)-C(13)	51.94(12)
C(42)-Zr(1)-C(13)	120.53(12)
N(1)-Zr(1)-C(34)	111.24(13)
Cl(1)-Zr(1)-C(34)	79.80(8)
C(11)-Zr(1)-C(34)	117.92(12)
C(32)-Zr(1)-C(34)	52.39(12)
C(31)-Zr(1)-C(34)	53.57(11)
C(12)-Zr(1)-C(34)	120.58(12)
C(33)-Zr(1)-C(34)	31.29(12)
C(22)-Zr(1)-C(34)	142.45(12)
C(42)-Zr(1)-C(34)	31.70(11)
C(13)-Zr(1)-C(34)	144.89(12)
N(1)-Zr(1)-C(14)	76.83(12)
Cl(1)-Zr(1)-C(14)	102.54(8)
C(11)-Zr(1)-C(14)	53.47(12)
C(32)-Zr(1)-C(14)	125.10(12)
C(31)-Zr(1)-C(14)	119.06(12)
C(12)-Zr(1)-C(14)	51.59(12)
C(33)-Zr(1)-C(14)	151.27(12)
C(22)-Zr(1)-C(14)	31.45(11)
C(42)-Zr(1)-C(14)	139.47(12)
C(13)-Zr(1)-C(14)	30.55(11)
C(34)-Zr(1)-C(14)	171.16(12)
C(30)-Si(1)-C(50)	105.5(2)
C(30)-Si(1)-C(31)	114.65(19)
C(50)-Si(1)-C(31)	114.08(19)
C(30)-Si(1)-C(11)	113.40(19)
C(50)-Si(1)-C(11)	112.76(19)
C(31)-Si(1)-C(11)	96.68(17)
C(1)-N(1)-Zr(1)	147.7(3)
C(1)-N(1)-H(1)	106.1
Zr(1)-N(1)-H(1)	106.1
N(1)-C(1)-C(3)	110.4(4)
N(1)-C(1)-C(2)	110.1(4)
C(3)-C(1)-C(2)	111.2(4)
N(1)-C(1)-C(4)	107.4(3)
C(3)-C(1)-C(4)	108.0(4)
C(2)-C(1)-C(4)	109.7(4)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(1)-C(4)-H(4A)	109.5

C (1) -C (4) -H (4B)	109.5
H (4A) -C (4) -H (4B)	109.5
C (1) -C (4) -H (4C)	109.5
H (4A) -C (4) -H (4C)	109.5
H (4B) -C (4) -H (4C)	109.5
C (22) -C (11) -C (12)	105.4 (3)
C (22) -C (11) -Si (1)	126.2 (3)
C (12) -C (11) -Si (1)	126.0 (3)
C (22) -C (11) -Zr (1)	77.6 (2)
C (12) -C (11) -Zr (1)	75.7 (2)
Si (1) -C (11) -Zr (1)	98.73 (16)
C (13) -C (12) -C (11)	109.4 (3)
C (13) -C (12) -C (29)	121.7 (4)
C (11) -C (12) -C (29)	128.9 (4)
C (13) -C (12) -Zr (1)	79.0 (2)
C (11) -C (12) -Zr (1)	70.8 (2)
C (29) -C (12) -Zr (1)	118.8 (3)
C (12) -C (13) -C (14)	109.5 (3)
C (12) -C (13) -Zr (1)	70.0 (2)
C (14) -C (13) -Zr (1)	77.3 (2)
C (12) -C (13) -H (13)	125.2
C (14) -C (13) -H (13)	125.2
Zr (1) -C (13) -H (13)	119.1
C (13) -C (14) -C (15)	131.1 (4)
C (13) -C (14) -C (22)	106.6 (3)
C (15) -C (14) -C (22)	122.3 (3)
C (13) -C (14) -Zr (1)	72.1 (2)
C (15) -C (14) -Zr (1)	125.5 (3)
C (22) -C (14) -Zr (1)	69.0 (2)
C (16) -C (15) -C (14)	116.4 (4)
C (16) -C (15) -C (23)	122.7 (4)
C (14) -C (15) -C (23)	120.9 (3)
C (15) -C (16) -C (20)	121.8 (4)
C (15) -C (16) -C (17)	128.8 (4)
C (20) -C (16) -C (17)	109.4 (3)
C (16) -C (17) -C (18)	103.0 (3)
C (16) -C (17) -H (17A)	111.2
C (18) -C (17) -H (17A)	111.2
C (16) -C (17) -H (17B)	111.2
C (18) -C (17) -H (17B)	111.2
H (17A) -C (17) -H (17B)	109.1
C (19) -C (18) -C (17)	104.5 (3)
C (19) -C (18) -H (18A)	110.8
C (17) -C (18) -H (18A)	110.8
C (19) -C (18) -H (18B)	110.8
C (17) -C (18) -H (18B)	110.8
H (18A) -C (18) -H (18B)	108.9
C (20) -C (19) -C (18)	103.8 (3)
C (20) -C (19) -H (19A)	111.0
C (18) -C (19) -H (19A)	111.0
C (20) -C (19) -H (19B)	111.0
C (18) -C (19) -H (19B)	111.0
H (19A) -C (19) -H (19B)	109.0
C (21) -C (20) -C (16)	122.4 (4)
C (21) -C (20) -C (19)	128.2 (4)
C (16) -C (20) -C (19)	109.4 (4)
C (20) -C (21) -C (22)	118.4 (4)
C (20) -C (21) -H (21)	120.8
C (22) -C (21) -H (21)	120.8
C (21) -C (22) -C (11)	132.3 (4)
C (21) -C (22) -C (14)	118.6 (4)
C (11) -C (22) -C (14)	109.1 (3)
C (21) -C (22) -Zr (1)	120.0 (2)
C (11) -C (22) -Zr (1)	69.4 (2)
C (14) -C (22) -Zr (1)	79.5 (2)
C (28) -C (23) -C (24)	117.8 (4)
C (28) -C (23) -C (15)	120.9 (4)

