

Support information for

Identification of 1,3-Dialkylimidazolium Salt Supramolecular Aggregates in Solution

Crestina S. Consorti,[†] Paulo A. Z. Suarez,[†] Roberto F. de Souza,[†] Robert A. Burrow,[‡] David H.

Farrar,⁺ Alan J. Lough,⁺ Watson Loh,[&] Luis H. M. da Silva,[&] and Jairton Dupont,^{†,}*

Laboratory of Molecular Catalysis, Institute of Chemistry, UFRGS, Av. Bento Gonçalves, 9500

Porto Alegre 91501-970 RS Brazil. Departamento de Química, UFSM, Santa Maria, RS, Brazil.

Department of Chemistry, University of Toronto, Canada. Instituto de Química, UNICAMP, CP

16154 Campinas 13083-970 SP, Brazil

1. CRYSTAL DATA FOR 1,3-DI-R-(+)-METHYL BENZYLIMIDAZOLIUM TETRAFLUOROBORATE ([DMBI]BF₄)

Table 1. Crystal data and structure refinement for [DMBI]BF₄.

| | | |
|----------------------|-----------------|--------------|
| Identification code | k99280 | |
| Empirical formula | C19 H21 B F4 N2 | |
| Formula weight | 364.19 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71069 Å | |
| Crystal system | Orthorhombic | |
| Space group | P 21 21 21 | |
| Unit cell dimensions | a = 10.721(5) Å | α = 90.000°. |
| | b = 10.854(5) Å | β = 90.000°. |
| | c = 15.484(5) Å | γ = 90.000°. |

| | |
|-----------------------------------|---|
| Volume | 1801.8(13) Å ³ |
| Z | 4 |
| Density (calculated) | 1.343 Mg/m ³ |
| Absorption coefficient | 0.107 mm ⁻¹ |
| F(000) | 760 |
| Crystal size | 0.30 x 0.30 x 0.25 mm ³ |
| Theta range for data collection | 2.63 to 27.49°. |
| Index ranges | 0<=h<=13, 0<=k<=14, 0<=l<=20 |
| Reflections collected | 2345 |
| Independent reflections | 2345 [R(int) = 0.0000] |
| Completeness to theta = 27.49° | 99.5 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9737 and 0.9685 |
| Refinement method | Full-matrix least-squares on F ² |
| Data / restraints / parameters | 2345 / 0 / 238 |
| Goodness-of-fit on F ² | 1.042 |
| Final R indices [I>2sigma(I)] | R1 = 0.0464, wR2 = 0.1166 |
| R indices (all data) | R1 = 0.0530, wR2 = 0.1210 |
| Absolute structure parameter | 0.2(13) |
| Extinction coefficient | 0.010(2) |
| Largest diff. peak and hole | 0.569 and -0.471 e.Å ⁻³ |

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

| | x | y | z | U(eq) |
|-------|---------|----------|----------|--------|
| N(1) | 4544(2) | 353(2) | 2071(1) | 25(1) |
| C(2) | 3437(2) | 56(2) | 1733(2) | 26(1) |
| N(3) | 3554(2) | -43(2) | 880(1) | 25(1) |
| C(4) | 4779(2) | 188(3) | 668(2) | 30(1) |
| C(5) | 5392(2) | 447(3) | 1404(2) | 30(1) |
| C(6) | 4761(2) | 618(2) | 3003(2) | 26(1) |
| C(7) | 4898(3) | 2011(2) | 3127(2) | 36(1) |
| C(8) | 5855(2) | -123(2) | 3339(2) | 26(1) |
| C(9) | 7087(2) | 207(3) | 3159(2) | 31(1) |
| C(10) | 8071(3) | -496(3) | 3475(2) | 38(1) |
| C(11) | 7832(3) | -1507(3) | 3997(2) | 42(1) |
| C(12) | 6623(3) | -1821(3) | 4194(2) | 40(1) |
| C(13) | 5633(3) | -1145(2) | 3863(2) | 32(1) |
| C(14) | 2547(2) | -280(2) | 226(2) | 28(1) |
| C(15) | 1274(2) | -280(3) | 662(2) | 35(1) |
| C(16) | 2840(2) | -1445(2) | -266(2) | 27(1) |
| C(17) | 2609(3) | -2613(3) | 79(2) | 36(1) |
| C(18) | 2903(3) | -3658(3) | -392(2) | 40(1) |
| C(19) | 3419(3) | -3566(3) | -1203(2) | 40(1) |
| C(20) | 3656(3) | -2413(3) | -1550(2) | 40(1) |
| C(21) | 3375(3) | -1366(3) | -1083(2) | 33(1) |
| B(1) | 1512(3) | -2209(3) | 3345(2) | 35(1) |
| F(1) | 814(2) | -1659(2) | 3980(1) | 50(1) |
| F(2) | 1105(4) | -3373(2) | 3230(2) | 113(1) |
| F(3) | 1347(3) | -1556(3) | 2600(2) | 106(1) |
| F(4) | 2732(2) | -2120(4) | 3556(2) | 115(1) |

Table 3. Bond lengths [Å] and angles [°].

| | | | |
|----------------|----------|-------------------|----------|
| N(1)-C(2) | 1.336(3) | C(2)-N(3)-C(4) | 108.2(2) |
| N(1)-C(5) | 1.380(3) | C(2)-N(3)-C(14) | 127.9(2) |
| N(1)-C(6) | 1.490(3) | C(4)-N(3)-C(14) | 123.8(2) |
| C(2)-N(3) | 1.331(3) | C(5)-C(4)-N(3) | 107.5(2) |
| N(3)-C(4) | 1.377(3) | C(4)-C(5)-N(1) | 107.3(2) |
| N(3)-C(14) | 1.502(3) | N(1)-C(6)-C(8) | 110.6(2) |
| C(4)-C(5) | 1.345(4) | N(1)-C(6)-C(7) | 109.1(2) |
| C(6)-C(8) | 1.514(4) | C(8)-C(6)-C(7) | 114.0(2) |
| C(6)-C(7) | 1.531(4) | C(13)-C(8)-C(9) | 118.8(2) |
| C(8)-C(13) | 1.395(4) | C(13)-C(8)-C(6) | 119.3(2) |
| C(8)-C(9) | 1.396(3) | C(9)-C(8)-C(6) | 121.8(2) |
| C(9)-C(10) | 1.391(4) | C(10)-C(9)-C(8) | 120.4(3) |
| C(10)-C(11) | 1.388(5) | C(11)-C(10)-C(9) | 119.9(3) |
| C(11)-C(12) | 1.373(5) | C(12)-C(11)-C(10) | 119.9(3) |
| C(12)-C(13) | 1.388(4) | C(11)-C(12)-C(13) | 120.6(3) |
| C(14)-C(16) | 1.510(4) | C(12)-C(13)-C(8) | 120.3(3) |
| C(14)-C(15) | 1.522(4) | N(3)-C(14)-C(16) | 109.5(2) |
| C(16)-C(21) | 1.391(4) | N(3)-C(14)-C(15) | 110.2(2) |
| C(16)-C(17) | 1.398(4) | C(16)-C(14)-C(15) | 114.2(2) |
| C(17)-C(18) | 1.384(4) | C(21)-C(16)-C(17) | 118.5(3) |
| C(18)-C(19) | 1.377(5) | C(21)-C(16)-C(14) | 119.6(2) |
| C(19)-C(20) | 1.385(4) | C(17)-C(16)-C(14) | 121.9(2) |
| C(20)-C(21) | 1.380(4) | C(18)-C(17)-C(16) | 120.1(3) |
| B(1)-F(2) | 1.349(4) | C(19)-C(18)-C(17) | 120.8(3) |
| B(1)-F(4) | 1.352(4) | C(18)-C(19)-C(20) | 119.5(3) |
| B(1)-F(3) | 1.365(4) | C(21)-C(20)-C(19) | 120.0(3) |
| B(1)-F(1) | 1.374(3) | C(20)-C(21)-C(16) | 121.0(3) |
| | | F(2)-B(1)-F(4) | 114.3(4) |
| C(2)-N(1)-C(5) | 108.0(2) | F(2)-B(1)-F(3) | 109.5(3) |
| C(2)-N(1)-C(6) | 124.4(2) | F(4)-B(1)-F(3) | 107.1(3) |
| C(5)-N(1)-C(6) | 127.4(2) | F(2)-B(1)-F(1) | 109.0(3) |
| N(3)-C(2)-N(1) | 108.9(2) | F(4)-B(1)-F(1) | 108.9(3) |
| | | F(3)-B(1)-F(1) | 108.0(3) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k99123. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

| | U ¹¹ | U ²² | U ³³ | U ²³ | U ¹³ | U ¹² |
|------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| N(1) | 24(1) | 27(1) | 24(1) | 0(1) | 1(1) | 0(1) |
| C(2) | 25(1) | 29(1) | 25(1) | 0(1) | 2(1) | -1(1) |
| N(3) | 25(1) | 26(1) | 25(1) | 1(1) | -1(1) | 0(1) |

