Article

**N,N-bis(2-quinolinylmethyl)benzylamine.**

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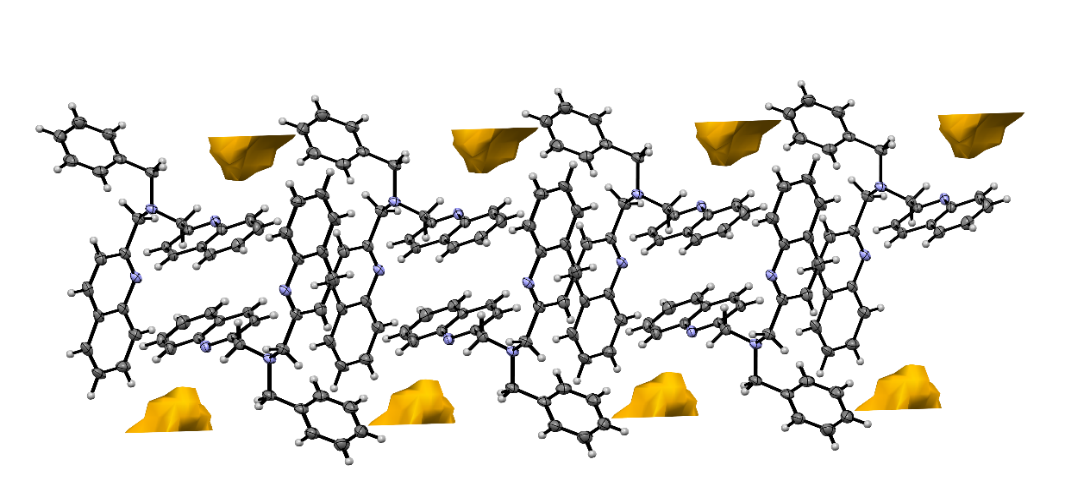
**Supplementary data**

Fig S1 1. The linear chains of the dimers of **1**, showing the exogenous voids that can include solvent molecules.

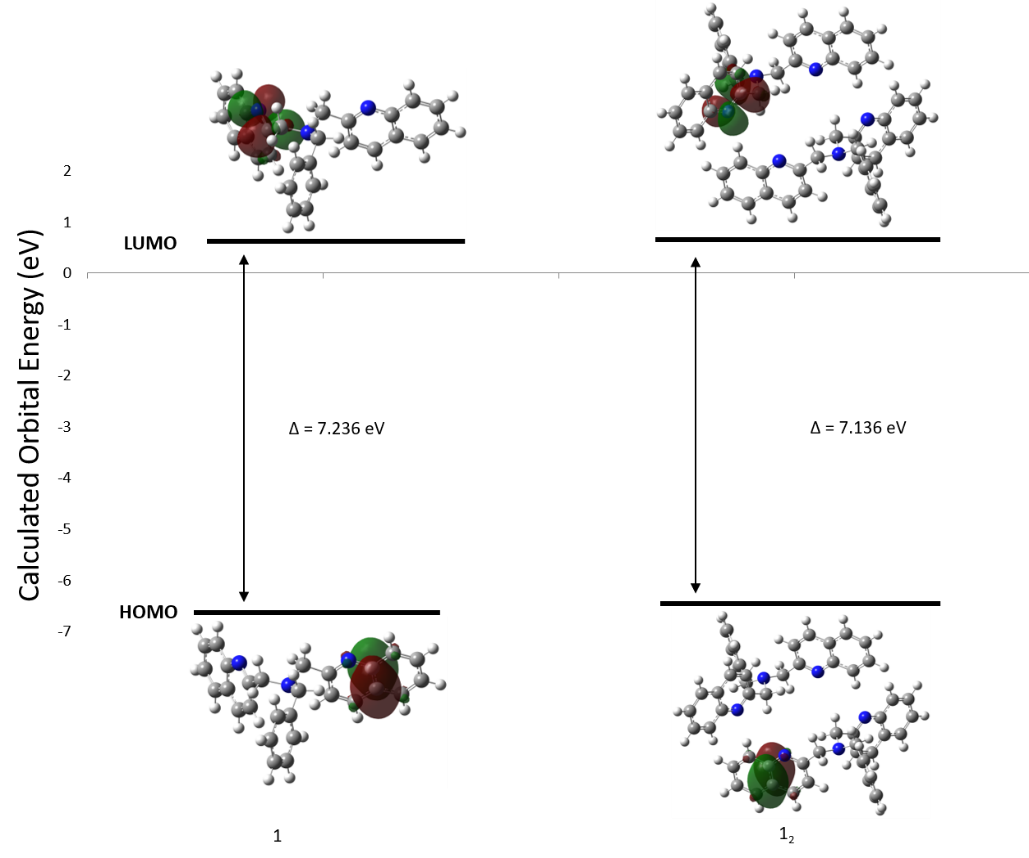


Fig. SI 2. The DFT HOMO-LUMO energy-band diagram for **1**.