C (24) -C (23) -C (15)	121.3 (4)
C (25) -C (24) -C (23)	120.2 (4)
C (25) -C (24) -H (24)	119.9
C (23) -C (24) -H (24)	119.9
C (26) -C (25) -C (24)	120.6 (4)
C (26) -C (25) -H (25)	119.7
C (24) -C (25) -H (25)	119.7
C (27) -C (26) -C (25)	120.3 (4)
C (27) -C (26) -H (26)	119.8
C (25) -C (26) -H (26)	119.8
C (26) -C (27) -C (28)	119.8 (4)
C (26) -C (27) -H (27)	120.1
C (28) -C (27) -H (27)	120.1
C (23) -C (28) -C (27)	121.2 (4)
C (23) -C (28) -H (28)	119.4
C (27) -C (28) -H (28)	119.4
C (12) -C (29) -H (29A)	109.5
C (12) -C (29) -H (29B)	109.5
H (29A) -C (29) -H (29B)	109.5
C (12) -C (29) -H (29C)	109.5
H (29A) -C (29) -H (29C)	109.5
H (29B) -C (29) -H (29C)	109.5
Si (1) -C (30) -H (30A)	109.5
Si (1) -C (30) -H (30B)	109.5
H (30A) -C (30) -H (30B)	109.5
Si (1) -C (30) -H (30C)	109.5
H (30A) -C (30) -H (30C)	109.5
H (30B) -C (30) -H (30C)	109.5
C (32) -C (31) -C (42)	105.6 (3)
C (32) -C (31) -Si (1)	125.6 (3)
C (42) -C (31) -Si (1)	124.2 (3)
C (32) -C (31) -Zr (1)	73.2 (2)
C (42) -C (31) -Zr (1)	76.8 (2)
Si (1) -C (31) -Zr (1)	96.72 (16)
C (33) -C (32) -C (31)	109.4 (3)
C (33) -C (32) -C (49)	123.5 (4)
C (31) -C (32) -C (49)	127.0 (3)
C (33) -C (32) -Zr (1)	75.5 (2)
C (31) -C (32) -Zr (1)	73.8 (2)
C (49) -C (32) -Zr (1)	120.3 (3)
C (32) -C (33) -C (34)	109.2 (3)
C (32) -C (33) -Zr (1)	72.5 (2)
C (34) -C (33) -Zr (1)	78.1 (2)
C (32) -C (33) -H (33)	125.4
C (34) -C (33) -H (33)	125.4
Zr (1) -C (33) -H (33)	115.9
C (33) -C (34) -C (42)	106.9 (3)
C (33) -C (34) -C (35)	131.7 (4)
C (42) -C (34) -C (35)	121.4 (4)
C (33) -C (34) -Zr (1)	70.6 (2)
C (42) -C (34) -Zr (1)	72.4 (2)
C (35) -C (34) -Zr (1)	121.1 (3)
C (36) -C (35) -C (34)	116.6 (4)
C (36) -C (35) -C (43)	124.3 (4)
C (34) -C (35) -C (43)	119.0 (4)
C (35) -C (36) -C (40)	122.8 (4)
C (35) -C (36) -C (37)	128.4 (4)
C (40) -C (36) -C (37)	108.9 (3)
C (36) -C (37) -C (38)	102.9 (3)
C (36) -C (37) -H (37A)	111.2
C (38) -C (37) -H (37A)	111.2
C (36) -C (37) -H (37B)	111.2
C (38) -C (37) -H (37B)	111.2
H (37A) -C (37) -H (37B)	109.1
C (39) -C (38) -C (37)	105.9 (4)
C (39) -C (38) -H (38A)	110.6
C (37) -C (38) -H (38A)	110.6

C (39) -C (38) -H (38B)	110.6
C (37) -C (38) -H (38B)	110.6
H (38A) -C (38) -H (38B)	108.7
C (40) -C (39) -C (38)	103.7 (3)
C (40) -C (39) -H (39A)	111.0
C (38) -C (39) -H (39A)	111.0
C (40) -C (39) -H (39B)	111.0
C (38) -C (39) -H (39B)	111.0
H (39A) -C (39) -H (39B)	109.0
C (41) -C (40) -C (36)	121.7 (4)
C (41) -C (40) -C (39)	128.5 (4)
C (36) -C (40) -C (39)	109.9 (3)
C (40) -C (41) -C (42)	118.7 (4)
C (40) -C (41) -H (41)	120.7
C (42) -C (41) -H (41)	120.7
C (41) -C (42) -C (34)	118.8 (3)
C (41) -C (42) -C (31)	132.5 (4)
C (34) -C (42) -C (31)	108.7 (3)
C (41) -C (42) -Zr (1)	121.2 (3)
C (34) -C (42) -Zr (1)	75.9 (2)
C (31) -C (42) -Zr (1)	70.7 (2)
C (44) -C (43) -C (48)	118.4 (4)
C (44) -C (43) -C (35)	121.8 (4)
C (48) -C (43) -C (35)	119.7 (4)
C (45) -C (44) -C (43)	120.7 (5)
C (45) -C (44) -H (44)	119.6
C (43) -C (44) -H (44)	119.6
C (44) -C (45) -C (46)	119.7 (5)
C (44) -C (45) -H (45)	120.2
C (46) -C (45) -H (45)	120.2
C (47) -C (46) -C (45)	119.9 (5)
C (47) -C (46) -H (46)	120.0
C (45) -C (46) -H (46)	120.0
C (46) -C (47) -C (48)	120.6 (5)
C (46) -C (47) -H (47)	119.7
C (48) -C (47) -H (47)	119.7
C (47) -C (48) -C (43)	120.7 (5)
C (47) -C (48) -H (48)	119.7
C (43) -C (48) -H (48)	119.7
C (32) -C (49) -H (49A)	109.5
C (32) -C (49) -H (49B)	109.5
H (49A) -C (49) -H (49B)	109.5
C (32) -C (49) -H (49C)	109.5
H (49A) -C (49) -H (49C)	109.5
H (49B) -C (49) -H (49C)	109.5
Si (1) -C (50) -H (50A)	109.5
Si (1) -C (50) -H (50B)	109.5
H (50A) -C (50) -H (50B)	109.5
Si (1) -C (50) -H (50C)	109.5
H (50A) -C (50) -H (50C)	109.5
H (50B) -C (50) -H (50C)	109.5
Cl (2) -C (10) -Cl (3)	113.4 (5)
Cl (2) -C (10) -H (10A)	108.9
Cl (3) -C (10) -H (10A)	108.9
Cl (2) -C (10) -H (10B)	108.9
Cl (3) -C (10) -H (10B)	108.9
H (10A) -C (10) -H (10B)	107.7

Table S11. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **16**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
Zr (1)	18 (1)	15 (1)	14 (1)	-1 (1)	1 (1)	1 (1)
Cl (1)	22 (1)	31 (1)	28 (1)	-8 (1)	5 (1)	4 (1)
Si (1)	20 (1)	23 (1)	17 (1)	-1 (1)	2 (1)	-3 (1)
N (1)	29 (2)	17 (2)	21 (2)	0 (1)	-4 (2)	-2 (1)
C (1)	38 (2)	19 (2)	21 (2)	7 (2)	-3 (2)	-4 (2)
C (2)	55 (3)	31 (3)	55 (4)	10 (3)	7 (3)	7 (2)
C (3)	46 (3)	49 (3)	33 (3)	8 (2)	6 (2)	-13 (2)
C (4)	86 (4)	39 (3)	23 (3)	2 (2)	1 (3)	-13 (3)
C (11)	18 (2)	18 (2)	21 (2)	1 (2)	-1 (2)	-4 (2)
C (12)	24 (2)	15 (2)	23 (2)	1 (2)	-2 (2)	-2 (2)
C (13)	21 (2)	17 (2)	22 (2)	-4 (2)	-2 (2)	0 (2)
C (14)	17 (2)	16 (2)	19 (2)	-4 (2)	-3 (2)	-3 (2)
C (15)	19 (2)	19 (2)	20 (2)	-5 (2)	-4 (2)	-2 (2)
C (16)	25 (2)	18 (2)	19 (2)	-2 (2)	-5 (2)	0 (2)
C (17)	27 (2)	31 (2)	21 (2)	2 (2)	-6 (2)	5 (2)
C (18)	39 (3)	33 (2)	30 (3)	2 (2)	-9 (2)	11 (2)
C (19)	30 (2)	31 (2)	28 (3)	-6 (2)	-7 (2)	13 (2)
C (20)	19 (2)	18 (2)	28 (2)	-4 (2)	-2 (2)	0 (2)
C (21)	20 (2)	19 (2)	22 (2)	-5 (2)	3 (2)	-1 (2)
C (22)	17 (2)	14 (2)	23 (2)	-1 (2)	-1 (2)	-5 (2)
C (23)	22 (2)	19 (2)	19 (2)	0 (2)	-3 (2)	1 (2)
C (24)	29 (2)	37 (2)	25 (2)	-4 (2)	-1 (2)	-1 (2)
C (25)	31 (3)	52 (3)	33 (3)	-9 (2)	7 (2)	8 (2)
C (26)	48 (3)	51 (3)	32 (3)	-12 (2)	5 (2)	15 (3)
C (27)	44 (3)	35 (3)	23 (3)	-14 (2)	-6 (2)	6 (2)
C (28)	26 (2)	27 (2)	27 (3)	-2 (2)	-5 (2)	1 (2)
C (29)	33 (2)	18 (2)	25 (2)	2 (2)	-4 (2)	3 (2)
C (30)	24 (2)	38 (2)	26 (2)	-6 (2)	5 (2)	-1 (2)
C (31)	19 (2)	22 (2)	16 (2)	-4 (2)	1 (2)	-1 (2)
C (32)	21 (2)	20 (2)	16 (2)	-6 (2)	-1 (2)	1 (2)
C (33)	22 (2)	16 (2)	17 (2)	0 (2)	1 (2)	-2 (2)
C (34)	20 (2)	20 (2)	15 (2)	-1 (2)	1 (2)	-2 (2)
C (35)	21 (2)	25 (2)	15 (2)	-7 (2)	4 (2)	-4 (2)
C (36)	17 (2)	30 (2)	19 (2)	-5 (2)	-1 (2)	3 (2)
C (37)	21 (2)	43 (3)	34 (3)	6 (2)	1 (2)	3 (2)
C (38)	26 (2)	48 (3)	49 (3)	11 (3)	-9 (2)	8 (2)
C (39)	28 (2)	32 (2)	29 (3)	5 (2)	-4 (2)	6 (2)
C (40)	23 (2)	23 (2)	15 (2)	-2 (2)	-1 (2)	1 (2)
C (41)	26 (2)	18 (2)	15 (2)	2 (2)	2 (2)	-2 (2)
C (42)	21 (2)	21 (2)	13 (2)	-5 (2)	3 (2)	-3 (2)
C (43)	15 (2)	32 (2)	22 (2)	5 (2)	0 (2)	-2 (2)
C (44)	25 (2)	33 (2)	42 (3)	8 (2)	1 (2)	-6 (2)
C (45)	41 (3)	40 (3)	61 (4)	21 (3)	2 (3)	-11 (2)
C (46)	35 (3)	63 (4)	56 (4)	28 (3)	7 (3)	-16 (3)
C (47)	31 (3)	80 (4)	32 (3)	19 (3)	9 (2)	-6 (3)
C (48)	27 (2)	48 (3)	28 (3)	5 (2)	2 (2)	3 (2)
C (49)	21 (2)	21 (2)	35 (3)	-2 (2)	0 (2)	4 (2)
C (50)	36 (2)	30 (2)	20 (2)	2 (2)	5 (2)	-8 (2)
C (10)	91 (6)	111 (7)	89 (6)	20 (5)	11 (5)	19 (5)
Cl (2)	119 (2)	117 (2)	158 (3)	67 (2)	35 (2)	35 (2)
Cl (3)	119 (2)	101 (2)	118 (2)	-11 (2)	4 (2)	24 (1)