| | | | | | | |
|-------|--------|--------|--------|--------|--------|--------|
| C(4) | 26(1) | 38(1) | 26(1) | 2(1) | 5(1) | 1(1) |
| C(5) | 24(1) | 39(1) | 28(1) | 2(1) | 3(1) | -1(1) |
| C(6) | 26(1) | 29(1) | 24(1) | -2(1) | 2(1) | -1(1) |
| C(7) | 42(2) | 31(1) | 35(1) | -6(1) | -3(1) | 4(1) |
| C(8) | 30(1) | 28(1) | 21(1) | -4(1) | 1(1) | -1(1) |
| C(9) | 30(1) | 37(1) | 26(1) | 0(1) | -1(1) | -2(1) |
| C(10) | 31(1) | 52(2) | 31(1) | -6(1) | -5(1) | 4(1) |
| C(11) | 48(2) | 37(2) | 40(2) | -5(1) | -14(1) | 11(1) |
| C(12) | 58(2) | 26(1) | 35(1) | 0(1) | -7(1) | 2(1) |
| C(13) | 38(1) | 29(1) | 28(1) | -1(1) | -1(1) | -6(1) |
| C(14) | 26(1) | 32(1) | 27(1) | 5(1) | -3(1) | 0(1) |
| C(15) | 25(1) | 47(2) | 34(1) | 3(1) | -3(1) | 3(1) |
| C(16) | 24(1) | 31(1) | 28(1) | 3(1) | -6(1) | -1(1) |
| C(17) | 40(2) | 36(1) | 32(1) | 5(1) | -8(1) | -3(1) |
| C(18) | 43(2) | 28(1) | 48(2) | 3(1) | -18(1) | -2(1) |
| C(19) | 38(2) | 37(2) | 45(2) | -11(1) | -13(1) | 7(1) |
| C(20) | 39(2) | 43(2) | 38(2) | -6(1) | -3(1) | 2(1) |
| C(21) | 32(1) | 33(1) | 34(1) | 2(1) | 0(1) | -1(1) |
| B(1) | 38(2) | 37(2) | 30(2) | -3(1) | 7(1) | 1(1) |
| F(1) | 46(1) | 49(1) | 54(1) | -14(1) | 10(1) | 7(1) |
| F(2) | 177(3) | 39(1) | 123(2) | -27(1) | 86(2) | -29(2) |
| F(3) | 126(2) | 145(3) | 46(1) | 38(2) | -12(1) | -64(2) |
| F(4) | 31(1) | 181(3) | 133(3) | -33(3) | -9(1) | 30(2) |

2. CRYSTAL DATA FOR 1,3-DI-R-(+)-METHYL BENZYLIMIDAZOLIUM HEXAFLUOROPHOSPHATE ([DMBI]PF₆)

Table 5. Crystal data and structure refinement for [DMBI]PF₆.

| | | |
|-----------------------------------|---|----------|
| Identification code | k9999 | |
| Empirical formula | C ₁₉ H ₂₁ F ₆ N ₂ P | |
| Formula weight | 422.35 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Orthorhombic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 10.2149(5) Å | α = 90°. |
| | b = 12.5025(4) Å | β = 90°. |
| | c = 15.0057(6) Å | γ = 90°. |
| Volume | 1916.40(14) Å ³ | |
| Z | 4 | |
| Density (calculated) | 1.464 Mg/m ³ | |
| Absorption coefficient | 0.207 mm ⁻¹ | |
| F(000) | 872 | |
| Crystal size | 0.20 x 0.10 x 0.05 mm ³ | |
| Theta range for data collection | 4.21 to 27.49°. | |
| Index ranges | -13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -19 ≤ l ≤ 19 | |
| Reflections collected | 4379 | |
| Independent reflections | 4379 [R(int) = 0.0000] | |
| Absorption correction | Semi-empirical from equivalents | |
| Refinement method | Full-matrix least-squares on F ² | |
| Data / restraints / parameters | 4379 / 0 / 257 | |
| Goodness-of-fit on F ² | 0.883 | |
| Final R indices [I > 2σ(I)] | R1 = 0.0434, wR2 = 0.0736 | |
| R indices (all data) | R1 = 0.0897, wR2 = 0.0818 | |
| Absolute structure parameter | 0.16(11) | |
| Extinction coefficient | 0.0049(7) | |
| Largest diff. peak and hole | 0.210 and -0.192 e.Å ⁻³ | |

Table 6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|---------|-------|
| C(1) | 1515(3) | 3864(2) | 5039(2) | 27(1) |
| N(2) | 2281(2) | 4725(1) | 5056(1) | 25(1) |
| C(3) | 3120(3) | 4684(2) | 4343(2) | 27(1) |
| C(4) | 2847(3) | 3772(2) | 3898(2) | 26(1) |
| N(5) | 1846(2) | 3268(1) | 4338(1) | 24(1) |
| C(10) | 2158(3) | 5623(2) | 5705(2) | 25(1) |
| C(11) | 3410(3) | 5732(2) | 6250(2) | 25(1) |
| C(12) | 4425(3) | 6410(2) | 5996(2) | 34(1) |
| C(13) | 5541(3) | 6486(2) | 6509(2) | 37(1) |
| C(14) | 5671(3) | 5884(2) | 7273(2) | 37(1) |
| C(15) | 4672(3) | 5207(2) | 7531(2) | 37(1) |
| C(16) | 3541(3) | 5136(2) | 7024(2) | 33(1) |
| C(17) | 1746(3) | 6623(2) | 5195(2) | 31(1) |
| C(20) | 1221(3) | 2233(2) | 4060(2) | 29(1) |
| C(21) | 1871(3) | 1293(2) | 4533(2) | 26(1) |
| C(22) | 2733(3) | 641(2) | 4069(2) | 33(1) |
| C(23) | 3295(3) | -236(2) | 4481(2) | 38(1) |
| C(24) | 2993(3) | -479(2) | 5355(2) | 40(1) |
| C(25) | 2129(3) | 164(2) | 5818(2) | 35(1) |
| C(26) | 1581(3) | 1048(2) | 5413(2) | 30(1) |
| C(27) | -249(3) | 2295(2) | 4195(2) | 36(1) |
| P | 323(1) | 2905(1) | 7701(1) | 27(1) |
| F(1) | 577(2) | 2928(1) | 8752(1) | 44(1) |
| F(2) | 201(2) | 1632(1) | 7727(1) | 42(1) |
| F(3) | -1221(1) | 2995(1) | 7863(1) | 36(1) |
| F(4) | 56(1) | 2887(1) | 6642(1) | 34(1) |
| F(5) | 428(2) | 4180(1) | 7662(1) | 37(1) |
| F(6) | 1856(2) | 2811(1) | 7522(1) | 45(1) |

Table 7. Bond lengths [Å] and angles [°].

| | | | |
|-----------------|------------|-------------------|-----------|
| | | C(4)-C(3)-N(2) | 106.7(2) |
| C(1)-N(2) | 1.331(3) | C(3)-C(4)-N(5) | 107.8(2) |
| C(1)-N(5) | 1.333(3) | C(1)-N(5)-C(4) | 108.2(2) |
| N(2)-C(3) | 1.372(3) | C(1)-N(5)-C(20) | 126.3(2) |
| N(2)-C(10) | 1.492(3) | C(4)-N(5)-C(20) | 125.5(2) |
| C(3)-C(4) | 1.350(3) | N(2)-C(10)-C(17) | 108.2(2) |
| C(4)-N(5) | 1.370(3) | N(2)-C(10)-C(11) | 110.3(2) |
| N(5)-C(20) | 1.501(3) | C(17)-C(10)-C(11) | 115.3(2) |
| C(10)-C(17) | 1.525(3) | C(16)-C(11)-C(12) | 119.0(3) |
| C(10)-C(11) | 1.525(4) | C(16)-C(11)-C(10) | 118.9(2) |
| C(11)-C(16) | 1.386(3) | C(12)-C(11)-C(10) | 122.2(2) |
| C(11)-C(12) | 1.392(4) | C(13)-C(12)-C(11) | 120.3(2) |
| C(12)-C(13) | 1.379(4) | C(14)-C(13)-C(12) | 120.4(3) |
| C(13)-C(14) | 1.378(3) | C(13)-C(14)-C(15) | 119.8(3) |
| C(14)-C(15) | 1.381(4) | C(14)-C(15)-C(16) | 120.1(2) |
| C(15)-C(16) | 1.386(4) | C(15)-C(16)-C(11) | 120.4(2) |
| C(20)-C(27) | 1.517(4) | N(5)-C(20)-C(27) | 109.9(2) |
| C(20)-C(21) | 1.525(3) | N(5)-C(20)-C(21) | 110.5(2) |
| C(21)-C(22) | 1.387(3) | C(27)-C(20)-C(21) | 114.1(2) |
| C(21)-C(26) | 1.389(3) | C(22)-C(21)-C(26) | 118.9(2) |
| C(22)-C(23) | 1.384(3) | C(22)-C(21)-C(20) | 119.7(2) |
| C(23)-C(24) | 1.381(4) | C(26)-C(21)-C(20) | 121.3(2) |
| C(24)-C(25) | 1.382(4) | C(23)-C(22)-C(21) | 120.3(3) |
| C(25)-C(26) | 1.379(3) | C(24)-C(23)-C(22) | 120.4(3) |
| P-F(6) | 1.593(2) | C(23)-C(24)-C(25) | 119.5(3) |
| P-F(2) | 1.5975(14) | C(26)-C(25)-C(24) | 120.3(3) |
| P-F(1) | 1.5981(14) | C(25)-C(26)-C(21) | 120.6(3) |
| P-F(5) | 1.5983(14) | F(6)-P-F(2) | 90.40(9) |
| P-F(3) | 1.599(2) | F(6)-P-F(1) | 90.48(9) |
| P-F(4) | 1.6120(15) | F(2)-P-F(1) | 90.36(8) |
| N(2)-C(1)-N(5) | 108.5(2) | F(6)-P-F(5) | 90.08(9) |
| C(1)-N(2)-C(3) | 108.8(2) | F(2)-P-F(5) | 179.05(9) |
| C(1)-N(2)-C(10) | 124.8(2) | F(1)-P-F(5) | 90.45(8) |
| C(3)-N(2)-C(10) | 126.2(2) | F(6)-P-F(3) | 178.99(9) |

