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[5] Fluorescence properties of representative compounds: Anthranilic acid ($\lambda_{ex} = 327$ nm; $\lambda_{em} = 392$ nm; $\Phi_f = 0.01$); ethyl anthranilate ($\lambda_{ex} = 339$ nm; $\lambda_{em} = 404$ nm; $\Phi_f = 0.11$).

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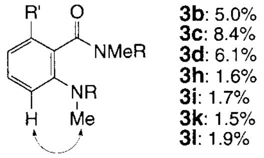
[7] The aryne precursors used in this study are readily available from the corresponding 2-halophenols or phenols. For detailed procedures, see Supporting Information.

[8] Although the reaction of benzyne (from **2a** and CsF) with a small excess of ureas in THF also gave moderate yields of products (e.g. with 2 equiv of **1a**, 20 °C, 27 h, 41 % yield of **3a**), we employed ureas as a solvent, as the yields were considerably improved.

[9] The structure of the products was determined by NOE in ^{1}H NMR spectra (Scheme 4). Furthermore, the crystal structure of **3b** was determined by an X-ray diffraction study. CCDC-185541 (**3b**)contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax: (+44)1223-336-033; or deposit@ccdc.cam.ac.uk).



Scheme 4. Determination of the structures of **3** by measuring the magnitude of the NOE denoted by the double-headed arrow.

[10] Although the regioisomeric ratio of **3e** and **3f** was elucidated to be 52:48 by ^{1}H NMR, we did not pursue the exact position of the methyl substituent of each compound, because separation of the regioisomers was difficult.

[11] 2-Amino-1-naphthamide **3l** was produced solely, regardless of the precursor (**2d** or **2e**) employed, which indicates that the reaction of an acyclic urea also proceeds through an aryne intermediate.

[12] In this reaction, 2-(dimethylcarbamoyl)phenyl triflate, which should be produced by the reaction of **1d** with the aryl anion derived from Ar-TMS and a fluoride ion, was also formed as a by-product.

[13] Because the urea oxygen atom is often considered to be more nucleophilic than the urea nitrogen atom, we cannot rule out the possibility that the reaction proceeds through other pathways, triggered by the nucleophilic addition of the urea oxygen atom to an aryne.

[14] It is well-known that electronic effects also favor nucleophilic attack at this *m*-position (see ref. [1]).

[15] The generation of 2-(dimethylcarbamoyl)phenyl triflate (see ref. [12]) may imply that the reaction of **1d** proceeds through a pathway which does not involve an aryne intermediate: The reaction of the primarily formed aryl anion (from Ar–TMS with a fluoride ion) with **1d** and subsequent aromatic nucleophilic substitution at a C–OTf moiety with an amide anion (R_2N^-). However, this pathway can be discounted, at least in the case of **1a**, because, according to this pathway, the reaction of **1a** with a 1,2-naphthalyne precursor (**2d** or **2e**) should afford the corresponding regioisomeric product. This conclusion contrasts with the results in entries 4 and 5 of Table 1.

Pyrazolate Coordination Continues To Amaze—The New μ-η^2:η^1 Binding Mode and the First Case of Unidentate Coordination to a Rare Earth Metal[**]

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Despite the recent transformations of pyrazolate coordination chemistry by the discovery of a range of new binding modes[1–4] and by extension of η^2-bonding from f-block elements[5] to early[6] and mid[7] d-block transition elements and main group metals,[8] surprising discoveries are still possible. Thus, we now report the preparation of $[Sc_2(Ph_2pz)_6]$ (**1**; Ph_2pz = 3,5-diphenylpyrazolate) with the new pyrazolate coordination mode, μ-η^2:η^1, which is intermediate between the common μ-η^1:η^1[9] and the recently reported μ-η^2:η^2[2,3a] ligation, and the first example of $\eta^1(N)$ coordination of a pyrazolate to a lanthanoid ion in $[Nd(\eta^2\text{-}Me_2pz)_2(\eta^1\text{-}Me_2pz)(Me_2pzH)_2py)]$ (**2**; Me_2pz = 3,5-dimethylpyrazolate; py = pyridine). Normally and expectedly, the large size and high Lewis acidity of Ln^{3+} favor chelation (η^2) and/or double bridging (μ-η^1:η^1, μ-η^2:η^2, μ-η^2:η^5 etc.).[2,3a,9]