Table S12. Hydrogen coordinates ($\text{\AA} \times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **16**.

x	y	z	U (eq)
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H (1)	4486	9377	7401	27
H (2A)	4547	12702	7670	70
H (2B)	3994	11980	7199	70
H (2C)	4606	13133	7045	70
H (3A)	5869	12023	7768	64
H (3B)	5973	12325	7139	64
H (3C)	6167	10748	7400	64
H (4A)	5334	9735	6622	74
H (4B)	5125	11359	6414	74
H (4C)	4485	10237	6539	74
H (13)	5077	5453	7781	24
H (17A)	2639	7618	6257	32
H (17B)	3356	8596	6161	32
H (18A)	2853	10690	6505	42
H (18B)	2093	9909	6269	42
H (19A)	2298	10563	7299	36
H (19B)	1846	9098	7112	36
H (21)	2881	8976	8192	24
H (24)	5377	6832	6977	37
H (25)	5963	5498	6337	46
H (26)	5278	4144	5670	52
H (27)	4000	4085	5638	42
H (28)	3395	5385	6281	33
H (29A)	4878	4485	9082	38
H (29B)	5418	5864	9191	38
H (29C)	5551	4723	8716	38
H (30A)	2940	9570	9063	44
H (30B)	3016	9221	9704	44
H (30C)	2679	8015	9277	44
H (33)	5455	11979	8523	22
H (37A)	8175	9820	9506	39
H (37B)	8070	8399	9116	39
H (38A)	8382	7202	9921	50
H (38B)	8058	8487	10278	50
H (39A)	7253	6148	9729	36
H (39B)	7113	6871	10308	36
H (41)	5691	7438	9863	24
H (44)	6676	13213	9080	40
H (45)	7208	14909	8525	57
H (46)	7931	14088	7846	62
H (47)	8108	11594	7724	57
H (48)	7587	9902	8276	41
H (49A)	3694	11812	9038	39
H (49B)	3634	11005	8458	39
H (49C)	4080	12516	8541	39
H (50A)	4609	6195	9839	43
H (50B)	3743	6173	9917	43
H (50C)	4270	7388	10221	43
H (10A)	1212	6744	777	116
H (10B)	951	5152	565	116

Table S13. Torsion angles [deg] for **16**.

C1 (1) -Zr (1) -N (1) -C (1)	-67.6 (5)
C (11) -Zr (1) -N (1) -C (1)	158.3 (5)
C (32) -Zr (1) -N (1) -C (1)	66.9 (5)
C (31) -Zr (1) -N (1) -C (1)	75.4 (5)
C (12) -Zr (1) -N (1) -C (1)	-162.5 (5)
C (33) -Zr (1) -N (1) -C (1)	35.8 (5)
C (22) -Zr (1) -N (1) -C (1)	161.7 (5)
C (42) -Zr (1) -N (1) -C (1)	34.1 (6)
C (13) -Zr (1) -N (1) -C (1)	-148.0 (5)