| | | | |
|-------------|----------|-------------|------------|
| F(2)-P-F(3) | 89.37(9) | F(2)-P-F(4) | 89.80(8) |
| F(1)-P-F(3) | 90.50(9) | F(1)-P-F(4) | 179.55(10) |
| F(5)-P-F(3) | 90.13(9) | F(5)-P-F(4) | 89.39(8) |
| F(6)-P-F(4) | 89.94(8) | F(3)-P-F(4) | 89.08(8) |

Symmetry transformations used to generate equivalent atoms:

Table 8. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k9999. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

| | U ¹¹ | U ²² | U ³³ | U ²³ | U ¹³ | U ¹² |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| C(1) | 26(2) | 26(1) | 27(1) | 3(1) | 1(1) | -4(1) |
| N(2) | 24(1) | 25(1) | 25(1) | 1(1) | 0(1) | 1(1) |
| C(3) | 23(2) | 26(1) | 31(2) | 2(1) | 2(1) | -2(1) |
| C(4) | 25(2) | 27(1) | 26(1) | 4(1) | 6(1) | 4(1) |
| N(5) | 23(1) | 23(1) | 27(1) | -1(1) | 0(1) | -1(1) |
| C(10) | 25(2) | 23(1) | 29(1) | -2(1) | 6(1) | -1(1) |
| C(11) | 25(2) | 25(1) | 27(1) | -5(1) | 5(1) | 0(1) |
| C(12) | 35(2) | 34(1) | 33(1) | 4(1) | -2(1) | -3(1) |
| C(13) | 29(2) | 42(2) | 40(2) | 0(1) | 0(1) | -8(1) |
| C(14) | 31(2) | 48(2) | 32(2) | -9(1) | -3(1) | 5(1) |
| C(15) | 42(2) | 41(2) | 28(1) | 2(1) | -1(2) | 5(2) |
| C(16) | 34(2) | 33(1) | 33(2) | 1(1) | 5(1) | -5(1) |
| C(17) | 28(2) | 28(1) | 39(2) | -3(1) | 2(1) | 1(1) |
| C(20) | 33(2) | 27(1) | 25(1) | -5(1) | 1(1) | -8(1) |
| C(21) | 23(2) | 22(1) | 33(1) | -3(1) | 0(1) | -4(1) |
| C(22) | 32(2) | 30(1) | 37(2) | -7(1) | 8(1) | -8(1) |
| C(23) | 29(2) | 31(1) | 55(2) | -13(1) | 4(2) | 1(1) |
| C(24) | 34(2) | 24(1) | 62(2) | 1(1) | -9(2) | -2(1) |
| C(25) | 33(2) | 34(1) | 38(2) | 2(1) | -5(1) | -10(1) |
| C(26) | 29(2) | 30(1) | 30(2) | -2(1) | 0(1) | -1(1) |
| C(27) | 33(2) | 31(1) | 45(2) | 4(1) | -8(1) | -6(1) |
| P | 27(1) | 26(1) | 26(1) | 1(1) | -1(1) | -3(1) |
| F(1) | 50(1) | 53(1) | 27(1) | 2(1) | -12(1) | -15(1) |

| | | | | | | |
|------|-------|-------|-------|------|--------|-------|
| F(2) | 55(1) | 27(1) | 45(1) | 6(1) | -12(1) | -6(1) |
| F(3) | 23(1) | 52(1) | 33(1) | 2(1) | 5(1) | -4(1) |
| F(4) | 42(1) | 37(1) | 23(1) | 1(1) | 5(1) | 1(1) |
| F(5) | 41(1) | 25(1) | 46(1) | 0(1) | -2(1) | -4(1) |
| F(6) | 23(1) | 47(1) | 64(1) | 9(1) | -1(1) | 4(1) |

Table 9. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$).

| | x | y | z | U(eq) |
|--------|----------|----------|---------|-------|
| H(1A) | 845(3) | 3702(2) | 5456(2) | 32 |
| H(3A) | 3768(3) | 5198(2) | 4191(2) | 32 |
| H(4A) | 3273(3) | 3524(2) | 3375(2) | 31 |
| H(10A) | 1433(3) | 5439(2) | 6126(2) | 30 |
| H(12A) | 4348(3) | 6822(2) | 5467(2) | 41 |
| H(13A) | 6225(3) | 6957(2) | 6334(2) | 44 |
| H(14A) | 6446(3) | 5933(2) | 7621(2) | 45 |
| H(15A) | 4760(3) | 4790(2) | 8056(2) | 44 |
| H(16A) | 2852(3) | 4677(2) | 7208(2) | 40 |
| H(17A) | 922(8) | 6485(4) | 4881(8) | 47 |
| H(17B) | 2427(7) | 6812(7) | 4763(7) | 47 |
| H(17C) | 1624(15) | 7216(4) | 5614(2) | 47 |
| H(20A) | 1381(3) | 2144(2) | 3407(2) | 34 |
| H(22A) | 2939(3) | 798(2) | 3465(2) | 40 |
| H(23A) | 3891(3) | -674(2) | 4161(2) | 46 |
| H(24A) | 3376(3) | -1084(2) | 5635(2) | 48 |
| H(25A) | 1911(3) | -2(2) | 6417(2) | 42 |
| H(26A) | 999(3) | 1493(2) | 5740(2) | 36 |
| H(27A) | -600(3) | 2905(7) | 3861(8) | 55 |
| H(27B) | -441(3) | 2387(11) | 4830(2) | 55 |
| H(27C) | -656(3) | 1634(5) | 3981(9) | 55 |

3. CRYSTAL DATA FOR 1,3-DI-R-(+)-METHYL BENZYLIMIDAZOLIUM TETRAPHENYLBORATE ([DMBI]BPh₄)

Table 10. Crystal data and structure refinement for [DMBI]BPh₄

| | | |
|-----------------------------------|---|-----------------|
| Identification code | k99128 | |
| Empirical formula | C ₄₃ H ₄₁ BN ₂ | |
| Formula weight | 596.59 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21 | |
| Unit cell dimensions | a = 8.484(5) Å | α = 90°. |
| | b = 19.347(5) Å | β = 90.506(5)°. |
| | c = 19.586(5) Å | γ = 90°. |
| Volume | 3215(2) Å ³ | |
| Z | 4 | |
| Density (calculated) | 1.233 Mg/m ³ | |
| Absorption coefficient | 0.070 mm ⁻¹ | |
| F(000) | 1272 | |
| Theta range for data collection | 2.96 to 26.35°. | |
| Index ranges | 0 ≤ h ≤ 10, 0 ≤ k ≤ 23, -23 ≤ l ≤ 23 | |
| Reflections collected | 6087 | |
| Independent reflections | 6087 [R(int) = 0.0000] | |
| Completeness to theta = 26.35° | 89.9 % | |
| Refinement method | Full-matrix least-squares on F ² | |
| Data / restraints / parameters | 6087 / 1 / 834 | |
| Goodness-of-fit on F ² | 1.032 | |
| Final R indices [I > 2σ(I)] | R1 = 0.0461, wR2 = 0.1036 | |
| R indices (all data) | R1 = 0.0692, wR2 = 0.1112 | |
| Absolute structure parameter | -3(3) | |
| Extinction coefficient | 0.0125(12) | |
| Largest diff. peak and hole | 0.208 and -0.207 e.Å ⁻³ | |

