# Electronic Supplementary Information

## Routes to new tetrazole compounds: Synthesis, characterization and crystal structure

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**Table S1.** Selected bond lengths (Å) and angles (°) for **2**

| | | | | | |
|---|---|---|---|---|---|
| *Bond lengths* | | | | | |
| O(17)–C(16) | 1.221(3) | N(4)–C(5) | 1.299(3) | N(11)–C(15) | 1.326(3) |
| N(1)–N(2) | 1.344(3) | N(8)–C(7) | 1.455(3) | N(12)–N(13) | 1.299(3) |
| N(1)–C(5) | 1.314(3) | N(8)–C(9) | 1.454(3) | N(13)–N(14) | 1.351(3) |
| N(1)–C(6) | 1.456(3) | N(8)–C(16) | 1.337(3) | N(14)–C(15) | 1.305(3) |
| N(2)–N(3) | 1.282(3) | N(11)–N(12) | 1.336(2) | C(6)–C(7) | 1.514(3) |
| N(3)–N(4) | 1.358(3) | N(11)–C(10) | 1.462(3) | C(9)–C(10) | 1.520(3) |
| *Bond angles* | | | | | |
| N(2)–N(1)–C(5) | 107.63(19) | C(9)–N(8)–C(16) | 121.52(18) | N(1)–C(5)–N(4) | 110.2(2) |
| N(2)–N(1)–C(6) | 121.14(18) | N(12)–N(11)–C(10) | 121.67(18) | N(1)–C(6)–C(7) | 111.78(19) |
| C(5)–N(1–C(6) | 131.2(2) | N(12)–N(11)–C(15) | 107.92(18) | N(8)–C(7)–C(6) | 112.3(2) |
| N(1)–N(2)–N(3) | 106.6(2) | C(10)–N(11)–C(15) | 130.40(18) | N(8)–C(9)–C(10) | 113.05(17) |
| N(2)–N(3)–N(4) | 110.5(2) | N(11)–N(12)–N(13) | 106.07(19) | N(11)–C(10)–C(9) | 111.48(18) |
| N(3)–N(4)–C(5) | 105.0(2) | N(12)–N(13)–N(14) | 111.2(2) | N(11)–C(15)–N(14) | 110.10(19) |
| C(7)–N(8)–C(9) | 118.49(17) | N(13)–N(14)–C(15) | 104.8(2) | O(17)–C(16)–N(8) | 125.1(2) |
| C(7)–N(8)–C(16) | 119.98(19) | | | | |
| *Torsion angles* | | | | | |
| C(5)–N(1)–N(2)–N(3) | –0.2(2) | C(9)–N(8)–C(7)–C(6) | 81.5(2) | C(15)–N(11)–C(10)–C(9) | 83.5(3) |
| C(6)–N(1)–N(2)–N(3) | –177.98(19) | C(16)–N(8)–C(7)–C(6) | –99.4(2) | N(12)–N(11)–C(15)–N(14) | 0.0(3) |
| N(2)–N(1)–C(5)–N(4) | 0.1(3) | C(7)–N(8)–C(9)–C(10) | 78.0(2) | C(10)–N(11)–C(15)–N(14) | –178.9(2) |
| C(6)–N(1)–C(5)–N(4) | 177.5(2) | C(16)–N(8)–C(9)–C(10) | –101.1(2) | N(11)–N(12)–N(13)–N(14) | 0.1(3) |
| N(2)–N(1)–C(6)–C(7) | 81.7(2) | C(7)–N(8)–C(16)–O(17) | –1.8(4) | N(12)–N(13)–N(14)–C(15) | –0.1(3) |
| C(5)–N(1)–C(6)–C(7) | –95.5(3) | C(9)–N(8)–C(16)–O(17) | 177.3(2) | N(13)–N(14)–C(15)–N(11) | 0.1(3) |
| N(1)–N(2)–N(3)–N(4) | 0.3(3) | C(10)–N(11)–N(12)–N(13) | 179.0(2) | N(1)–C(6)–C(7)–N(8) | 56.0(3) |
| N(2)–N(3)–N(4)–C(5) | –0.3(3) | C(15)–N(11)–N(12)–N(13) | 0.0(3) | N(8)–C(9)–C(10)–N(11) | 67.0(2) |
| N(3)–N(4)–C(5)–N(1) | 0.1(3) | N(12)–N(11)–C(10)–C(9) | –95.2(2) | | |