C(34)-Zr(1)-N(1)-C(1)	15.8(5)
C(14)-Zr(1)-N(1)-C(1)	-168.0(5)
Zr(1)-N(1)-C(1)-C(3)	22.6(7)
Zr(1)-N(1)-C(1)-C(2)	-100.5(5)
Zr(1)-N(1)-C(1)-C(4)	140.1(4)
C(30)-Si(1)-C(11)-C(22)	37.9(4)
C(50)-Si(1)-C(11)-C(22)	157.7(3)
C(31)-Si(1)-C(11)-C(22)	-82.7(3)
C(30)-Si(1)-C(11)-C(12)	-162.6(3)
C(50)-Si(1)-C(11)-C(12)	-42.7(4)
C(31)-Si(1)-C(11)-C(12)	76.9(3)
C(30)-Si(1)-C(11)-Zr(1)	118.87(19)
C(50)-Si(1)-C(11)-Zr(1)	-121.32(18)
C(31)-Si(1)-C(11)-Zr(1)	-1.68(18)
N(1)-Zr(1)-C(11)-C(22)	6.2(3)
Cl(1)-Zr(1)-C(11)-C(22)	-119.5(2)
C(32)-Zr(1)-C(11)-C(22)	100.7(2)
C(31)-Zr(1)-C(11)-C(22)	126.6(2)
C(12)-Zr(1)-C(11)-C(22)	-109.7(3)
C(33)-Zr(1)-C(11)-C(22)	110.5(2)
C(42)-Zr(1)-C(11)-C(22)	153.6(2)
C(13)-Zr(1)-C(11)-C(22)	-74.3(2)
C(34)-Zr(1)-C(11)-C(22)	146.3(2)
C(14)-Zr(1)-C(11)-C(22)	-36.0(2)
N(1)-Zr(1)-C(11)-C(12)	115.9(2)
Cl(1)-Zr(1)-C(11)-C(12)	-9.9(3)
C(32)-Zr(1)-C(11)-C(12)	-149.7(2)
C(31)-Zr(1)-C(11)-C(12)	-123.7(3)
C(33)-Zr(1)-C(11)-C(12)	-139.8(2)
C(22)-Zr(1)-C(11)-C(12)	109.7(3)
C(42)-Zr(1)-C(11)-C(12)	-96.7(2)
C(13)-Zr(1)-C(11)-C(12)	35.4(2)
C(34)-Zr(1)-C(11)-C(12)	-104.0(2)
C(14)-Zr(1)-C(11)-C(12)	73.6(2)
N(1)-Zr(1)-C(11)-Si(1)	-119.04(16)
Cl(1)-Zr(1)-C(11)-Si(1)	115.18(13)
C(32)-Zr(1)-C(11)-Si(1)	-24.62(16)
C(31)-Zr(1)-C(11)-Si(1)	1.33(14)
C(12)-Zr(1)-C(11)-Si(1)	125.1(3)
C(33)-Zr(1)-C(11)-Si(1)	-14.8(2)
C(22)-Zr(1)-C(11)-Si(1)	-125.3(3)
C(42)-Zr(1)-C(11)-Si(1)	28.36(16)
C(13)-Zr(1)-C(11)-Si(1)	160.4(2)
C(34)-Zr(1)-C(11)-Si(1)	21.0(2)
C(14)-Zr(1)-C(11)-Si(1)	-161.3(2)
C(22)-C(11)-C(12)-C(13)	2.2(4)
Si(1)-C(11)-C(12)-C(13)	-160.8(3)
Zr(1)-C(11)-C(12)-C(13)	-70.3(3)
C(22)-C(11)-C(12)-C(29)	-175.5(4)
Si(1)-C(11)-C(12)-C(29)	21.5(6)
Zr(1)-C(11)-C(12)-C(29)	111.9(4)
C(22)-C(11)-C(12)-Zr(1)	72.6(2)
Si(1)-C(11)-C(12)-Zr(1)	-90.5(3)
N(1)-Zr(1)-C(12)-C(13)	28.7(3)
Cl(1)-Zr(1)-C(12)-C(13)	-73.4(2)
C(11)-Zr(1)-C(12)-C(13)	115.2(3)
C(32)-Zr(1)-C(12)-C(13)	149.9(2)
C(31)-Zr(1)-C(12)-C(13)	165.6(2)
C(33)-Zr(1)-C(12)-C(13)	178.6(2)
C(22)-Zr(1)-C(12)-C(13)	75.4(2)
C(42)-Zr(1)-C(12)-C(13)	-162.0(2)
C(34)-Zr(1)-C(12)-C(13)	-149.5(2)
C(14)-Zr(1)-C(12)-C(13)	35.5(2)
N(1)-Zr(1)-C(12)-C(11)	-86.5(3)
Cl(1)-Zr(1)-C(12)-C(11)	171.4(2)
C(32)-Zr(1)-C(12)-C(11)	34.7(3)
C(31)-Zr(1)-C(12)-C(11)	50.4(2)

C(33)-Zr(1)-C(12)-C(11)	63.4(3)
C(22)-Zr(1)-C(12)-C(11)	-39.7(2)
C(42)-Zr(1)-C(12)-C(11)	82.8(2)
C(13)-Zr(1)-C(12)-C(11)	-115.2(3)
C(34)-Zr(1)-C(12)-C(11)	95.3(2)
C(14)-Zr(1)-C(12)-C(11)	-79.7(2)
N(1)-Zr(1)-C(12)-C(29)	148.9(3)
Cl(1)-Zr(1)-C(12)-C(29)	46.9(3)
C(11)-Zr(1)-C(12)-C(29)	-124.5(4)
C(32)-Zr(1)-C(12)-C(29)	-89.8(3)
C(31)-Zr(1)-C(12)-C(29)	-74.1(3)
C(33)-Zr(1)-C(12)-C(29)	-61.1(4)
C(22)-Zr(1)-C(12)-C(29)	-164.3(4)
C(42)-Zr(1)-C(12)-C(29)	-41.8(3)
C(13)-Zr(1)-C(12)-C(29)	120.3(4)
C(34)-Zr(1)-C(12)-C(29)	-29.2(3)
C(14)-Zr(1)-C(12)-C(29)	155.8(4)
C(11)-C(12)-C(13)-C(14)	-2.9(4)
C(29)-C(12)-C(13)-C(14)	175.0(3)
Zr(1)-C(12)-C(13)-C(14)	-67.9(3)
C(11)-C(12)-C(13)-Zr(1)	64.9(3)
C(29)-C(12)-C(13)-Zr(1)	-117.1(4)
N(1)-Zr(1)-C(13)-C(12)	-157.5(2)
Cl(1)-Zr(1)-C(13)-C(12)	102.7(2)
C(11)-Zr(1)-C(13)-C(12)	-38.4(2)
C(32)-Zr(1)-C(13)-C(12)	-46.7(3)
C(31)-Zr(1)-C(13)-C(12)	-16.4(3)
C(22)-Zr(1)-C(13)-C(12)	-80.1(3)
C(42)-Zr(1)-C(13)-C(12)	21.0(3)
C(34)-Zr(1)-C(13)-C(12)	49.5(3)
C(14)-Zr(1)-C(13)-C(12)	-116.5(3)
N(1)-Zr(1)-C(13)-C(14)	-41.0(2)
Cl(1)-Zr(1)-C(13)-C(14)	-140.9(2)
C(11)-Zr(1)-C(13)-C(14)	78.1(2)
C(32)-Zr(1)-C(13)-C(14)	69.8(3)
C(31)-Zr(1)-C(13)-C(14)	100.1(2)
C(12)-Zr(1)-C(13)-C(14)	116.5(3)
C(22)-Zr(1)-C(13)-C(14)	36.4(2)
C(42)-Zr(1)-C(13)-C(14)	137.5(2)
C(34)-Zr(1)-C(13)-C(14)	166.0(2)
C(12)-C(13)-C(14)-C(15)	-175.0(4)
Zr(1)-C(13)-C(14)-C(15)	121.8(4)
C(12)-C(13)-C(14)-C(22)	2.4(4)
Zr(1)-C(13)-C(14)-C(22)	-60.7(2)
C(12)-C(13)-C(14)-Zr(1)	63.1(3)
N(1)-Zr(1)-C(14)-C(13)	138.4(2)
Cl(1)-Zr(1)-C(14)-C(13)	39.3(2)
C(11)-Zr(1)-C(14)-C(13)	-78.6(2)
C(32)-Zr(1)-C(14)-C(13)	-135.6(2)
C(31)-Zr(1)-C(14)-C(13)	-97.0(2)
C(12)-Zr(1)-C(14)-C(13)	-36.1(2)
C(33)-Zr(1)-C(14)-C(13)	-164.4(2)
C(22)-Zr(1)-C(14)-C(13)	-116.4(3)
C(42)-Zr(1)-C(14)-C(13)	-63.7(3)
N(1)-Zr(1)-C(14)-C(15)	10.3(3)
Cl(1)-Zr(1)-C(14)-C(15)	-88.8(3)
C(11)-Zr(1)-C(14)-C(15)	153.2(4)
C(32)-Zr(1)-C(14)-C(15)	96.2(3)
C(31)-Zr(1)-C(14)-C(15)	134.8(3)
C(12)-Zr(1)-C(14)-C(15)	-164.2(4)
C(33)-Zr(1)-C(14)-C(15)	67.4(4)
C(22)-Zr(1)-C(14)-C(15)	115.4(4)
C(42)-Zr(1)-C(14)-C(15)	168.2(3)
C(13)-Zr(1)-C(14)-C(15)	-128.2(4)
N(1)-Zr(1)-C(14)-C(22)	-105.1(2)
Cl(1)-Zr(1)-C(14)-C(22)	155.8(2)
C(11)-Zr(1)-C(14)-C(22)	37.8(2)

