Electronic Supplementary Information

Copper-mediated imine–nitrile coupling leading to unsymmetric 1,3,5-triazapentadienato complexes containing the incorporated iminoisoindolin-1-one moiety

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[\text{Cu}\{\text{HN=CH}_{\text{3}}\text{CN=C}({\text{C}}_{\text{6}}\text{H}_{\text{4}}\text{CO})\}_2\} (3). \text{C}_{24}\text{H}_{24}\text{N}_6\text{CuO}_2 (492.0): \text{calcd.} \text{ C 58.59, H 4.92, N 17.08; found: C 58.26, H 4.86, N 16.92}. \text{FAB}^+\text{-MS, } m/z: 492 \text{ [M]}^+. \text{IR (KBr): } 3203 \text{ [(s) } \nu(\text{NH})], 2960 \text{ and 2931 [(m-w) } \nu_{\text{as}}(\text{CH})], 2873 [(m) } \nu_{\text{d}}(\text{CH})], 1695 [(s) } \nu(\text{C}=\text{O})], 1616 (s) \text{ and 1602 [(vs) } \nu(\text{C}=\text{N})], 1553 [(vs) } \delta(\text{NH})] \text{ cm}^{-1}.

[\text{Cu}\{\text{HN=CH}_{\text{3}}\text{CN=C}({\text{C}}_{\text{6}}\text{H}_{\text{4}}\text{CO})\}_2\} (5). \text{C}_{30}\text{H}_{32}\text{N}_6\text{CuO}_2 (572.2): \text{calcd.} \text{ C 62.98, H 5.64, N 14.69; found: C 62.80, H 5.80, N 14.79}. \text{FAB}^+-\text{MS, } m/z: 572 \text{ [M]}^+. \text{IR (KBr): } 3203 [(vs) \nu(\text{NH})], 2934 [(vs) \nu_{\text{as}}(\text{CH})], 2851 [(s) \nu_{\text{d}}(\text{CH})], 1698 [(vs) \nu(\text{C}=\text{O})], 1618 (vs) \text{ and 1602 [(vs) } \nu(\text{C}=\text{N})], 1552 [(vs) } \delta(\text{NH})] \text{ cm}^{-1}.

[\text{Cu}\{\text{HN=CH}_{\text{3}}\text{CN=C}({\text{C}}_{\text{6}}\text{H}_{\text{4}}\text{CO})\}_2\} (6). \text{C}_{32}\text{H}_{24}\text{N}_6\text{CuO}_2 (588.1): \text{calcd.} \text{ C 65.35, H 4.11, N 14.29; found: C 65.08, H 4.96, N 14.17}. \text{FAB}^+-\text{MS, } m/z: 588 \text{ [M]}^+. \text{IR (KBr): } 3192 [(s) \nu(\text{NH})], 3028 \text{ and 2925 [(m-w) } \nu_{\text{as}}(\text{CH})], 2853 [(m) \nu_{\text{d}}(\text{CH})], 1695 [(vs) \nu(\text{C}=\text{O})], 1620 (vs) \text{ and 1597 [(vs) } \nu(\text{C}=\text{N})], 1545 \text{ vs } \delta(\text{NH})] \text{ cm}^{-1}.

[\text{Cu}\{\text{HN=CH}_{\text{3}}\text{CN=C}({\text{C}}_{\text{6}}\text{H}_{\text{4}}\text{CO})\}_2\} (7). \text{C}_{22}\text{H}_{20}\text{N}_6\text{CuO}_2 (464.0): \text{calcd.} \text{ C 56.95, H 4.35, N 18.11; found: C 57.05, H 4.44, N 18.07}. \text{FAB}^+-\text{MS, } m/z: 464 \text{ [M]}^+. \text{IR (KBr): } 3202 [(s) \nu(\text{NH})], 2963 \text{ and 2924 [(m-w) } \nu_{\text{as}}(\text{CH})], 2855 [(m) \nu_{\text{d}}(\text{CH})], 1687 [(s) \nu(\text{C}=\text{O})], 1610 (s) \text{ and 1602 [(vs) } \nu(\text{C}=\text{N})], 1548 [(vs) } \delta(\text{NH})], 747 [(s) } \delta(\text{CH from Ar})] \text{ cm}^{-1}.