Compound **1** was synthesized by the direct reaction between scandium metal and 3,5-diphenylpyrazole at 270–300 °C [Eq. (1)], and was isolated by extraction with toluene from which single crystals were obtained.

$$2\,Sc + 6\,Ph_2pzH \rightarrow [Sc_2(Ph_2pz)_6]\ (\mathbf{1}) + 3\,H_2 \qquad (1)$$

On the other hand, **2** was a minor product of the redox transmetalation/ligand exchange reaction between neodymium metal, $Hg(C_6F_5)_2$, and 3,5-dimethylpyrazole in pyridine, a reaction giving $[Nd(Me_2pz)_3(py)]$ (**3**) as the main product [Eq. (2)].

$$2\,Nd + 3\,Hg(C_6F_5)_2 + 6\ (\text{or } 8)\ Me_2pzH \xrightarrow{py} 2\,\mathbf{3}\ (\text{or } \mathbf{2}) + 6\,C_6F_5H + 3\,Hg \qquad (2)$$

A few single crystals of **2** deposited amidst bulk impure **3** and were separated for structure determination.

The structure of **1**[10a] comprises a dimer (Figure 1). Each scandium center is seven-coordinate with two terminal η^2-Ph_2pz ligands and two bridging Ph_2pz ligands, one of which ($3n$) is η^1-bonded by N(32) to Sc(1) and η^2-linked through

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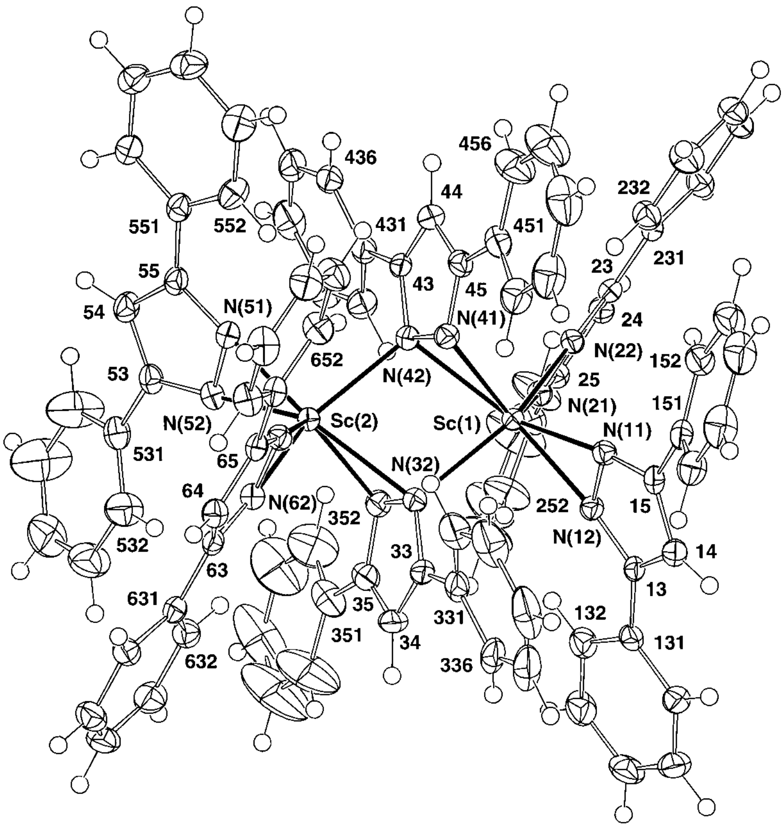

Figure 1. Projection of **1**, with the Sc···Sc vector in the page, showing the inclinations of the central planes of ligands 3 and 4. Selected bond lengths [Å] and angles [°]: Sc(1)-N(11,12,21,22,31*,32,41,42) 2.126(2), 2.116(2), 2.145(2), 2.114(2) 3.011(2), 2.250(2), 2.226(2), 2.349(2); Sc(2)-N(31,32,41*,42,51,52,61,62) 2.222(2), 2.365(2), 3.092(2), 2.271(2), 2.112(2), 2.135(2), 2.125(2), 2.128(2); Sc(1)-N(31,32,41,42)-Sc(2) 85.37(6), 102.27(7), 83.34(6), 102.14(7) Sc(1)···Sc(2)* 3.5943(6). * Nonbonding separations.