Table 11. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k99128 - DMBI-BPh4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|----------|-------|
| C(11) | 9078(4) | 3034(2) | 9895(2) | 25(1) |
| N(12) | 9951(4) | 2922(2) | 10437(2) | 25(1) |
| C(13) | 10486(5) | 2261(2) | 10396(2) | 37(1) |
| C(14) | 9914(5) | 1972(2) | 9824(2) | 36(1) |
| N(15) | 9020(4) | 2465(2) | 9515(2) | 25(1) |
| C(30) | 8208(4) | 2421(2) | 8843(2) | 26(1) |
| C(31) | 8853(4) | 2946(2) | 8356(2) | 25(1) |
| C(32) | 10257(4) | 2850(2) | 8058(2) | 30(1) |
| C(33) | 10840(5) | 3344(2) | 7619(2) | 34(1) |
| C(34) | 10040(5) | 3937(2) | 7482(2) | 33(1) |
| C(35) | 8644(5) | 4036(2) | 7771(2) | 34(1) |
| C(36) | 8048(5) | 3545(2) | 8210(2) | 30(1) |
| C(37) | 8227(5) | 1686(2) | 8576(2) | 32(1) |
| C(40) | 10225(5) | 3447(2) | 10985(2) | 26(1) |
| C(41) | 9224(4) | 3307(2) | 11595(2) | 25(1) |
| C(42) | 8029(4) | 3750(2) | 11719(2) | 27(1) |
| C(43) | 7124(5) | 3656(2) | 12289(2) | 33(1) |
| C(44) | 7399(5) | 3124(2) | 12736(2) | 37(1) |
| C(45) | 8550(6) | 2665(2) | 12601(2) | 43(1) |
| C(46) | 9465(5) | 2759(2) | 12039(2) | 36(1) |
| C(47) | 11898(5) | 3467(2) | 11157(2) | 36(1) |
| C(21) | 9111(4) | 973(2) | 5094(2) | 26(1) |
| N(22) | 9759(4) | 1100(2) | 4495(2) | 24(1) |
| C(23) | 9869(5) | 1805(2) | 4423(2) | 35(1) |
| C(24) | 9264(5) | 2098(2) | 4987(2) | 33(1) |
| N(25) | 8793(3) | 1565(2) | 5408(2) | 24(1) |
| C(50) | 10311(4) | 574(2) | 4016(2) | 26(1) |
| C(51) | 9549(4) | 664(2) | 3325(2) | 24(1) |
| C(52) | 8018(4) | 525(2) | 3266(2) | 34(1) |
| C(53) | 7282(5) | 561(2) | 2640(2) | 38(1) |
| C(54) | 8067(5) | 736(2) | 2062(2) | 36(1) |

| | | | | |
|--------|----------|---------|----------|-------|
| C(55) | 9608(5) | 877(2) | 2116(2) | 34(1) |
| C(56) | 10329(5) | 840(2) | 2743(2) | 30(1) |
| C(57) | 12024(5) | 580(2) | 4017(2) | 38(1) |
| C(60) | 8070(4) | 1609(2) | 6090(2) | 28(1) |
| C(61) | 8967(4) | 1146(2) | 6576(2) | 24(1) |
| C(62) | 10399(5) | 1340(2) | 6797(2) | 35(1) |
| C(63) | 11196(6) | 923(3) | 7231(2) | 51(1) |
| C(64) | 10591(7) | 307(3) | 7448(2) | 55(2) |
| C(65) | 9169(7) | 100(3) | 7234(2) | 54(1) |
| C(66) | 8360(5) | 530(2) | 6791(2) | 36(1) |
| C(67) | 7977(5) | 2348(2) | 6327(2) | 36(1) |
| B(1) | 6201(5) | 5276(2) | 10002(2) | 22(1) |
| C(111) | 5633(4) | 5487(2) | 10768(2) | 22(1) |
| C(112) | 4874(4) | 5050(2) | 11225(2) | 26(1) |
| C(113) | 4537(4) | 5253(2) | 11887(2) | 28(1) |
| C(114) | 4923(4) | 5900(2) | 12124(2) | 27(1) |
| C(115) | 5624(4) | 6352(2) | 11686(2) | 28(1) |
| C(116) | 5966(4) | 6149(2) | 11026(2) | 24(1) |
| C(121) | 5793(4) | 5928(2) | 9484(2) | 24(1) |
| C(122) | 4424(5) | 6290(2) | 9547(2) | 28(1) |
| C(123) | 3979(5) | 6817(2) | 9103(2) | 35(1) |
| C(124) | 4886(5) | 6996(2) | 8564(2) | 38(1) |
| C(125) | 6229(5) | 6645(2) | 8479(2) | 40(1) |
| C(126) | 6667(5) | 6123(2) | 8932(2) | 31(1) |
| C(131) | 5425(4) | 4571(2) | 9684(2) | 21(1) |
| C(132) | 4594(4) | 4560(2) | 9070(2) | 26(1) |
| C(133) | 3945(4) | 3965(2) | 8805(2) | 29(1) |
| C(134) | 4080(4) | 3340(2) | 9147(2) | 30(1) |
| C(135) | 4912(5) | 3320(2) | 9750(2) | 30(1) |
| C(136) | 5569(4) | 3929(2) | 10002(2) | 25(1) |
| C(141) | 8050(4) | 5140(2) | 10034(2) | 21(1) |
| C(142) | 8805(4) | 4862(2) | 9470(2) | 26(1) |
| C(143) | 10361(4) | 4747(2) | 9464(2) | 31(1) |
| C(144) | 11232(4) | 4903(2) | 10027(2) | 28(1) |
| C(145) | 10543(4) | 5154(2) | 10600(2) | 24(1) |
| C(146) | 8977(4) | 5275(2) | 10601(2) | 22(1) |

| | | | | |
|--------|----------|----------|---------|-------|
| B(2) | 6563(5) | 8652(2) | 5087(2) | 21(1) |
| C(211) | 6243(4) | 8012(2) | 5618(2) | 23(1) |
| C(212) | 4917(5) | 7612(2) | 5564(2) | 27(1) |
| C(213) | 4523(5) | 7109(2) | 6035(2) | 30(1) |
| C(214) | 5451(5) | 6985(2) | 6601(2) | 32(1) |
| C(215) | 6763(5) | 7367(2) | 6673(2) | 33(1) |
| C(216) | 7141(4) | 7860(2) | 6193(2) | 28(1) |
| C(221) | 5747(4) | 9355(2) | 5385(2) | 20(1) |
| C(222) | 4910(4) | 9376(2) | 5987(2) | 23(1) |
| C(223) | 4202(4) | 9975(2) | 6229(2) | 26(1) |
| C(224) | 4314(4) | 10583(2) | 5863(2) | 28(1) |
| C(225) | 5153(4) | 10594(2) | 5268(2) | 26(1) |
| C(226) | 5870(4) | 9995(2) | 5052(2) | 25(1) |
| C(231) | 5959(4) | 8434(2) | 4321(2) | 22(1) |
| C(232) | 5184(4) | 8868(2) | 3868(2) | 25(1) |
| C(233) | 4840(4) | 8674(2) | 3197(2) | 30(1) |
| C(234) | 5227(4) | 8031(2) | 2955(2) | 29(1) |
| C(235) | 5970(4) | 7576(2) | 3390(2) | 29(1) |
| C(236) | 6325(4) | 7779(2) | 4055(2) | 26(1) |
| C(241) | 8388(4) | 8835(2) | 5034(2) | 22(1) |
| C(242) | 9177(4) | 9121(2) | 5596(2) | 26(1) |
| C(243) | 10702(4) | 9245(2) | 5596(2) | 30(1) |
| C(244) | 11557(4) | 9121(2) | 5014(2) | 29(1) |
| C(245) | 10815(4) | 8880(2) | 4441(2) | 26(1) |
| C(246) | 9274(4) | 8732(2) | 4452(2) | 23(1) |

Table 12. Bond lengths [\AA] and angles [$^\circ$] for k99128 - DMBI·BPh₄.