[\text{Cu}\{\text{HN=CH}_{\text{3}}\text{CN=C}({\text{C}}_{\text{6}}\text{H}_{\text{4}}\text{CO})\}_2\} (8). \text{C}_{24}\text{H}_{24}\text{N}_6\text{CuO}_2 (492.0): \text{calcd.} \text{ C 58.59, H 4.92, N 17.08; found: C 58.66, H 4.87, N 17.23}. \text{FAB}^+-\text{MS, } m/z: 492 \text{ [M]}^+. \text{IR (KBr): } 3194 [(s) \nu(\text{NH})], 2974 \text{ and 2922 [(m-w) } \nu_{\text{as}}(\text{CH})], 2885 [(m) \nu_{\text{d}}(\text{CH})], 1697 [(s) \nu(\text{C}=\text{O})], 1617 (s) \text{ and 1606 [(vs) } \nu(\text{C}=\text{N})], 1554 \text{ vs } \delta(\text{NH}), 744 [(s) } \delta(\text{CH from Ar})] \text{ cm}^{-1}.

[\text{Cu}\{\text{HN=CH}_{\text{3}}\text{CN=C}({\text{C}}_{\text{6}}\text{H}_{\text{4}}\text{CO})\}_2\} (9). \text{C}_{24}\text{H}_{24}\text{N}_6\text{CuO}_2 (520.1): \text{calcd.} \text{ C 60.04, H 5.43, N 16.16; found: C 59.88, H 5.55, N 16.02}. \text{FAB}^+-\text{MS, } m/z: 520 \text{ [M]}^+. \text{IR (KBr): } 3204 [(vs) \nu(\text{NH})],
2968 and 2924 [(m-w) $\nu_{as}(CH)$], 2870 [(m) $\nu_{s}(CH)$], 1698 [(vs) $\nu(C=O)$], 1603 [(vs) $\nu(C=N)$], 1548 [(vs) $\delta(NH)$], 760 [(s) $\delta(CH$ from Ar)] cm\(^{-1}\).

[Cu\{H\N=C(Et)N=C(C_6H_2Cl_2CO)\N\}$_2$] (10). C$_{22}$H$_{16}$N$_6$CuO$_2$Cl$_4$ (601.8): calcd. C 43.91, H 2.68, N 13.97; found: C 44.04, H 2.60, N 14.12%. FAB\(^{-}\)-MS, $m/z$: 602 [M$^+$]. IR (KBr): 3190 [(m-w) $\nu(NH)$], 2975 [(w) $\nu_{as}(CH)$], 2937 [(w) $\nu_{s}(CH)$], 1696 [(vs) $\nu(C=O)$], 1612 (vs) and 1598 [(vs) $\nu(C=N)$], 1558 [(vs) $\delta(NH)$] cm\(^{-1}\).

[Cu\{H\N=C(Et)N=C(C_6F_4CO)\N\}$_2$] (11). C$_{22}$H$_{12}$N$_6$CuO$_2$F$_8$ (607.9): calcd. C 43.47, H 1.99, N 13.83; found: C 43.27, H 1.90, N 14.00%. FAB\(^{-}\)-MS, $m/z$: 608 [M$^+$]. IR (KBr): 3204 [(m-w) $\nu(NH)$], 2989 [(w) $\nu_{as}(CH)$], 2921 [(w) $\nu_{s}(CH)$], 1708 [(s) $\nu(C=O)$], 1609 [(vs) $\nu(C=N)$], 1568 [(s) $\delta(NH)$] cm\(^{-1}\).