C(32)-Zr(1)-C(14)-C(22)	-19.1(3)
C(31)-Zr(1)-C(14)-C(22)	19.4(3)
C(12)-Zr(1)-C(14)-C(22)	80.4(2)
C(33)-Zr(1)-C(14)-C(22)	-48.0(3)
C(42)-Zr(1)-C(14)-C(22)	52.8(3)
C(13)-Zr(1)-C(14)-C(22)	116.4(3)
C(13)-C(14)-C(15)-C(16)	178.5(4)
C(22)-C(14)-C(15)-C(16)	1.4(5)
Zr(1)-C(14)-C(15)-C(16)	-84.5(4)
C(13)-C(14)-C(15)-C(23)	0.1(6)
C(22)-C(14)-C(15)-C(23)	-177.1(3)
Zr(1)-C(14)-C(15)-C(23)	97.0(4)
C(14)-C(15)-C(16)-C(20)	-0.7(6)
C(23)-C(15)-C(16)-C(20)	177.7(4)
C(14)-C(15)-C(16)-C(17)	178.6(4)
C(23)-C(15)-C(16)-C(17)	-2.9(6)
C(15)-C(16)-C(17)-C(18)	-160.7(4)
C(20)-C(16)-C(17)-C(18)	18.7(4)
C(16)-C(17)-C(18)-C(19)	-30.0(4)
C(17)-C(18)-C(19)-C(20)	30.2(5)
C(15)-C(16)-C(20)-C(21)	-0.4(6)
C(17)-C(16)-C(20)-C(21)	-179.9(4)
C(15)-C(16)-C(20)-C(19)	179.6(4)
C(17)-C(16)-C(20)-C(19)	0.1(5)
C(18)-C(19)-C(20)-C(21)	160.7(4)
C(18)-C(19)-C(20)-C(16)	-19.2(5)
C(16)-C(20)-C(21)-C(22)	0.8(6)
C(19)-C(20)-C(21)-C(22)	-179.1(4)
C(20)-C(21)-C(22)-C(11)	-177.2(4)
C(20)-C(21)-C(22)-C(14)	-0.2(5)
C(20)-C(21)-C(22)-Zr(1)	94.2(4)
C(12)-C(11)-C(22)-C(21)	176.6(4)
Si(1)-C(11)-C(22)-C(21)	-20.4(6)
Zr(1)-C(11)-C(22)-C(21)	-112.3(4)
C(12)-C(11)-C(22)-C(14)	-0.7(4)
Si(1)-C(11)-C(22)-C(14)	162.3(3)
Zr(1)-C(11)-C(22)-C(14)	70.4(3)
C(12)-C(11)-C(22)-Zr(1)	-71.1(2)
Si(1)-C(11)-C(22)-Zr(1)	91.8(3)
C(13)-C(14)-C(22)-C(21)	-178.7(3)
C(15)-C(14)-C(22)-C(21)	-1.0(5)
Zr(1)-C(14)-C(22)-C(21)	118.5(3)
C(13)-C(14)-C(22)-C(11)	-1.0(4)
C(15)-C(14)-C(22)-C(11)	176.7(3)
Zr(1)-C(14)-C(22)-C(11)	-63.8(2)
C(13)-C(14)-C(22)-Zr(1)	62.7(3)
C(15)-C(14)-C(22)-Zr(1)	-119.5(3)
N(1)-Zr(1)-C(22)-C(21)	-46.8(3)
Cl(1)-Zr(1)-C(22)-C(21)	-148.9(3)
C(11)-Zr(1)-C(22)-C(21)	127.8(4)
C(32)-Zr(1)-C(22)-C(21)	47.3(3)
C(31)-Zr(1)-C(22)-C(21)	79.7(3)
C(12)-Zr(1)-C(22)-C(21)	168.3(4)
C(33)-Zr(1)-C(22)-C(21)	36.9(4)
C(42)-Zr(1)-C(22)-C(21)	98.1(3)
C(13)-Zr(1)-C(22)-C(21)	-152.4(4)
C(34)-Zr(1)-C(22)-C(21)	74.2(4)
C(14)-Zr(1)-C(22)-C(21)	-117.1(4)
N(1)-Zr(1)-C(22)-C(11)	-174.5(2)
Cl(1)-Zr(1)-C(22)-C(11)	83.3(2)
C(32)-Zr(1)-C(22)-C(11)	-80.5(2)
C(31)-Zr(1)-C(22)-C(11)	-48.0(2)
C(12)-Zr(1)-C(22)-C(11)	40.5(2)
C(33)-Zr(1)-C(22)-C(11)	-90.9(2)
C(42)-Zr(1)-C(22)-C(11)	-29.6(2)
C(13)-Zr(1)-C(22)-C(11)	79.8(2)
C(34)-Zr(1)-C(22)-C(11)	-53.6(3)

C(14)-Zr(1)-C(22)-C(11)	115.1(3)
N(1)-Zr(1)-C(22)-C(14)	70.4(2)
Cl(1)-Zr(1)-C(22)-C(14)	-31.8(3)
C(11)-Zr(1)-C(22)-C(14)	-115.1(3)
C(32)-Zr(1)-C(22)-C(14)	164.4(2)
C(31)-Zr(1)-C(22)-C(14)	-163.1(2)
C(12)-Zr(1)-C(22)-C(14)	-74.6(2)
C(33)-Zr(1)-C(22)-C(14)	154.0(2)
C(42)-Zr(1)-C(22)-C(14)	-144.7(2)
C(13)-Zr(1)-C(22)-C(14)	-35.3(2)
C(34)-Zr(1)-C(22)-C(14)	-168.7(2)
C(16)-C(15)-C(23)-C(28)	-51.0(6)
C(14)-C(15)-C(23)-C(28)	127.4(4)
C(16)-C(15)-C(23)-C(24)	131.9(4)
C(14)-C(15)-C(23)-C(24)	-49.7(6)
C(28)-C(23)-C(24)-C(25)	0.4(6)
C(15)-C(23)-C(24)-C(25)	177.6(4)
C(23)-C(24)-C(25)-C(26)	0.2(7)
C(24)-C(25)-C(26)-C(27)	-0.4(8)
C(25)-C(26)-C(27)-C(28)	-0.1(8)
C(24)-C(23)-C(28)-C(27)	-0.9(6)
C(15)-C(23)-C(28)-C(27)	-178.1(4)
C(26)-C(27)-C(28)-C(23)	0.7(7)
C(30)-Si(1)-C(31)-C(32)	-43.9(4)
C(50)-Si(1)-C(31)-C(32)	-165.7(3)
C(11)-Si(1)-C(31)-C(32)	75.7(4)
C(30)-Si(1)-C(31)-C(42)	163.4(3)
C(50)-Si(1)-C(31)-C(42)	41.6(4)
C(11)-Si(1)-C(31)-C(42)	-77.0(3)
C(30)-Si(1)-C(31)-Zr(1)	-117.95(18)
C(50)-Si(1)-C(31)-Zr(1)	120.25(18)
C(11)-Si(1)-C(31)-Zr(1)	1.63(17)
N(1)-Zr(1)-C(31)-C(32)	-15.7(3)
Cl(1)-Zr(1)-C(31)-C(32)	121.0(2)
C(11)-Zr(1)-C(31)-C(32)	-126.5(2)
C(12)-Zr(1)-C(31)-C(32)	-153.9(2)
C(33)-Zr(1)-C(31)-C(32)	36.1(2)
C(22)-Zr(1)-C(31)-C(32)	-100.6(2)
C(42)-Zr(1)-C(31)-C(32)	111.1(3)
C(13)-Zr(1)-C(31)-C(32)	-145.6(2)
C(34)-Zr(1)-C(31)-C(32)	75.2(2)
C(14)-Zr(1)-C(31)-C(32)	-110.6(2)
N(1)-Zr(1)-C(31)-C(42)	-126.8(2)
Cl(1)-Zr(1)-C(31)-C(42)	9.9(2)
C(11)-Zr(1)-C(31)-C(42)	122.3(2)
C(32)-Zr(1)-C(31)-C(42)	-111.1(3)
C(12)-Zr(1)-C(31)-C(42)	95.0(2)
C(33)-Zr(1)-C(31)-C(42)	-75.0(2)
C(22)-Zr(1)-C(31)-C(42)	148.2(2)
C(13)-Zr(1)-C(31)-C(42)	103.3(2)
C(34)-Zr(1)-C(31)-C(42)	-35.9(2)
C(14)-Zr(1)-C(31)-C(42)	138.3(2)
N(1)-Zr(1)-C(31)-Si(1)	109.49(17)
Cl(1)-Zr(1)-C(31)-Si(1)	-113.77(13)
C(11)-Zr(1)-C(31)-Si(1)	-1.32(14)
C(32)-Zr(1)-C(31)-Si(1)	125.2(3)
C(12)-Zr(1)-C(31)-Si(1)	-28.69(16)
C(33)-Zr(1)-C(31)-Si(1)	161.3(2)
C(22)-Zr(1)-C(31)-Si(1)	24.58(16)
C(42)-Zr(1)-C(31)-Si(1)	-123.7(3)
C(13)-Zr(1)-C(31)-Si(1)	-20.3(2)
C(34)-Zr(1)-C(31)-Si(1)	-159.6(2)
C(14)-Zr(1)-C(31)-Si(1)	14.6(2)
C(42)-C(31)-C(32)-C(33)	2.8(4)
Si(1)-C(31)-C(32)-C(33)	-154.0(3)
Zr(1)-C(31)-C(32)-C(33)	-67.8(3)
C(42)-C(31)-C(32)-C(49)	-173.3(4)