N(31,32) to Sc(2) and the other ($4n$) η^2-bonded by N(41,42) to Sc(1) and η^1-linked through N(42) to Sc(2). As the Sc(2)···N(41) and Sc(1)···N(31) separations are 0.76–0.82 Å longer than the bonding Sc(2)–N(42) and Sc(1)–N(32) distances (Figure 1), they are convincingly nonbonding, thereby establishing μ-η^2:η^1 ligation. Moreover, the nonbonding separations are greater by over 0.3 Å than the average bonding distances for the bridging ligands of eight-coordinate $[La_2(\eta^2\text{-}t\text{Bu}_2\text{pz})_4(\mu\text{-}\eta^2\text{:}\eta^2\text{-}t\text{Bu}_2\text{pz})_2]$ (**4**; tBu$_2$pz = 3,5-di-*tert*-butylpyrazolate)[3a] despite the much smaller size (ca. 0.3 Å) of Sc^{3+} than La^{3+}.[11] For each μ-η^2:η^1 ligand, the Sc–η^1(N) length lies between the two Sc–η^2(N) distances, the latter two differing by 0.12–0.15 Å, slightly more than the differences between each pair of bridging Sc(1,2)–N(n2) (n = 4,3) distances. The C_3N_2 planes of the bridging ligands are near parallel (dihedral angle 1.8(1)°) and they intersect the Sc···Sc axis at 62.69(8) and 60.96(7)° (cf. parallel with Sc···Sc for μ-η^1:η^1- or 90° for μ-η^2:η^2-ligation). Parallel stacking of ligand Ph substituent planes about $x = 0$, 0.5 is a significant lattice motif.

Although the ^{1}H NMR spectrum of **1** in C_6D_6 differs significantly from that in coordinating (and presumably bridge splitting) C_4D_8O, only one H4(pz) resonance signal was observed by contrast with two for the μ-η^2:η^2 bridged **4**.[3a] Possibly the chemical shifts of the terminal and bridging ligands overlap (difference only 0.24 ppm for **4**),[3a] but cleavage of the η^1 bridge or exchange cannot be ruled out. Two C4(pz) resonance signals are observed in the solid-state ^{13}C NMR spectrum of **1**, but the solubility in C_6D_6 was insufficient for a satisfactory spectrum.

The structure of **2** (Figure 2) features an eight-coordinate neodymium center with two η^2-Me$_2$pz, one η^1-Me$_2$pz, one η^1-py, and two η^1-Me$_2$pzH ligands. For the unidentate ligand (3n), the Nd–N(31) bond length is 0.83 Å shorter than the Nd···N(32) separation, completely excluding the latter as a bonding contact, and establishing η^1-ligation. Stronger (by ca. 0.15 Å) bonds are observed for η^2-binding than the η^1-linked Nd-N(31) which is only 0.05–0.08 Å shorter than the Nd–N(Me$_2$pzH) distances. Location of the H(-N) atoms of the Me$_2$pzH ligands provides a clear reason for noncoordination of N(32) of the η^1-bonded Me$_2$pz, as it is held in a hydrogen-bonding chelate by cisoid pyrazole hydrogen atoms H(12, 22) (Figure 2).

Overall, the structure of **1** with μ-η^2:η^1-Ph$_2$pz groups results from effective steric engineering. Seven-coordination by comparison with six-coordination in monomeric $[Sc(\eta^2\text{-}t\text{Bu}_2\text{pz})_3]$[3a] can be attributed to the lower bulkiness of Ph$_2$pz than tBu$_2$pz (e.g. tBu$_2$pz gives the eight-coordinate dimer **4**,[3a] but Ph$_2$pz gives the ten-coordinate trimer $[La_3(Ph_2pz)_9]$[12]). However, Sc^{3+} is too small to sustain eight-coordination which would result from μ-η^2:η^2 bonding, as observed for a larger metal in **4** (or the isostructural Lu ana-