| | | | |
|--------------|----------|--------------|----------|
| C(11)-N(12) | 1.308(4) | C(43)-C(44) | 1.370(6) |
| C(11)-N(15) | 1.330(5) | C(43)-H(43) | 0.9500 |
| C(11)-H(11) | 0.9500 | C(44)-C(45) | 1.347(6) |
| N(12)-C(13) | 1.360(5) | C(44)-H(44) | 0.9500 |
| N(12)-C(40) | 1.494(4) | C(45)-C(46) | 1.366(6) |
| C(13)-C(14) | 1.340(5) | C(45)-H(45) | 0.9500 |
| C(13)-H(13) | 0.9500 | C(46)-H(46) | 0.9500 |
| C(14)-N(15) | 1.359(5) | C(47)-H(47A) | 0.9800 |
| C(14)-H(14) | 0.9500 | C(47)-H(47B) | 0.9800 |
| N(15)-C(30) | 1.482(4) | C(47)-H(47C) | 0.9800 |
| C(30)-C(31) | 1.501(5) | C(21)-N(22) | 1.322(5) |
| C(30)-C(37) | 1.515(5) | C(21)-N(25) | 1.328(5) |
| C(30)-H(30) | 1.0000 | C(21)-H(21) | 0.9500 |
| C(31)-C(32) | 1.345(5) | N(22)-C(23) | 1.375(5) |
| C(31)-C(36) | 1.375(5) | N(22)-C(50) | 1.464(5) |
| C(32)-C(33) | 1.380(6) | C(23)-C(24) | 1.348(6) |
| C(32)-H(32) | 0.9500 | C(23)-H(23) | 0.9500 |
| C(33)-C(34) | 1.359(6) | C(24)-N(25) | 1.381(5) |
| C(33)-H(33) | 0.9500 | C(24)-H(24) | 0.9500 |
| C(34)-C(35) | 1.332(6) | N(25)-C(60) | 1.478(5) |
| C(34)-H(34) | 0.9500 | C(50)-C(57) | 1.453(5) |
| C(35)-C(36) | 1.380(6) | C(50)-C(51) | 1.504(5) |
| C(35)-H(35) | 0.9500 | C(50)-H(50) | 1.0000 |
| C(36)-H(36) | 0.9500 | C(51)-C(52) | 1.331(5) |
| C(37)-H(37A) | 0.9800 | C(51)-C(56) | 1.367(5) |
| C(37)-H(37B) | 0.9800 | C(52)-C(53) | 1.374(5) |
| C(37)-H(37C) | 0.9800 | C(52)-H(52) | 0.9500 |
| C(40)-C(47) | 1.457(6) | C(53)-C(54) | 1.361(6) |
| C(40)-C(41) | 1.496(5) | C(53)-H(53) | 0.9500 |
| C(40)-H(40) | 1.0000 | C(54)-C(55) | 1.338(6) |
| C(41)-C(42) | 1.351(5) | C(54)-H(54) | 0.9500 |
| C(41)-C(46) | 1.386(5) | C(55)-C(56) | 1.368(5) |
| C(42)-C(43) | 1.372(6) | C(55)-H(55) | 0.9500 |
| C(42)-H(42) | 0.9500 | C(56)-H(56) | 0.9500 |

| | | | |
|---------------|----------|---------------|----------|
| C(57)-H(57A) | 0.9800 | C(121)-C(126) | 1.369(5) |
| C(57)-H(57B) | 0.9800 | C(122)-C(123) | 1.391(5) |
| C(57)-H(57C) | 0.9800 | C(122)-H(122) | 0.9500 |
| C(60)-C(67) | 1.506(5) | C(123)-C(124) | 1.356(6) |
| C(60)-C(61) | 1.508(5) | C(123)-H(123) | 0.9500 |
| C(60)-H(60) | 1.0000 | C(124)-C(125) | 1.337(6) |
| C(61)-C(62) | 1.341(5) | C(124)-H(124) | 0.9500 |
| C(61)-C(66) | 1.365(6) | C(125)-C(126) | 1.393(5) |
| C(62)-C(63) | 1.348(6) | C(125)-H(125) | 0.9500 |
| C(62)-H(62) | 0.9500 | C(126)-H(126) | 0.9500 |
| C(63)-C(64) | 1.367(8) | C(131)-C(132) | 1.388(5) |
| C(63)-H(63) | 0.9500 | C(131)-C(136) | 1.396(5) |
| C(64)-C(65) | 1.336(8) | C(132)-C(133) | 1.377(5) |
| C(64)-H(64) | 0.9500 | C(132)-H(132) | 0.9500 |
| C(65)-C(66) | 1.381(6) | C(133)-C(134) | 1.387(5) |
| C(65)-H(65) | 0.9500 | C(133)-H(133) | 0.9500 |
| C(66)-H(66) | 0.9500 | C(134)-C(135) | 1.371(5) |
| C(67)-H(67A) | 0.9800 | C(134)-H(134) | 0.9500 |
| C(67)-H(67B) | 0.9800 | C(135)-C(136) | 1.392(5) |
| C(67)-H(67C) | 0.9800 | C(135)-H(135) | 0.9500 |
| B(1)-C(141) | 1.591(5) | C(136)-H(136) | 0.9500 |
| B(1)-C(111) | 1.632(5) | C(141)-C(146) | 1.380(4) |
| B(1)-C(131) | 1.635(5) | C(141)-C(142) | 1.389(5) |
| B(1)-C(121) | 1.653(5) | C(142)-C(143) | 1.339(5) |
| C(111)-C(112) | 1.394(5) | C(142)-H(142) | 0.9500 |
| C(111)-C(116) | 1.403(5) | C(143)-C(144) | 1.357(5) |
| C(112)-C(113) | 1.385(5) | C(143)-H(143) | 0.9500 |
| C(112)-H(112) | 0.9500 | C(144)-C(145) | 1.360(5) |
| C(113)-C(114) | 1.374(5) | C(144)-H(144) | 0.9500 |
| C(113)-H(113) | 0.9500 | C(145)-C(146) | 1.348(5) |
| C(114)-C(115) | 1.366(6) | C(145)-H(145) | 0.9500 |
| C(114)-H(114) | 0.9500 | C(146)-H(146) | 0.9500 |
| C(115)-C(116) | 1.384(5) | B(2)-C(241) | 1.592(5) |
| C(115)-H(115) | 0.9500 | B(2)-C(221) | 1.636(5) |
| C(116)-H(116) | 0.9500 | B(2)-C(231) | 1.637(5) |
| C(121)-C(122) | 1.363(5) | B(2)-C(211) | 1.642(5) |

| | | | |
|---------------|----------|-------------------|----------|
| C(211)-C(212) | 1.368(5) | C(242)-H(242) | 0.9500 |
| C(211)-C(216) | 1.385(5) | C(243)-C(244) | 1.378(6) |
| C(212)-C(213) | 1.382(5) | C(243)-H(243) | 0.9500 |
| C(212)-H(212) | 0.9500 | C(244)-C(245) | 1.363(5) |
| C(213)-C(214) | 1.376(6) | C(244)-H(244) | 0.9500 |
| C(213)-H(213) | 0.9500 | C(245)-C(246) | 1.338(5) |
| C(214)-C(215) | 1.342(6) | C(245)-H(245) | 0.9500 |
| C(214)-H(214) | 0.9500 | C(246)-H(246) | 0.9500 |
| C(215)-C(216) | 1.379(5) | | |
| C(215)-H(215) | 0.9500 | N(12)-C(11)-N(15) | 109.6(3) |
| C(216)-H(216) | 0.9500 | N(12)-C(11)-H(11) | 125.2 |
| C(221)-C(222) | 1.382(5) | N(15)-C(11)-H(11) | 125.2 |
| C(221)-C(226) | 1.404(5) | C(11)-N(12)-C(13) | 107.2(3) |
| C(222)-C(223) | 1.391(5) | C(11)-N(12)-C(40) | 123.7(3) |
| C(222)-H(222) | 0.9500 | C(13)-N(12)-C(40) | 129.1(3) |
| C(223)-C(224) | 1.380(5) | C(14)-C(13)-N(12) | 108.9(3) |
| C(223)-H(223) | 0.9500 | C(14)-C(13)-H(13) | 125.6 |
| C(224)-C(225) | 1.371(6) | N(12)-C(13)-H(13) | 125.6 |
| C(224)-H(224) | 0.9500 | C(13)-C(14)-N(15) | 106.0(3) |
| C(225)-C(226) | 1.377(5) | C(13)-C(14)-H(14) | 127.0 |
| C(225)-H(225) | 0.9500 | N(15)-C(14)-H(14) | 127.0 |
| C(226)-H(226) | 0.9500 | C(11)-N(15)-C(14) | 108.3(3) |
| C(231)-C(232) | 1.383(5) | C(11)-N(15)-C(30) | 124.0(3) |
| C(231)-C(236) | 1.406(5) | C(14)-N(15)-C(30) | 127.5(3) |
| C(232)-C(233) | 1.394(5) | N(15)-C(30)-C(31) | 110.8(3) |
| C(232)-H(232) | 0.9500 | N(15)-C(30)-C(37) | 110.8(3) |
| C(233)-C(234) | 1.373(6) | C(31)-C(30)-C(37) | 114.3(3) |
| C(233)-H(233) | 0.9500 | N(15)-C(30)-H(30) | 106.9 |
| C(234)-C(235) | 1.373(5) | C(31)-C(30)-H(30) | 106.9 |
| C(234)-H(234) | 0.9500 | C(37)-C(30)-H(30) | 106.9 |
| C(235)-C(236) | 1.391(5) | C(32)-C(31)-C(36) | 117.8(4) |
| C(235)-H(235) | 0.9500 | C(32)-C(31)-C(30) | 120.8(3) |
| C(236)-H(236) | 0.9500 | C(36)-C(31)-C(30) | 121.4(4) |
| C(241)-C(246) | 1.386(5) | C(31)-C(32)-C(33) | 119.9(4) |
| C(241)-C(242) | 1.398(5) | C(31)-C(32)-H(32) | 120.1 |
| C(242)-C(243) | 1.316(5) | C(33)-C(32)-H(32) | 120.1 |