Si (1)-C (31)-C (32)-C (49)	29.9 (6)
Zr (1)-C (31)-C (32)-C (49)	116.1 (4)
C (42)-C (31)-C (32)-Zr (1)	70.6 (3)
Si (1)-C (31)-C (32)-Zr (1)	-86.2 (3)
N (1)-Zr (1)-C (32)-C (33)	-77.1 (2)
Cl (1)-Zr (1)-C (32)-C (33)	32.7 (3)
C (11)-Zr (1)-C (32)-C (33)	163.7 (2)
C (31)-Zr (1)-C (32)-C (33)	115.6 (3)
C (12)-Zr (1)-C (32)-C (33)	145.3 (2)
C (22)-Zr (1)-C (32)-C (33)	-163.9 (2)
C (42)-Zr (1)-C (32)-C (33)	76.7 (2)
C (13)-Zr (1)-C (32)-C (33)	170.3 (2)
C (34)-Zr (1)-C (32)-C (33)	36.5 (2)
C (14)-Zr (1)-C (32)-C (33)	-154.0 (2)
N (1)-Zr (1)-C (32)-C (31)	167.4 (2)
Cl (1)-Zr (1)-C (32)-C (31)	-82.9 (2)
C (11)-Zr (1)-C (32)-C (31)	48.1 (2)
C (12)-Zr (1)-C (32)-C (31)	29.7 (3)
C (33)-Zr (1)-C (32)-C (31)	-115.6 (3)
C (22)-Zr (1)-C (32)-C (31)	80.6 (2)
C (42)-Zr (1)-C (32)-C (31)	-38.9 (2)
C (13)-Zr (1)-C (32)-C (31)	54.8 (3)
C (34)-Zr (1)-C (32)-C (31)	-79.0 (2)
C (14)-Zr (1)-C (32)-C (31)	90.4 (2)
N (1)-Zr (1)-C (32)-C (49)	43.5 (3)
Cl (1)-Zr (1)-C (32)-C (49)	153.3 (2)
C (11)-Zr (1)-C (32)-C (49)	-75.8 (3)
C (31)-Zr (1)-C (32)-C (49)	-123.8 (4)
C (12)-Zr (1)-C (32)-C (49)	-94.1 (3)
C (33)-Zr (1)-C (32)-C (49)	120.6 (4)
C (22)-Zr (1)-C (32)-C (49)	-43.3 (3)
C (42)-Zr (1)-C (32)-C (49)	-162.7 (4)
C (13)-Zr (1)-C (32)-C (49)	-69.1 (4)
C (34)-Zr (1)-C (32)-C (49)	157.1 (4)
C (14)-Zr (1)-C (32)-C (49)	-33.4 (4)
C (31)-C (32)-C (33)-C (34)	-3.6 (4)
C (49)-C (32)-C (33)-C (34)	172.7 (4)
Zr (1)-C (32)-C (33)-C (34)	-70.3 (3)
C (31)-C (32)-C (33)-Zr (1)	66.7 (3)
C (49)-C (32)-C (33)-Zr (1)	-117.0 (4)
N (1)-Zr (1)-C (33)-C (32)	103.3 (2)
Cl (1)-Zr (1)-C (33)-C (32)	-155.6 (2)
C (11)-Zr (1)-C (33)-C (32)	-18.9 (3)
C (31)-Zr (1)-C (33)-C (32)	-37.4 (2)
C (12)-Zr (1)-C (33)-C (32)	-53.5 (3)
C (22)-Zr (1)-C (33)-C (32)	19.9 (3)
C (42)-Zr (1)-C (33)-C (32)	-78.2 (2)
C (34)-Zr (1)-C (33)-C (32)	-114.7 (3)
C (14)-Zr (1)-C (33)-C (32)	48.3 (4)
N (1)-Zr (1)-C (33)-C (34)	-142.0 (2)
Cl (1)-Zr (1)-C (33)-C (34)	-40.9 (2)
C (11)-Zr (1)-C (33)-C (34)	95.9 (2)
C (32)-Zr (1)-C (33)-C (34)	114.7 (3)
C (31)-Zr (1)-C (33)-C (34)	77.4 (2)
C (12)-Zr (1)-C (33)-C (34)	61.2 (3)
C (22)-Zr (1)-C (33)-C (34)	134.6 (2)
C (42)-Zr (1)-C (33)-C (34)	36.6 (2)
C (14)-Zr (1)-C (33)-C (34)	163.0 (2)
C (32)-C (33)-C (34)-C (42)	2.8 (4)
Zr (1)-C (33)-C (34)-C (42)	-63.7 (3)
C (32)-C (33)-C (34)-C (35)	-178.7 (4)
Zr (1)-C (33)-C (34)-C (35)	114.8 (4)
C (32)-C (33)-C (34)-Zr (1)	66.5 (3)
N (1)-Zr (1)-C (34)-C (33)	41.3 (2)
Cl (1)-Zr (1)-C (34)-C (33)	139.8 (2)
C (11)-Zr (1)-C (34)-C (33)	-101.8 (2)
C (32)-Zr (1)-C (34)-C (33)	-37.3 (2)