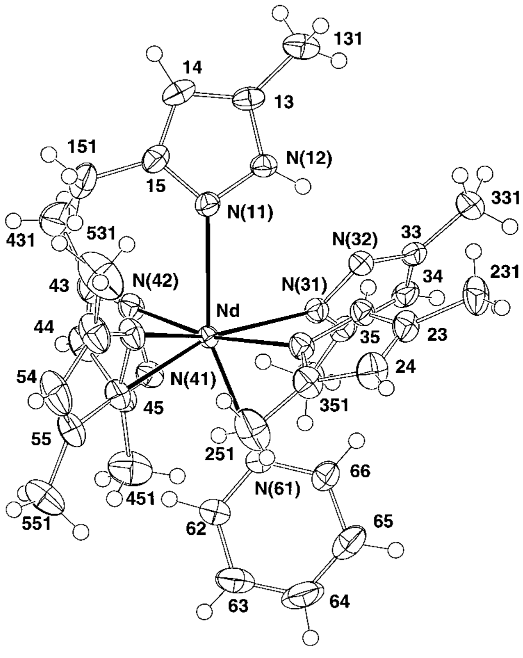

Figure 2. Projection of **2** normal to the Nd–N(11) vector. Selected bond lengths [Å] and angles [°]: Nd-N(11,21,31,32*,41,42,51,52,61) 2.621(1), 2.649(1), 2.564(1), 3.398(1), 2.412(1), 2.428(1), 2.447(1), 2.434(1), 2.626(1); N(12)-H(12) 0.88(2); N(22)-H(22) 0.85(3); N(32)···H(12,22) 1.96(2), 1.97(3); H(12)-N(32)-H(22) 88(1). * Nonbonding separations.

logue[3a]). On the other hand, the η^1-Me$_2$pz coordination of **2** is mainly a fortuitous result of a composition permitting significant hydrogen bonding to the uncoordinated nitrogen atom. This factor is far more important than the small reduction in crowding[13] caused by η^1- rather than η^2-Me$_2$pz bonding, and the sum of steric coordination numbers of the ligands[14] is not overlarge at 7.4 (or 7.6 with three η^2-Me$_2$pz groups).[15] Indeed the structure of **2** is so unusual as to confirm the normal unlikelihood of η^1-pyrazolate coordination to large Ln^{3+} ions.

Experimental Section

1: A mixture of Sc chunks (0.40 g, 8.90 mmol), Ph$_2$pzH (Lancaster) (0.66 g, 3.00 mmol), and mercury metal (two drops) was heated in a sealed tube between about 270 and 300 °C for a total of 111 h (minimum time for visual disappearance of Ph$_2$pzH). The reaction mixture was extracted twice with hot toluene (80 and 20 mL) and filtered giving a colorless solution which deposited some colorless single crystals of [Sc$_2$(Ph$_2$pz)$_6$] for the structure determination. The solution was then concentrated to 5 mL yielding large colorless crystals which were dried at 100 °C under vacuum affording [Sc$_2$(Ph$_2$pz)$_6$] (0.58 g, 83 %). M.p. (sealed tube/N$_2$): 318–321 °C (sublimation ~180 °C); IR (Nujol): $\tilde{\nu} = 1604$m, 1535m, 1422s, 1313m, 1283m, 1244m, 1164m, 1135w, 1100w, 1071m, 1020m, 985w, 965s, 952m, 910m, 814m, 803m, 757s, 686s cm^{-1}; ^{1}H NMR ([D$_8$]THF): $\delta = 7.10$–7.22 (m, 36 H; *m,p*-H(Ph)), 7.26 (s, 6 H; H-4(pz)), 7.71 ppm (dd, $^3J = 8.2$ Hz, $^4J = 1.2$ Hz, 24 H; *o*-H(Ph)); ^{1}H NMR ([D$_6$]benzene): $\delta = 6.56$ (s, 6 H; H-4(pz)), 6.89–6.92 (m, 36 H; *m,p*-H(Ph)), 7.54 ppm (d, $^3J = 7.9$ Hz, 24 H; *o*-H(Ph)); ^{13}C NMR (75.48 MHz CPMAS): $\delta = 105.4$ (s, C4; terminal-Me$_2$pz), 123.6–133.0 (complex m, *o,m,p*-Ph of terminal-/bridging-Me$_2$pz), 149.1 ppm (s, C4; bridging-Me$_2$pz), *ipso*-C unresolved; elemental analysis calcd (%) for $C_{90}H_{66}N_{12}Sc_2$ C 76.9, H 4.7, N 12.0, Sc, 6.4; found: C 76.7, H 5.0, N 12.0, Sc 6.6.