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|---------------------|----------|---------------------|----------|
| C(34)-C(33)-C(32) | 121.8(4) | C(44)-C(45)-C(46) | 119.2(4) |
| C(34)-C(33)-H(33) | 119.1 | C(44)-C(45)-H(45) | 120.4 |
| C(32)-C(33)-H(33) | 119.1 | C(46)-C(45)-H(45) | 120.4 |
| C(35)-C(34)-C(33) | 118.8(4) | C(45)-C(46)-C(41) | 121.7(4) |
| C(35)-C(34)-H(34) | 120.6 | C(45)-C(46)-H(46) | 119.1 |
| C(33)-C(34)-H(34) | 120.6 | C(41)-C(46)-H(46) | 119.1 |
| C(34)-C(35)-C(36) | 119.9(4) | C(40)-C(47)-H(47A) | 109.5 |
| C(34)-C(35)-H(35) | 120.1 | C(40)-C(47)-H(47B) | 109.5 |
| C(36)-C(35)-H(35) | 120.1 | H(47A)-C(47)-H(47B) | 109.5 |
| C(31)-C(36)-C(35) | 121.8(4) | C(40)-C(47)-H(47C) | 109.5 |
| C(31)-C(36)-H(36) | 119.1 | H(47A)-C(47)-H(47C) | 109.5 |
| C(35)-C(36)-H(36) | 119.1 | H(47B)-C(47)-H(47C) | 109.5 |
| C(30)-C(37)-H(37A) | 109.5 | N(22)-C(21)-N(25) | 109.8(3) |
| C(30)-C(37)-H(37B) | 109.5 | N(22)-C(21)-H(21) | 125.1 |
| H(37A)-C(37)-H(37B) | 109.5 | N(25)-C(21)-H(21) | 125.1 |
| C(30)-C(37)-H(37C) | 109.5 | C(21)-N(22)-C(23) | 107.7(3) |
| H(37A)-C(37)-H(37C) | 109.5 | C(21)-N(22)-C(50) | 125.3(3) |
| H(37B)-C(37)-H(37C) | 109.5 | C(23)-N(22)-C(50) | 126.9(3) |
| C(47)-C(40)-N(12) | 109.2(3) | C(24)-C(23)-N(22) | 107.8(4) |
| C(47)-C(40)-C(41) | 112.3(3) | C(24)-C(23)-H(23) | 126.1 |
| N(12)-C(40)-C(41) | 111.4(3) | N(22)-C(23)-H(23) | 126.1 |
| C(47)-C(40)-H(40) | 107.9 | C(23)-C(24)-N(25) | 106.8(3) |
| N(12)-C(40)-H(40) | 107.9 | C(23)-C(24)-H(24) | 126.6 |
| C(41)-C(40)-H(40) | 107.9 | N(25)-C(24)-H(24) | 126.6 |
| C(42)-C(41)-C(46) | 118.7(4) | C(21)-N(25)-C(24) | 107.9(3) |
| C(42)-C(41)-C(40) | 117.5(3) | C(21)-N(25)-C(60) | 123.8(3) |
| C(46)-C(41)-C(40) | 123.8(3) | C(24)-N(25)-C(60) | 128.4(3) |
| C(41)-C(42)-C(43) | 119.2(4) | C(57)-C(50)-N(22) | 108.6(3) |
| C(41)-C(42)-H(42) | 120.4 | C(57)-C(50)-C(51) | 114.9(3) |
| C(43)-C(42)-H(42) | 120.4 | N(22)-C(50)-C(51) | 111.0(3) |
| C(44)-C(43)-C(42) | 121.8(4) | C(57)-C(50)-H(50) | 107.3 |
| C(44)-C(43)-H(43) | 119.1 | N(22)-C(50)-H(50) | 107.3 |
| C(42)-C(43)-H(43) | 119.1 | C(51)-C(50)-H(50) | 107.3 |
| C(45)-C(44)-C(43) | 119.3(4) | C(52)-C(51)-C(56) | 117.2(3) |
| C(45)-C(44)-H(44) | 120.4 | C(52)-C(51)-C(50) | 117.7(3) |
| C(43)-C(44)-H(44) | 120.4 | C(56)-C(51)-C(50) | 124.9(3) |

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|---------------------|----------|----------------------|----------|
| C(51)-C(52)-C(53) | 120.1(4) | C(65)-C(64)-C(63) | 120.3(4) |
| C(51)-C(52)-H(52) | 119.9 | C(65)-C(64)-H(64) | 119.8 |
| C(53)-C(52)-H(52) | 119.9 | C(63)-C(64)-H(64) | 119.8 |
| C(54)-C(53)-C(52) | 122.3(4) | C(64)-C(65)-C(66) | 117.3(5) |
| C(54)-C(53)-H(53) | 118.9 | C(64)-C(65)-H(65) | 121.4 |
| C(52)-C(53)-H(53) | 118.9 | C(66)-C(65)-H(65) | 121.4 |
| C(55)-C(54)-C(53) | 118.0(4) | C(61)-C(66)-C(65) | 122.2(4) |
| C(55)-C(54)-H(54) | 121.0 | C(61)-C(66)-H(66) | 118.9 |
| C(53)-C(54)-H(54) | 121.0 | C(65)-C(66)-H(66) | 118.9 |
| C(54)-C(55)-C(56) | 119.3(4) | C(60)-C(67)-H(67A) | 109.5 |
| C(54)-C(55)-H(55) | 120.3 | C(60)-C(67)-H(67B) | 109.5 |
| C(56)-C(55)-H(55) | 120.3 | H(67A)-C(67)-H(67B) | 109.5 |
| C(51)-C(56)-C(55) | 123.1(4) | C(60)-C(67)-H(67C) | 109.5 |
| C(51)-C(56)-H(56) | 118.5 | H(67A)-C(67)-H(67C) | 109.5 |
| C(55)-C(56)-H(56) | 118.5 | H(67B)-C(67)-H(67C) | 109.5 |
| C(50)-C(57)-H(57A) | 109.5 | C(141)-B(1)-C(111) | 107.7(3) |
| C(50)-C(57)-H(57B) | 109.5 | C(141)-B(1)-C(131) | 105.7(3) |
| H(57A)-C(57)-H(57B) | 109.5 | C(111)-B(1)-C(131) | 116.0(3) |
| C(50)-C(57)-H(57C) | 109.5 | C(141)-B(1)-C(121) | 110.5(3) |
| H(57A)-C(57)-H(57C) | 109.5 | C(111)-B(1)-C(121) | 108.1(3) |
| H(57B)-C(57)-H(57C) | 109.5 | C(131)-B(1)-C(121) | 108.7(3) |
| N(25)-C(60)-C(67) | 110.9(3) | C(112)-C(111)-C(116) | 114.5(3) |
| N(25)-C(60)-C(61) | 109.0(3) | C(112)-C(111)-B(1) | 125.5(3) |
| C(67)-C(60)-C(61) | 113.4(3) | C(116)-C(111)-B(1) | 120.0(3) |
| N(25)-C(60)-H(60) | 107.8 | C(113)-C(112)-C(111) | 122.0(4) |
| C(67)-C(60)-H(60) | 107.8 | C(113)-C(112)-H(112) | 119.0 |
| C(61)-C(60)-H(60) | 107.8 | C(111)-C(112)-H(112) | 119.0 |
| C(62)-C(61)-C(66) | 119.2(4) | C(114)-C(113)-C(112) | 121.6(4) |
| C(62)-C(61)-C(60) | 119.2(4) | C(114)-C(113)-H(113) | 119.2 |
| C(66)-C(61)-C(60) | 121.6(3) | C(112)-C(113)-H(113) | 119.2 |
| C(61)-C(62)-C(63) | 118.9(4) | C(115)-C(114)-C(113) | 118.3(3) |
| C(61)-C(62)-H(62) | 120.5 | C(115)-C(114)-H(114) | 120.8 |
| C(63)-C(62)-H(62) | 120.5 | C(113)-C(114)-H(114) | 120.8 |
| C(62)-C(63)-C(64) | 122.0(5) | C(114)-C(115)-C(116) | 120.1(4) |
| C(62)-C(63)-H(63) | 119.0 | C(114)-C(115)-H(115) | 120.0 |
| C(64)-C(63)-H(63) | 119.0 | C(116)-C(115)-H(115) | 120.0 |