C(31)-Zr(1)-C(34)-C(33)	-79.0(2)
C(12)-Zr(1)-C(34)-C(33)	-140.3(2)
C(22)-Zr(1)-C(34)-C(33)	-72.1(3)
C(42)-Zr(1)-C(34)-C(33)	-115.8(3)
C(13)-Zr(1)-C(34)-C(33)	-167.4(2)
N(1)-Zr(1)-C(34)-C(42)	157.1(2)
Cl(1)-Zr(1)-C(34)-C(42)	-104.4(2)
C(11)-Zr(1)-C(34)-C(42)	14.1(3)
C(32)-Zr(1)-C(34)-C(42)	78.5(2)
C(31)-Zr(1)-C(34)-C(42)	36.9(2)
C(12)-Zr(1)-C(34)-C(42)	-24.4(3)
C(33)-Zr(1)-C(34)-C(42)	115.8(3)
C(22)-Zr(1)-C(34)-C(42)	43.8(3)
C(13)-Zr(1)-C(34)-C(42)	-51.5(3)
N(1)-Zr(1)-C(34)-C(35)	-86.4(3)
Cl(1)-Zr(1)-C(34)-C(35)	12.1(3)
C(11)-Zr(1)-C(34)-C(35)	130.6(3)
C(32)-Zr(1)-C(34)-C(35)	-165.0(4)
C(31)-Zr(1)-C(34)-C(35)	153.4(4)
C(12)-Zr(1)-C(34)-C(35)	92.1(3)
C(33)-Zr(1)-C(34)-C(35)	-127.6(4)
C(22)-Zr(1)-C(34)-C(35)	160.3(3)
C(42)-Zr(1)-C(34)-C(35)	116.5(4)
C(13)-Zr(1)-C(34)-C(35)	65.0(4)
C(33)-C(34)-C(35)-C(36)	-177.6(4)
C(42)-C(34)-C(35)-C(36)	0.8(6)
Zr(1)-C(34)-C(35)-C(36)	-86.6(4)
C(33)-C(34)-C(35)-C(43)	-0.7(6)
C(42)-C(34)-C(35)-C(43)	177.6(4)
Zr(1)-C(34)-C(35)-C(43)	90.3(4)
C(34)-C(35)-C(36)-C(40)	-1.7(6)
C(43)-C(35)-C(36)-C(40)	-178.4(4)
C(34)-C(35)-C(36)-C(37)	179.1(4)
C(43)-C(35)-C(36)-C(37)	2.4(7)
C(35)-C(36)-C(37)-C(38)	162.1(4)
C(40)-C(36)-C(37)-C(38)	-17.2(5)
C(36)-C(37)-C(38)-C(39)	28.2(5)
C(37)-C(38)-C(39)-C(40)	-28.7(5)
C(35)-C(36)-C(40)-C(41)	-0.1(6)
C(37)-C(36)-C(40)-C(41)	179.2(4)
C(35)-C(36)-C(40)-C(39)	-179.9(4)
C(37)-C(36)-C(40)-C(39)	-0.6(5)
C(38)-C(39)-C(40)-C(41)	-161.4(4)
C(38)-C(39)-C(40)-C(36)	18.3(5)
C(36)-C(40)-C(41)-C(42)	3.0(6)
C(39)-C(40)-C(41)-C(42)	-177.4(4)
C(40)-C(41)-C(42)-C(34)	-3.8(6)
C(40)-C(41)-C(42)-C(31)	178.4(4)
C(40)-C(41)-C(42)-Zr(1)	86.7(4)
C(33)-C(34)-C(42)-C(41)	-179.4(3)
C(35)-C(34)-C(42)-C(41)	1.9(6)
Zr(1)-C(34)-C(42)-C(41)	118.1(3)
C(33)-C(34)-C(42)-C(31)	-1.0(4)
C(35)-C(34)-C(42)-C(31)	-179.7(3)
Zr(1)-C(34)-C(42)-C(31)	-63.6(3)
C(33)-C(34)-C(42)-Zr(1)	62.5(3)
C(35)-C(34)-C(42)-Zr(1)	-116.2(3)
C(32)-C(31)-C(42)-C(41)	177.0(4)
Si(1)-C(31)-C(42)-C(41)	-25.8(6)
Zr(1)-C(31)-C(42)-C(41)	-115.0(4)
C(32)-C(31)-C(42)-C(34)	-1.0(4)
Si(1)-C(31)-C(42)-C(34)	156.2(3)
Zr(1)-C(31)-C(42)-C(34)	67.0(3)
C(32)-C(31)-C(42)-Zr(1)	-68.0(3)
Si(1)-C(31)-C(42)-Zr(1)	89.2(3)
N(1)-Zr(1)-C(42)-C(41)	-149.2(3)
Cl(1)-Zr(1)-C(42)-C(41)	-42.9(3)

C (11)-Zr (1)-C (42)-C (41)	77.0 (3)
C (32)-Zr (1)-C (42)-C (41)	168.1 (4)
C (31)-Zr (1)-C (42)-C (41)	128.6 (4)
C (12)-Zr (1)-C (42)-C (41)	43.7 (3)
C (33)-Zr (1)-C (42)-C (41)	-151.4 (4)
C (22)-Zr (1)-C (42)-C (41)	92.7 (3)
C (13)-Zr (1)-C (42)-C (41)	33.1 (3)
C (34)-Zr (1)-C (42)-C (41)	-115.4 (4)
C (14)-Zr (1)-C (42)-C (41)	65.1 (4)
N (1)-Zr (1)-C (42)-C (34)	-33.9 (3)
Cl (1)-Zr (1)-C (42)-C (34)	72.5 (2)
C (11)-Zr (1)-C (42)-C (34)	-167.6 (2)
C (32)-Zr (1)-C (42)-C (34)	-76.5 (2)
C (31)-Zr (1)-C (42)-C (34)	-116.0 (3)
C (12)-Zr (1)-C (42)-C (34)	159.1 (2)
C (33)-Zr (1)-C (42)-C (34)	-36.1 (2)
C (22)-Zr (1)-C (42)-C (34)	-152.0 (2)
C (13)-Zr (1)-C (42)-C (34)	148.5 (2)
C (14)-Zr (1)-C (42)-C (34)	-179.6 (2)
N (1)-Zr (1)-C (42)-C (31)	82.2 (3)
Cl (1)-Zr (1)-C (42)-C (31)	-171.5 (2)
C (11)-Zr (1)-C (42)-C (31)	-51.6 (2)
C (32)-Zr (1)-C (42)-C (31)	39.5 (2)
C (12)-Zr (1)-C (42)-C (31)	-84.9 (2)
C (33)-Zr (1)-C (42)-C (31)	79.9 (2)
C (22)-Zr (1)-C (42)-C (31)	-35.9 (3)
C (13)-Zr (1)-C (42)-C (31)	-95.5 (2)
C (34)-Zr (1)-C (42)-C (31)	116.0 (3)
C (14)-Zr (1)-C (42)-C (31)	-63.6 (3)
C (36)-C (35)-C (43)-C (44)	-125.8 (5)
C (34)-C (35)-C (43)-C (44)	57.6 (6)
C (36)-C (35)-C (43)-C (48)	56.9 (6)
C (34)-C (35)-C (43)-C (48)	-119.7 (4)
C (48)-C (43)-C (44)-C (45)	1.0 (7)
C (35)-C (43)-C (44)-C (45)	-176.4 (4)
C (43)-C (44)-C (45)-C (46)	-0.5 (8)
C (44)-C (45)-C (46)-C (47)	0.1 (8)
C (45)-C (46)-C (47)-C (48)	-0.3 (8)
C (46)-C (47)-C (48)-C (43)	0.8 (8)
C (44)-C (43)-C (48)-C (47)	-1.1 (7)
C (35)-C (43)-C (48)-C (47)	176.3 (4)

Propylene homopolymerization using 14. *Preparation of the catalyst system.* Complex **14** (0.206 mmol) was added at room temperature to 4.33 mmol of MAO (30% strength solution in toluene, Albemarle). The solution was allowed to stand overnight at room temperature and was subsequently diluted with 10.9 ml of toluene. The diluted solution was carefully added to a log of silica (Sylopol 948, calcined at 600 °C, Grace). Particular care was taken to ensure that the solution was uniformly distributed over the support material. After 10 minutes, the flask containing the catalyst suspension was connected to a vacuum line and dried until the content of volatile material was reduced to less than 5% by weight. *Propylene homopolymerization.* Homopolymerization reactions were carried out in a 10 L

reactor, previously flushed with nitrogen, charged with 3.5 kg of liquid propene. Eight milliliters of a 20% (by weight) solution of triethylaluminum in Exxsol (Witco) was introduced into the reactor and the mixture was stirred at 30 °C for 15 minutes. A suspension of the catalyst in 20 ml of Exxsol was introduced into the reactor. The reactor temperature was increased to 65 °C and maintained at this temperature for 60 minutes. The polymerizations were halted by venting the reactor. The polymers were dried overnight under reduced pressure before being analyzed.