2: Neodymium metal powder (0.93 g, 6.45 mmol), Me$_2$pzH (1.08 g, 11.23 mmol), and Hg(C$_6$F$_5$)$_2$ (2.78 g, 5.20 mmol) were stirred and heated in pyridine (50 mL) at 70 °C. Filtration through a Celite pad, evaporation to about 5 mL, addition of hexane (40 mL), and standing at 30–35 °C produced a blue product containing brown impurities and some blue crystals of **2** (IR (Nujol): $\tilde{\nu} = 3289$w, 1570w, 1518vs, 1415s, 1310s, 1296s, 1242s, 1131m, 1026w, 1008m, 983w, 801w, 780w, 726w cm^{-1}), which were used for the structure determination.[10b] Addition of toluene dissolved the brown impuritiy leaving **3** as the bulk product (0.77 g, 44 %). M.p. (sealed tube/N$_2$): 213–215 (initial decomp at ca. 156 °C); IR (Nujol): $\tilde{\nu} = 1597$vs, 1513vs, 1481s (sh), 1444vs, 1417vs, 1363vs, 1351s (sh), 1333s, 1242s, 1218s, 1152s, 1096m, 1070s, 1035s, 1007vs, 961s, 809s, 778vs, 764vs, 755vs, 730vs, 696vs, 676m, 668m, 656m cm^{-1}; Vis/near IR (in PhMe λ_{max} (ε)) = 352 (10), 515 (12), 529 (5), 587 (9), 685 (33), 740 (1), 794 (11), 805 (22), 881 (14) nm; elemental analysis (%) calcd for $C_{20}H_{26}N_7Nd$: Nd 28.35; found: Nd 28.61. Deliberate syntheses of **2** have not yet succeeded.

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[10] Crystal structure analyses: Full spheres of absorption corrected data ($N_{t(otal)}$ reflections, merged to N unique (R_{int} cited), $N_o(F > 4\sigma(F))$ considered "observed"; Bruker AXS CCD instrument, monochromatic Mo$_{K\alpha}$ radiation, $\lambda = 0.71073$ Å; $T \approx 153$ K) were measured; in refinement anisotropic displacement parameter forms were refined for the non-hydrogen atoms. Conventional residuals R, R_w (weights: $(\sigma^2(F) + 0.0004\,F^2)^{-1}$) on $|F|$ at convergence are cited (neutral atom complex scattering factors). In the figures, displacement ellipsoids are shown with 50 % probability amplitude, hydrogen atoms having arbitrary radii of 0.1 Å. a) **1:** $C_{90}H_{66}N_{12}Sc_2$, $M_r = 1405.5$; monoclinic $P2_1/c$, $a = 26.637(2)$, $b = 11.5815(8)$, $c = 23.367(2)$ Å, $\beta = 91.335(2)°$, $V = 7207$ Å^3; ρ_{calcd} $(Z = 4) = 1.295$ g cm^{-3}; $N_t = 136159$, $N = 19142$ ($R_{int} = 0.067$), $N_o = 14237$ ($2\theta_{max} = 58°$); $R = 0.051$, $R_w = 0.061$ $(x, y, z, U_{iso})_H$ included as constrained estimates. b) **2:** $C_{30}H_{42}N_{11}Nd$, $M_r = 701.0$; monoclinic $P2_1/n$ $a = 12.3427(7)$, $b = 22.647(1)$, $c = 12.7239(7)$ Å, $\beta = 102.630(1)°$, $V = 3471$ Å^3; ρ_{calcd} $(Z = 4) = 1.341$ g cm^{-3}; $N_t = 71103$, $N = 18265$ ($R_{int} = 0.029$), $N_o = 14360$ ($2\theta_{max} = 75°$); $R = 0.026$, $R_w = 0.033$. $(x, y, z, U_{iso})_H$ refined. CCDC-184620 (**1**) and CCDC-184621 (**2**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax: (+44)1223-336-033; or deposit@ccdc.cam.ac.uk).

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[15] Asymmetry (ca. 0.20 Å) of η^2-*t*Bu$_2$pz binding in [Er(*t*Bu$_2$pz)$_3$(*t*-Bu$_2$pzH)] has been attributed to steric crowding[16] but a referee suggests (retrospectively) it may be due to hydrogen bonding from the NH group of the pyrazole to the most distant η^2-*t*Bu$_2$pz nitrogen atom. Interestingly, the same paper has a theoretical study of [Y(η^1-pz)Cl$_2$(NH$_3$)$_2$] with the uncoordinated nitrogen atom H-bonded to a hydrogen atom of NH$_3$.

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