Table SI 1. Atomic coordinates ( x 104) and equivalent isotropic displacement parameters (Å2x 103)

for l1\_sq (**1**). U(eq) is defined as one-third of the trace of the orthogonalized Uij tensor.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

N(1) 1275(1) 5529(1) 2873(1) 21(1)

C(1) 5772(2) 7548(2) 6655(1) 28(1)

N(2) 4883(1) 8183(1) 4699(1) 20(1)

C(2) 5579(2) 7672(2) 7727(1) 33(1)

N(3) 2765(1) 8324(1) 2385(1) 21(1)

C(3) 4251(2) 8590(2) 7944(1) 33(1)

C(4) 3148(2) 9377(2) 7093(1) 29(1)

C(5) 3304(2) 9272(1) 5977(1) 23(1)

C(6) 4643(2) 8346(1) 5760(1) 21(1)

C(7) 2188(2) 10034(1) 5057(1) 26(1)

C(8) 2434(2) 9860(1) 4018(1) 26(1)

C(9) 3820(2) 8918(1) 3870(1) 20(1)

C(10) 4073(2) 8760(1) 2701(1) 23(1)

C(11) -110(2) 5147(1) 3159(1) 21(1)

C(12) -313(2) 4070(1) 2866(1) 29(1)

C(13) -1676(2) 3661(2) 3138(1) 33(1)

C(14) -2896(2) 4302(2) 3707(1) 31(1)

C(15) -2730(2) 5345(1) 3998(1) 25(1)

C(16) -1342(2) 5794(1) 3726(1) 20(1)

C(17) -1126(2) 6885(1) 3987(1) 20(1)

C(18) 247(2) 7254(1) 3697(1) 20(1)

C(19) 1431(2) 6539(1) 3146(1) 19(1)

C(20) 2994(2) 6905(1) 2918(1) 22(1)

C(21) 2472(2) 8748(1) 1140(1) 26(1)

C(22) 1885(2) 10225(1) 643(1) 25(1)

C(23) 514(2) 10884(2) 1056(1) 30(1)

C(24) -26(2) 12241(2) 646(1) 34(1)

C(25) 795(2) 12970(2) -192(1) 38(1)

C(26) 2142(2) 12330(2) -620(1) 39(1)

C(27) 2684(2) 10967(2) -206(1) 32(1)

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\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

N(1)-C(19) 1.3165(16)

N(1)-C(11) 1.3772(17)

C(1)-C(2) 1.371(2)

C(1)-C(6) 1.411(2)

C(1)-H(1) 0.9500

N(2)-C(9) 1.3151(17)

N(2)-C(6) 1.3768(16)

C(2)-C(3) 1.408(2)

C(2)-H(2) 0.9500

N(3)-C(20) 1.4625(17)

N(3)-C(21) 1.4673(16)

N(3)-C(10) 1.4692(16)

C(3)-C(4) 1.363(2)

C(3)-H(3) 0.9500

C(4)-C(5) 1.4164(19)

C(4)-H(4) 0.9500

C(5)-C(7) 1.417(2)

C(5)-C(6) 1.4186(19)

C(7)-C(8) 1.356(2)

C(7)-H(7) 0.9500

C(8)-C(9) 1.4241(19)

C(8)-H(8) 0.9500

C(9)-C(10) 1.5082(17)

C(10)-H(10A) 0.9900

C(10)-H(10B) 0.9900

C(11)-C(12) 1.4156(18)

C(11)-C(16) 1.4166(19)

C(12)-C(13) 1.371(2)

C(12)-H(12) 0.9500

C(13)-C(14) 1.409(2)

C(13)-H(13) 0.9500

C(14)-C(15) 1.366(2)

C(14)-H(14) 0.9500

C(15)-C(16) 1.4138(19)

C(15)-H(15) 0.9500

C(16)-C(17) 1.4158(18)

C(17)-C(18) 1.3603(18)

C(17)-H(17) 0.9500

C(18)-C(19) 1.4171(18)

C(18)-H(18) 0.9500

C(19)-C(20) 1.5119(18)

C(20)-H(20A) 0.9900

C(20)-H(20B) 0.9900

C(21)-C(22) 1.508(2)