Propylene polymerization using **14** in slurry with hydrogen (see Table 2). The catalyst system was prepared as described above with the addition of hydrogen as indicated in table 2. The reactor was made inert before being charged using nitrogen. Eight milliliters of a 20% strength by weight solution of triethylaluminum in Exxsol (from Witco) was introduced into the reactor and the mixture was stirred at 30 °C for 15 minutes. Varied quantities of the catalyst system (table 5) in a suspension of 20 ml of Exxsol were introduced into the reactor. The reactor temperature was increased to 65 °C and maintained at this temperature for 60 minutes. The polymerizations were halted by venting the reactor. The polymers were dried overnight under reduced pressure before being analyzed.

Comparative two-stage polymerization for **14** and **17** (See Table 3). *Preparation of the supported catalyst system.* Thirty milliliters of toluene and 6.3 g SiO₂ were placed in a round flask equipped with a KPG stirrer at 0 °C. Using a dropping funnel, 15.1 ml of MAO was slowly added at 0 °C, and then, the suspension was allowed to warm to room temperature and was stirred for 2 h. The reaction mixture was placed in a stirred glass flask equipped with a filter (size P3) and the solvent was removed. The residue was resuspended in toluene (20 ml), stirred for 15 min at room temperature, and filtered. The support was suspended in toluene (20 ml), warmed to 80 °C, and then stirred for 30 min at this temperature before hot filtration. This step was repeated before the MAO/silica was suspended at 15 °C in toluene (20 ml). Under stirring, a solution of 0.25 mmol (40 µmol/g carrier) of the metallocene indicated in table 3 in 2 ml MAO and 2 ml toluene was slowly added. The reaction mixture was stirred for 1 h at 15 °C, and then for 2 h after raising the temperature to 40 °C. The resulting solid was filtered and washed 3

times at 60 °C with 20 ml toluene (stirring: 3 × 30 min). After the last filtration, the reaction product was transferred with an aliquot of toluene onto a glass frit (size P3) and filtered again. The catalyst was dried in high vacuum until the was weight constant. *Polymerization procedure. Step a)* A 2.5 L autoclave, previously kept overnight under nitrogen purge, was charged with 2 mmol triethylaluminum (TEA) (as a 10% hexane solution) as the reactor scavenger. In addition, 0.5 bar-g of propylene was added to prevent air insertion in the reactor. For the prepolymerization, 252 g of propylene was added to the autoclave at 0 °C. The catalytic system was injected into the reactor where the propylene was prepolymerized at 30 °C for 5 minutes. At the end of this step, the reactor temperature was raised from to 70 °C (in 10 minutes). During the temperature increase, 59 cc H₂, corresponding to 2.63 mmol of H₂, was fed into the reactor. Bulk propylene polymerization was carried out at 30 bar-g of pressure and 70 °C until the liquid propylene was totally consumed and the pressure inside the reactor began to decrease. When this step was completed, the PP matrix polymerization time was recorded, the pressure was released down to 0.1 bar-g propylene, and the temperature decreased to 30 °C. *Step b)* Ethylene and propylene at a 0.3 molar ratio ethylene(C2)/propylene(C3)+ethylene(C2) were added into the reactor to reach a pressure of 21 bar-g. The temperature was then raised to 60°C, and the mixture was fed at constant pressure until 232 g of monomers were consumed. Then, the reactor was vented and cooled down to room temperature, stopping the reaction. The polymer was collected and dried at reduced pressure and 60 °C. The resulting polymer was subjected to xylene extraction at 25 °C according to the procedure described above. The fraction of polymer soluble in xylene at 25 °C was taken as the amount of ethylene/propylene copolymers produced in the process.

Propylene/ethylene copolymerization using **14** (See Table 4). *Step a)* A 11.7 L autoclave, previously kept overnight under nitrogen purge, was added with 8 mmol triisobutylaluminum (TIBA) (as 20% by wt in Exxsol, 0.77 mol/L) as the reactor scavenger. The autoclave was filled with 550 g of propylene and 70 mg of hydrogen. At room temperature, the catalyst for propylene homopolymerization was injected in the reactor using an additional 150 g of liquid propylene. The temperature was increased

to 40 °C in 2-3 minutes, and the propylene was polymerized at this temperature for 5 minutes. *Step b)* At the end of the prepolymerization step, the monomer was totally flushed out. The reactor was filled with fresh ethylene/propylene monomer mixture and the temperature was increased in approximately 10 min to 60 °C to reach the desired polymerization pressure of 21 bar-g. *Step c)* The ethylene/propylene mixture was fed at constant pressure for 60 minutes. The reactor was vented and cooled down to room temperature to stop the reaction. The polymer was collected and dried at reduced pressure and 60 °C. The resulting polymer was subjected to xylene extraction at 25 °C according to the procedure described above. The fraction of polymer soluble in xylene at 25 °C was taken as the amount of ethylene/propylene copolymers produced in the process.

Polymer Analysis. *Intrinsic viscosity (I.V.) in decahydronaphthalene.* The I.V. in decahydronaphthalene (DHN) was determined on an Ubbelohde viscometer PVS 1 with an S 5 measuring head (both from Lauda) in decalin at 135 °C. To prepare the sample, 20 mg of polymer was dissolved in 20 ml of decalin at 135 °C over a period of 2 hours. Fifteen milliliters of the solution was placed in the viscometer; the instrument carried out a minimum of three running-out time measurements until a consistent result had been obtained. The I.V. was calculated from the running-out times according to $IV = (t/t_0 - 1) * l / c$, where t is the running-out time of the solution, t_0 is the mean of the running-out time of the solvent, and c is the concentration of the solution in g/ml.

Intrinsic viscosity (I.V.) in tetrahydronaphthalene. The measurement for ethylene/propylene copolymers were performed in tetrahydronaphthalene (THN) solution obtained by dissolving the polymer at 135 °C for 1 hour as described above.

Xylene soluble fraction at 25 °C. The polymer (2.5 g) was dissolved in 250 ml of o-xylene under stirring at 135 °C for 30 minutes, then the solution was cooled to 25 °C for 30 minutes and the insoluble polymer was filtered. The resulting solution was evaporated under flow of nitrogen, and the residue was dried and weighed to determine the percentage of soluble polymer.

Melting Temperature T_m . Calorimetric measurements were performed using a differential scanning calorimeter DSC Mettler. The instrument was calibrated with indium and tin standards. The weighted sample (5-10 mg) was sealed into aluminum pans, heated to 200 °C and maintained at that temperature for 5 minutes to allow complete melting of all the crystallites. After cooling at 20 °C/min to 0 °C and standing for 5 minutes at 0 °C, the sample was heated to 200 °C at a rate of 20 °C/min. In this second heating run, the peak temperature was assumed to be the melting temperature (T_m) and the area was the global melting enthalpy (ΔH).

Gel permeation chromatography. Gel permeation chromatography (GPC) was carried out at 145 °C in 1,2,4-trichlorobenzene using a GPC apparatus 150 °C from Waters. The data were evaluated using Win-GPC software from HS-Entwicklungsgesellschaft für wissenschaftliche Hard- und Software mbH, Ober-Hilbersheim. The calibration of the columns was carried out by means of polypropylene standards having molar masses from 100 to 107 g/mol. The mass average molar masses (M_w) and the number average molar masses (M_n) of the polymers were determined.