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| C(115)-C(116)-C(111) | 123.5(4) | C(135)-C(136)-C(131) | 124.1(3) |
| C(115)-C(116)-H(116) | 118.2 | C(135)-C(136)-H(136) | 117.9 |
| C(111)-C(116)-H(116) | 118.2 | C(131)-C(136)-H(136) | 117.9 |
| C(122)-C(121)-C(126) | 113.4(3) | C(146)-C(141)-C(142) | 116.6(3) |
| C(122)-C(121)-B(1) | 120.7(3) | C(146)-C(141)-B(1) | 123.7(3) |
| C(126)-C(121)-B(1) | 125.7(3) | C(142)-C(141)-B(1) | 119.6(3) |
| C(121)-C(122)-C(123) | 123.1(4) | C(143)-C(142)-C(141) | 122.3(3) |
| C(121)-C(122)-H(122) | 118.4 | C(143)-C(142)-H(142) | 118.9 |
| C(123)-C(122)-H(122) | 118.4 | C(141)-C(142)-H(142) | 118.9 |
| C(124)-C(123)-C(122) | 121.4(4) | C(142)-C(143)-C(144) | 119.0(4) |
| C(124)-C(123)-H(123) | 119.3 | C(142)-C(143)-H(143) | 120.5 |
| C(122)-C(123)-H(123) | 119.3 | C(144)-C(143)-H(143) | 120.5 |
| C(125)-C(124)-C(123) | 117.3(4) | C(143)-C(144)-C(145) | 121.0(3) |
| C(125)-C(124)-H(124) | 121.4 | C(143)-C(144)-H(144) | 119.5 |
| C(123)-C(124)-H(124) | 121.4 | C(145)-C(144)-H(144) | 119.5 |
| C(124)-C(125)-C(126) | 120.7(4) | C(146)-C(145)-C(144) | 119.5(3) |
| C(124)-C(125)-H(125) | 119.6 | C(146)-C(145)-H(145) | 120.2 |
| C(126)-C(125)-H(125) | 119.6 | C(144)-C(145)-H(145) | 120.2 |
| C(121)-C(126)-C(125) | 124.1(4) | C(145)-C(146)-C(141) | 121.5(3) |
| C(121)-C(126)-H(126) | 118.0 | C(145)-C(146)-H(146) | 119.3 |
| C(125)-C(126)-H(126) | 118.0 | C(141)-C(146)-H(146) | 119.3 |
| C(132)-C(131)-C(136) | 114.6(3) | C(241)-B(2)-C(221) | 104.7(3) |
| C(132)-C(131)-B(1) | 122.9(3) | C(241)-B(2)-C(231) | 107.1(3) |
| C(136)-C(131)-B(1) | 122.6(3) | C(221)-B(2)-C(231) | 114.3(3) |
| C(133)-C(132)-C(131) | 122.6(3) | C(241)-B(2)-C(211) | 112.0(3) |
| C(133)-C(132)-H(132) | 118.7 | C(221)-B(2)-C(211) | 109.2(3) |
| C(131)-C(132)-H(132) | 118.7 | C(231)-B(2)-C(211) | 109.5(3) |
| C(132)-C(133)-C(134) | 121.0(3) | C(212)-C(211)-C(216) | 112.8(3) |
| C(132)-C(133)-H(133) | 119.5 | C(212)-C(211)-B(2) | 121.3(3) |
| C(134)-C(133)-H(133) | 119.5 | C(216)-C(211)-B(2) | 125.6(3) |
| C(135)-C(134)-C(133) | 118.7(3) | C(211)-C(212)-C(213) | 123.4(3) |
| C(135)-C(134)-H(134) | 120.6 | C(211)-C(212)-H(212) | 118.3 |
| C(133)-C(134)-H(134) | 120.6 | C(213)-C(212)-H(212) | 118.3 |
| C(134)-C(135)-C(136) | 118.9(4) | C(214)-C(213)-C(212) | 121.3(4) |
| C(134)-C(135)-H(135) | 120.5 | C(214)-C(213)-H(213) | 119.3 |
| C(136)-C(135)-H(135) | 120.5 | C(212)-C(213)-H(213) | 119.3 |

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| C(215)-C(214)-C(213) | 117.2(4) | C(233)-C(232)-H(232) | 118.8 |
| C(215)-C(214)-H(214) | 121.4 | C(234)-C(233)-C(232) | 121.3(3) |
| C(213)-C(214)-H(214) | 121.4 | C(234)-C(233)-H(233) | 119.3 |
| C(214)-C(215)-C(216) | 120.4(4) | C(232)-C(233)-H(233) | 119.3 |
| C(214)-C(215)-H(215) | 119.8 | C(233)-C(234)-C(235) | 118.4(3) |
| C(216)-C(215)-H(215) | 119.8 | C(233)-C(234)-H(234) | 120.8 |
| C(215)-C(216)-C(211) | 124.8(4) | C(235)-C(234)-H(234) | 120.8 |
| C(215)-C(216)-H(216) | 117.6 | C(234)-C(235)-C(236) | 119.6(4) |
| C(211)-C(216)-H(216) | 117.6 | C(234)-C(235)-H(235) | 120.2 |
| C(222)-C(221)-C(226) | 114.3(3) | C(236)-C(235)-H(235) | 120.2 |
| C(222)-C(221)-B(2) | 123.4(3) | C(235)-C(236)-C(231) | 123.7(3) |
| C(226)-C(221)-B(2) | 122.3(3) | C(235)-C(236)-H(236) | 118.2 |
| C(221)-C(222)-C(223) | 122.8(3) | C(231)-C(236)-H(236) | 118.2 |
| C(221)-C(222)-H(222) | 118.6 | C(246)-C(241)-C(242) | 116.4(3) |
| C(223)-C(222)-H(222) | 118.6 | C(246)-C(241)-B(2) | 123.9(3) |
| C(224)-C(223)-C(222) | 120.1(4) | C(242)-C(241)-B(2) | 119.7(3) |
| C(224)-C(223)-H(223) | 120.0 | C(243)-C(242)-C(241) | 122.5(4) |
| C(222)-C(223)-H(223) | 120.0 | C(243)-C(242)-H(242) | 118.8 |
| C(225)-C(224)-C(223) | 119.6(4) | C(241)-C(242)-H(242) | 118.8 |
| C(225)-C(224)-H(224) | 120.2 | C(242)-C(243)-C(244) | 119.5(4) |
| C(223)-C(224)-H(224) | 120.2 | C(242)-C(243)-H(243) | 120.2 |
| C(224)-C(225)-C(226) | 118.8(4) | C(244)-C(243)-H(243) | 120.2 |
| C(224)-C(225)-H(225) | 120.6 | C(245)-C(244)-C(243) | 119.9(3) |
| C(226)-C(225)-H(225) | 120.6 | C(245)-C(244)-H(244) | 120.1 |
| C(225)-C(226)-C(221) | 124.4(4) | C(243)-C(244)-H(244) | 120.1 |
| C(225)-C(226)-H(226) | 117.8 | C(246)-C(245)-C(244) | 120.3(4) |
| C(221)-C(226)-H(226) | 117.8 | C(246)-C(245)-H(245) | 119.9 |
| C(232)-C(231)-C(236) | 114.5(3) | C(244)-C(245)-H(245) | 119.9 |
| C(232)-C(231)-B(2) | 125.1(3) | C(245)-C(246)-C(241) | 121.3(3) |
| C(236)-C(231)-B(2) | 120.2(3) | C(245)-C(246)-H(246) | 119.4 |
| C(231)-C(232)-C(233) | 122.4(3) | C(241)-C(246)-H(246) | 119.4 |
| C(231)-C(232)-H(232) | 118.8 | | |

Symmetry transformations used to generate equivalent atoms:

Table 13. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k99128 - DMBI·BPh4. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

| | U^{11} | U^{22} | U^{33} | U^{23} | U^{13} | U^{12} |
|-------|----------|----------|----------|----------|----------|----------|
| C(11) | 24(2) | 23(2) | 29(2) | 2(2) | 2(2) | 2(2) |
| N(12) | 29(2) | 22(2) | 23(2) | -2(1) | 3(1) | 1(1) |
| C(13) | 51(3) | 28(2) | 33(2) | -1(2) | -9(2) | 12(2) |
| C(14) | 49(2) | 23(2) | 35(2) | -3(2) | -10(2) | 11(2) |
| N(15) | 28(2) | 21(2) | 24(2) | -1(1) | 3(1) | 2(1) |
| C(30) | 20(2) | 32(2) | 24(2) | 1(2) | -1(2) | 2(2) |
| C(31) | 23(2) | 27(2) | 25(2) | -6(2) | -5(2) | 1(2) |
| C(32) | 27(2) | 27(2) | 36(2) | -4(2) | -1(2) | -1(2) |
| C(33) | 27(2) | 46(2) | 29(2) | -11(2) | 4(2) | -8(2) |
| C(34) | 39(2) | 33(2) | 27(2) | 2(2) | -1(2) | -12(2) |
| C(35) | 33(2) | 34(2) | 35(2) | 3(2) | -7(2) | -3(2) |
| C(36) | 31(2) | 29(2) | 30(2) | -3(2) | -7(2) | -1(2) |
| C(37) | 35(2) | 31(2) | 31(2) | -1(2) | -4(2) | -5(2) |
| C(40) | 34(2) | 16(2) | 27(2) | -4(1) | 4(2) | -1(2) |
| C(41) | 31(2) | 21(2) | 23(2) | 0(2) | -2(2) | -4(2) |
| C(42) | 30(2) | 27(2) | 25(2) | 0(2) | 1(2) | -2(2) |
| C(43) | 32(2) | 30(2) | 36(2) | -6(2) | 5(2) | 0(2) |
| C(44) | 43(2) | 34(2) | 32(2) | -1(2) | 13(2) | -1(2) |
| C(45) | 54(3) | 39(3) | 37(3) | 11(2) | 8(2) | 6(2) |
| C(46) | 38(2) | 34(2) | 36(2) | 1(2) | 4(2) | 9(2) |
| C(47) | 32(2) | 34(2) | 42(2) | -7(2) | 7(2) | -6(2) |
| C(21) | 25(2) | 27(2) | 26(2) | 5(2) | -4(2) | -5(2) |
| N(22) | 29(2) | 22(2) | 22(2) | 2(1) | -2(1) | -5(1) |
| C(23) | 49(3) | 25(2) | 31(2) | 1(2) | 3(2) | -12(2) |
| C(24) | 42(2) | 23(2) | 33(2) | 1(2) | 1(2) | -5(2) |
| N(25) | 23(2) | 25(2) | 24(2) | -1(1) | -1(1) | -4(1) |
| C(50) | 28(2) | 21(2) | 27(2) | -2(2) | 2(2) | -1(2) |
| C(51) | 26(2) | 18(2) | 26(2) | -3(2) | 1(2) | 4(2) |
| C(52) | 26(2) | 51(3) | 24(2) | 1(2) | 6(2) | 2(2) |
| C(53) | 20(2) | 58(3) | 36(2) | -6(2) | -4(2) | 4(2) |
| C(54) | 46(3) | 36(2) | 25(2) | -1(2) | -7(2) | 6(2) |

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|--------|-------|-------|-------|--------|--------|-------|
| C(55) | 44(2) | 33(2) | 26(2) | 1(2) | 10(2) | 0(2) |
| C(56) | 31(2) | 28(2) | 30(2) | -2(2) | 5(2) | -4(2) |
| C(57) | 29(2) | 35(2) | 48(3) | 6(2) | -6(2) | -3(2) |
| C(60) | 20(2) | 32(2) | 30(2) | 1(2) | 1(2) | 1(2) |
| C(61) | 23(2) | 31(2) | 19(2) | -4(2) | 2(2) | 5(2) |
| C(62) | 27(2) | 38(2) | 40(2) | -8(2) | -4(2) | 5(2) |
| C(63) | 43(3) | 70(4) | 40(3) | -13(3) | -12(2) | 25(3) |
| C(64) | 74(4) | 65(3) | 25(2) | 2(2) | -1(2) | 49(3) |
| C(65) | 81(4) | 42(3) | 39(3) | 10(2) | 25(3) | 20(3) |
| C(66) | 39(2) | 34(2) | 35(2) | -3(2) | 10(2) | -2(2) |
| C(67) | 41(2) | 35(2) | 33(2) | 0(2) | 4(2) | 10(2) |
| B(1) | 21(2) | 21(2) | 23(2) | 0(2) | 0(2) | 0(2) |
| C(111) | 13(2) | 26(2) | 28(2) | 0(2) | -3(1) | 6(2) |
| C(112) | 20(2) | 28(2) | 29(2) | 5(2) | 0(2) | 3(2) |
| C(113) | 24(2) | 34(2) | 26(2) | 5(2) | 3(2) | 5(2) |
| C(114) | 24(2) | 36(2) | 22(2) | -2(2) | -1(2) | 10(2) |
| C(115) | 26(2) | 30(2) | 28(2) | -4(2) | -6(2) | 7(2) |
| C(116) | 26(2) | 24(2) | 23(2) | -1(2) | -3(2) | 2(2) |
| C(121) | 27(2) | 23(2) | 24(2) | -1(2) | -6(2) | -3(2) |
| C(122) | 31(2) | 27(2) | 26(2) | -2(2) | -3(2) | 5(2) |
| C(123) | 45(3) | 25(2) | 36(2) | -4(2) | -13(2) | 11(2) |
| C(124) | 51(3) | 26(2) | 37(2) | 8(2) | -20(2) | -4(2) |
| C(125) | 40(2) | 44(3) | 35(2) | 11(2) | -7(2) | -9(2) |
| C(126) | 27(2) | 33(2) | 31(2) | 8(2) | -6(2) | -2(2) |
| C(131) | 16(2) | 24(2) | 25(2) | -2(2) | 4(1) | 3(1) |
| C(132) | 24(2) | 28(2) | 25(2) | -3(2) | -2(2) | 3(2) |
| C(133) | 25(2) | 33(2) | 29(2) | -8(2) | -3(2) | 1(2) |
| C(134) | 28(2) | 25(2) | 37(2) | -11(2) | 6(2) | -5(2) |
| C(135) | 29(2) | 25(2) | 36(2) | -1(2) | 9(2) | -1(2) |
| C(136) | 22(2) | 28(2) | 26(2) | -2(2) | 1(2) | 4(2) |
| C(141) | 21(2) | 19(2) | 24(2) | 4(1) | -1(2) | -7(2) |
| C(142) | 26(2) | 29(2) | 22(2) | 1(2) | 1(2) | 0(2) |
| C(143) | 25(2) | 33(2) | 35(2) | 7(2) | 6(2) | 7(2) |
| C(144) | 15(2) | 28(2) | 41(2) | 8(2) | 3(2) | -2(2) |
| C(145) | 23(2) | 18(2) | 32(2) | 4(2) | -3(2) | -5(2) |
| C(146) | 22(2) | 18(2) | 25(2) | 3(1) | 0(2) | 0(2) |

| | | | | | | |
|--------|-------|-------|-------|-------|-------|-------|
| B(2) | 19(2) | 19(2) | 25(2) | 0(2) | 0(2) | 1(2) |
| C(211) | 24(2) | 23(2) | 24(2) | -4(2) | 4(2) | 2(2) |
| C(212) | 28(2) | 27(2) | 26(2) | -5(2) | 0(2) | -2(2) |
| C(213) | 33(2) | 25(2) | 32(2) | -2(2) | 10(2) | -7(2) |
| C(214) | 42(2) | 24(2) | 31(2) | 5(2) | 14(2) | 5(2) |
| C(215) | 34(2) | 34(2) | 30(2) | 9(2) | 3(2) | 6(2) |
| C(216) | 28(2) | 30(2) | 25(2) | 4(2) | -1(2) | 1(2) |
| C(221) | 15(2) | 26(2) | 20(2) | 0(2) | -3(1) | -2(1) |
| C(222) | 21(2) | 22(2) | 26(2) | -1(2) | -4(2) | -3(2) |
| C(223) | 21(2) | 31(2) | 26(2) | -6(2) | -1(2) | -2(2) |
| C(224) | 24(2) | 24(2) | 35(2) | -8(2) | -9(2) | 2(2) |
| C(225) | 28(2) | 21(2) | 30(2) | 3(2) | -9(2) | -3(2) |
| C(226) | 22(2) | 28(2) | 24(2) | 0(2) | -4(2) | -2(2) |
| C(231) | 12(2) | 26(2) | 27(2) | 2(2) | 2(1) | -3(1) |
| C(232) | 22(2) | 26(2) | 27(2) | -2(2) | -1(2) | -1(2) |
| C(233) | 23(2) | 37(2) | 32(2) | 3(2) | -4(2) | 0(2) |
| C(234) | 27(2) | 36(2) | 22(2) | -1(2) | -1(2) | -8(2) |
| C(235) | 25(2) | 34(2) | 27(2) | -7(2) | 1(2) | -1(2) |
| C(236) | 24(2) | 28(2) | 25(2) | 3(2) | -2(2) | -1(2) |
| C(241) | 19(2) | 20(2) | 26(2) | 5(1) | 0(2) | 2(1) |
| C(242) | 26(2) | 28(2) | 23(2) | 1(2) | 0(2) | -2(2) |
| C(243) | 26(2) | 34(2) | 29(2) | 1(2) | -7(2) | 0(2) |
| C(244) | 19(2) | 30(2) | 38(2) | 7(2) | -2(2) | 0(2) |
| C(245) | 24(2) | 23(2) | 31(2) | 2(2) | 7(2) | 2(2) |
| C(246) | 25(2) | 18(2) | 25(2) | 4(2) | -1(2) | -3(2) |