C(21)-H(21A) 0.9900

C(21)-H(21B) 0.9900

C(22)-C(27) 1.389(2)

C(22)-C(23) 1.394(2)

C(23)-C(24) 1.383(2)

C(23)-H(23) 0.9500

C(24)-C(25) 1.386(2)

C(24)-H(24) 0.9500

C(25)-C(26) 1.381(2)

C(25)-H(25) 0.9500

C(26)-C(27) 1.390(2)

C(26)-H(26) 0.9500

C(27)-H(27) 0.9500

C(19)-N(1)-C(11) 117.47(11)

C(2)-C(1)-C(6) 120.20(14)

C(2)-C(1)-H(1) 119.9

C(6)-C(1)-H(1) 119.9

C(9)-N(2)-C(6) 118.00(11)

C(1)-C(2)-C(3) 120.29(15)

C(1)-C(2)-H(2) 119.9

C(3)-C(2)-H(2) 119.9

C(20)-N(3)-C(21) 112.04(10)

C(20)-N(3)-C(10) 111.57(10)

C(21)-N(3)-C(10) 112.74(10)

C(4)-C(3)-C(2) 120.69(13)

C(4)-C(3)-H(3) 119.7

C(2)-C(3)-H(3) 119.7

C(3)-C(4)-C(5) 120.56(14)

C(3)-C(4)-H(4) 119.7

C(5)-C(4)-H(4) 119.7

C(4)-C(5)-C(7) 123.76(13)

C(4)-C(5)-C(6) 118.69(13)

C(7)-C(5)-C(6) 117.55(12)

N(2)-C(6)-C(1) 118.16(12)

N(2)-C(6)-C(5) 122.27(12)

C(1)-C(6)-C(5) 119.56(12)

C(8)-C(7)-C(5) 119.60(13)

C(8)-C(7)-H(7) 120.2

C(5)-C(7)-H(7) 120.2

C(7)-C(8)-C(9) 119.24(13)

C(7)-C(8)-H(8) 120.4

C(9)-C(8)-H(8) 120.4

N(2)-C(9)-C(8) 123.34(12)

N(2)-C(9)-C(10) 118.61(12)

C(8)-C(9)-C(10) 118.05(12)

N(3)-C(10)-C(9) 109.90(10)

N(3)-C(10)-H(10A) 109.7

C(9)-C(10)-H(10A) 109.7

N(3)-C(10)-H(10B) 109.7

C(9)-C(10)-H(10B) 109.7

H(10A)-C(10)-H(10B) 108.2

N(1)-C(11)-C(12) 118.63(12)

N(1)-C(11)-C(16) 122.62(11)

C(12)-C(11)-C(16) 118.75(12)

C(13)-C(12)-C(11) 120.25(14)

C(13)-C(12)-H(12) 119.9

C(11)-C(12)-H(12) 119.9

C(12)-C(13)-C(14) 120.84(13)

C(12)-C(13)-H(13) 119.6

C(14)-C(13)-H(13) 119.6

C(15)-C(14)-C(13) 120.09(13)

C(15)-C(14)-H(14) 120.0

C(13)-C(14)-H(14) 120.0

C(14)-C(15)-C(16) 120.43(14)

C(14)-C(15)-H(15) 119.8

C(16)-C(15)-H(15) 119.8

C(15)-C(16)-C(17) 122.67(12)

C(15)-C(16)-C(11) 119.64(12)

C(17)-C(16)-C(11) 117.69(12)

C(18)-C(17)-C(16) 119.03(12)

C(18)-C(17)-H(17) 120.5

C(16)-C(17)-H(17) 120.5

C(17)-C(18)-C(19) 119.65(12)

C(17)-C(18)-H(18) 120.2

C(19)-C(18)-H(18) 120.2

N(1)-C(19)-C(18) 123.53(12)

N(1)-C(19)-C(20) 117.97(11)

C(18)-C(19)-C(20) 118.42(11)

N(3)-C(20)-C(19) 112.01(10)

N(3)-C(20)-H(20A) 109.2

C(19)-C(20)-H(20A) 109.2

N(3)-C(20)-H(20B) 109.2

C(19)-C(20)-H(20B) 109.2

H(20A)-C(20)-H(20B) 107.9

N(3)-C(21)-C(22) 111.29(11)

N(3)-C(21)-H(21A) 109.4

C(22)-C(21)-H(21A) 109.4

N(3)-C(21)-H(21B) 109.4

C(22)-C(21)-H(21B) 109.4

H(21A)-C(21)-H(21B) 108.0

C(27)-C(22)-C(23) 118.19(14)

C(27)-C(22)-C(21) 122.11(13)