**Table S2.** Selected bond lengths (Å) and angles (°) for **13**

| | | | | | |
|---|---|---|---|---|---|
| *Bond lengths* | | | | | |
| O(10)–C(9) | 1.358(2) | N(1)–C(6) | 1.461(2) | N(8)–C(9) | 1.351(2) |
| O(10)–C(11) | 1.458(2) | N(2)–N(3) | 1.294(2) | N(8)–C(12) | 1.456(2) |
| O(13)–C(9) | 1.214(2) | N(3)–N(4) | 1.363(2) | C(6)–C(7) | 1.525(2) |
| N(1)–N(2) | 1.3474(16) | N(4)–C(5) | 1.315(2) | C(11)–C(12) | 1.522(2) |
| N(1)–C(5) | 1.334(2) | N(8)–C(7) | 1.448(2) | | |
| *Bond angles* | | | | | |
| C(9)–O(10)–C(11) | 108.36(12) | N(3)–N(4)–C(5) | 105.17(14) | N(8)–C(7)–C(6) | 113.34(13) |
| N(2)–N(1)–C(5) | 108.14(13) | C(7)–N(8)–C(9) | 122.01(13) | O(10)–C(9)–O(13) | 122.26(15) |
| N(2)–N(1)–C(6) | 121.37(13) | C(7)–N(8)–C(12) | 123.44(13) | O(10)–C(9)–N(8) | 109.91(14) |
| C(5)–N(1)–C(6) | 130.40(13) | C(9)–N(8)–C(12) | 111.31(12) | O(13)–C(9)–N(8) | 127.82(15) |
| N(1)–N(2)–N(3) | 106.36(13) | N(1)–C(5)–N(4) | 109.36(14) | O(10)–C(11)–C(12) | 104.54(13) |
| N(2)–N(3)–N(4) | 110.96(14) | N(1)–C(6)–C(7) | 111.85(13) | N(8)–C(12)–C(11) | 100.15(14) |
| *Torsion angles* | | | | | |
| C(5)–N(1)–N(2)–N(3) | –0.03(17) | N(3)–N(4)–C(5)–N(1) | 0.40(17) | C(7)–N(8)–C(12)–C(11) | 178.93(13) |
| C(6)–N(1)–N(2)–N(3) | 176.81(13) | C(9)–N(8)–C(7)–C(6) | –90.14(18) | C(9)–N(8)–C(12)–C(11) | –21.10(16) |
| N(2)–N(1)–C(5)–N(4) | –0.24(18) | C(12)–N(8)–C(7)–C(6) | 67.75(19) | N(1)–C(6)–C(7)–N(8) | 63.41(17) |
| C(6)–N(1)–C(5)–N(4) | –176.71(15) | C(7)–N(8)–C(9)–O(10) | 171.01(13) | O(13)–C(9)–O(10)–C(11) | –173.16(15) |
| N(2)–N(1)–C(6)–C(7) | –85.93(17) | C(7)–N(8)–C(9)–O(13) | –10.2(2) | N(8)–C(9)–O(10)–C(11) | 5.67(17) |
| C(5)–N(1)–C(6)–C(7) | 90.15(19) | C(12)–N(8)–C(9)–O(10) | 10.71(18) | C(12)–C(11)–O(10)–C(9) | –18.63(16) |
| N(1)–N(2)–N(3)–N(4) | 0.30(17) | C(12)–N(8)–C(9)–O(13) | –170.53(16) | O(10)–C(11)–C(12)–N(8) | 22.98(15) |
| N(2)–N(3)–N(4)–C(5) | –0.44(18) | | | | |