C(23)-C(22)-C(21) 119.69(12)

C(24)-C(23)-C(22) 121.13(14)

C(24)-C(23)-H(23) 119.4

C(22)-C(23)-H(23) 119.4

C(23)-C(24)-C(25) 120.02(15)

C(23)-C(24)-H(24) 120.0

C(25)-C(24)-H(24) 120.0

C(26)-C(25)-C(24) 119.54(15)

C(26)-C(25)-H(25) 120.2

C(24)-C(25)-H(25) 120.2

C(25)-C(26)-C(27) 120.33(15)

C(25)-C(26)-H(26) 119.8

C(27)-C(26)-H(26) 119.8

C(22)-C(27)-C(26) 120.78(15)

C(22)-C(27)-H(27) 119.6

C(26)-C(27)-H(27) 119.6

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Symmetry transformations used to generate equivalent atoms:

Table SI 3. Anisotropic displacement parameters (Å2x 103)for l1\_sq. The anisotropic

displacement factor exponent takes the form: -22[ h2a\*2U11 + ... + 2 h k a\* b\* U12 ]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

U11 U22 U33 U23 U13 U12

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N(1) 21(1) 20(1) 24(1) -11(1) -3(1) -2(1)

C(1) 30(1) 32(1) 25(1) -12(1) 2(1) -9(1)

N(2) 19(1) 26(1) 22(1) -13(1) 5(1) -11(1)

C(2) 44(1) 37(1) 22(1) -9(1) -1(1) -18(1)

N(3) 23(1) 26(1) 18(1) -10(1) 1(1) -12(1)

C(3) 52(1) 40(1) 21(1) -18(1) 14(1) -28(1)

C(4) 36(1) 33(1) 32(1) -22(1) 16(1) -20(1)

C(5) 26(1) 25(1) 27(1) -16(1) 10(1) -16(1)

C(6) 23(1) 24(1) 23(1) -12(1) 6(1) -14(1)

C(7) 22(1) 28(1) 38(1) -20(1) 6(1) -7(1)

C(8) 23(1) 28(1) 30(1) -13(1) -2(1) -7(1)

C(9) 19(1) 26(1) 22(1) -11(1) 4(1) -13(1)

C(10) 22(1) 32(1) 22(1) -12(1) 4(1) -14(1)

C(11) 23(1) 18(1) 22(1) -7(1) -5(1) -3(1)

C(12) 33(1) 24(1) 34(1) -15(1) -4(1) -6(1)

C(13) 43(1) 25(1) 38(1) -13(1) -6(1) -15(1)

C(14) 33(1) 31(1) 32(1) -6(1) -3(1) -18(1)

C(15) 24(1) 25(1) 25(1) -5(1) -1(1) -9(1)

C(16) 22(1) 18(1) 19(1) -4(1) -4(1) -5(1)

C(17) 20(1) 18(1) 21(1) -8(1) 2(1) -2(1)

C(18) 23(1) 17(1) 22(1) -9(1) 1(1) -6(1)

C(19) 19(1) 18(1) 18(1) -6(1) -2(1) -3(1)

C(20) 18(1) 25(1) 24(1) -12(1) 1(1) -4(1)

C(21) 32(1) 33(1) 20(1) -13(1) 2(1) -14(1)

C(22) 30(1) 33(1) 18(1) -11(1) -2(1) -14(1)

C(23) 29(1) 40(1) 22(1) -8(1) -2(1) -13(1)

C(24) 35(1) 41(1) 26(1) -14(1) -4(1) -5(1)

C(25) 57(1) 30(1) 27(1) -10(1) -4(1) -12(1)

C(26) 56(1) 39(1) 26(1) -9(1) 9(1) -24(1)

C(27) 40(1) 37(1) 22(1) -12(1) 5(1) -15(1)

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1. Kryatov, S. V. *et al.* Dioxygen binding to complexes with FeII2(μ-OH)2 cores: Steric control of

activation barrier and O2-adduct formation*. Inorg. Chem*. 2005, *44,* 85-99.

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| Identification code for 1 | l1\_sq |
| Empirical formula | C27H23N3 |
| Formula weight | 389.48 |
| Temperature | 100(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Triclinic |
| Space group | *P -1* |
| Unit cell dimensions | a = 8.7296(6) Å |
|  | b = 11.1447(6) Å |
|  | c = 12.3411(6) Å |
| Volume | 1093.45(11) Å3 |
| Z | 2 |
| Density (calculated) | 1.183 Mg/m3 |
| Absorption coefficient | 0.070 mm-1 |
| F(000) | 412 |