Electronic Supplementary Information

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

Maximilian N. Kopylovich,[1] Konstantin V. Luzyanin,[1] Matti Haukka,[2] Armando J. L. Pombeiro*[1] and Vadim Yu. Kukushkin*[3,4]

[1] *Centro de Química Estrutural, Complexo I, Instituto Superior Técnico, TU Lisbon, Av. Rovisco Pais, 1049–001 Lisbon, Portugal. E-mail: pombeiro@ist.utl.pt*
[2] *Department of Chemistry, University of Joensuu, Department of Chemistry, P.O. Box 111, FI-80101, Joensuu, Finland*
[3] *St.Petersburg State University, 198504 Stary Petergof, Russian Federation. E-mail: kukushkin@VK2100.spb.edu*
[4] *Institute of Macromolecular Compounds of the Russian Academy of Sciences, V. O. Bolshoi Pr. 31, 199004 St.Petersburg, Russian Federation*

[Cu{H*N*=C(Pr^n)N=C(C$_6$H$_4$CO)*N*}$_2$] (**3**). $C_{24}H_{24}N_6CuO_2$ (492.0): calcd. C 58.59, H 4.92, N 17.08; found: C 58.26, H 4.86, N 16.92%. FAB$^+$-MS, *m/z*: 492 $[M]^+$. IR (KBr): 3203 [(s) *ν*(NH)], 2960 and 2931 [(m-w) ν_{as}(CH)], 2873 [(m) ν_s(CH)], 1695 [(s) *ν*(C=O)], 1616 (s) and 1602 [(vs) *ν*(C=N)], 1553 [(vs) *δ*(NH)] cm^{-1}.

[Cu{H*N*=C(C$_6$H$_{11}$)N=C(C$_6$H$_4$CO)*N*}$_2$] (**5**). $C_{30}H_{32}N_6CuO_2$ (572.2): calcd. C 62.98, H 5.64, N 14.69; found: C 62.80, H 5.80, N 14.79%. FAB$^+$-MS, *m/z*: 572 $[M]^+$. IR (KBr): 3203 [(vs) *ν*(NH)], 2934 [(vs) ν_{as}(CH)], 2851 [(s) ν_s(CH)], 1698 [(vs) *ν*(C=O)], 1618 (vs) and 1602 [(vs) *ν*(C=N)], 1552 [(vs) *δ*(NH)] cm^{-1}.

[Cu{H*N*=C(CH$_2$Ph)N=C(C$_6$H$_4$CO)*N*}$_2$] (**6**). $C_{32}H_{24}N_6CuO_2$ (588.1): calcd. C 65.35, H 4.11, N 14.29; found: C 65.08, H 4.96, N 14.17%. FAB$^+$-MS, *m/z*: 588 $[M]^+$. IR (KBr): 3192 [(s) *ν*(NH)], 3028 and 2925 [(m-w) ν_{as}(CH)], 2853 [(m) ν_s(CH)], 1695 [(vs) *ν*(C=O)], 1620 (vs) and 1597 [(vs) *ν*(C=N)], 1545 vs *δ*(NH) cm^{-1}.

[Cu{*N*H=C(Me)N=C(C$_6$H$_3$(4-Me)CO*N*)$_2$] (**7**). $C_{22}H_{20}N_6CuO_2$ (464.0): calcd. C 56.95, H 4.35, N 18.11; found: C 57.05, H 4.44, N 18.07%. FAB$^+$-MS, *m/z*: 464 $[M]^+$. IR (KBr): 3202 [(s) *ν*(NH)], 2963 and 2924 [(m-w) ν_{as}(CH)], 2855 [(m) ν_s(CH)], 1687 [(s) *ν*(C=O)], 1610 (s) and 1602 [(vs) ν(C=N)], 1548 [(vs) *δ*(NH)], 747 [(s) *δ*(CH from Ar)] cm^{-1}.

[Cu{*N*H=C(Et)N=C(C$_6$H$_3$(4-Me)CO*N*)$_2$] (**8**). $C_{24}H_{24}N_6CuO_2$ (492.0): calcd. C 58.59, H 4.92, N 17.08; found: C 58.66, H 4.87, N 17.23%. FAB$^+$-MS, *m/z*: 492 $[M]^+$. IR (KBr): 3194 [(s) *ν*(NH)], 2974 and 2922 [(m-w) ν_{as}(CH)], 2885 [(m) ν_s(CH)], 1697 [(s) *ν*(C=O)], 1617 (s) and 1606 [(vs) *ν*(C=N)], 1554 vs *δ*(NH), 744 [(s) *δ*(CH from Ar)] cm^{-1}.

[Cu{*N*H=C(Pr^i)N=C(C$_6$H$_3$(4-Me)CO*N*)$_2$] (**9**). $C_{24}H_{24}N_6CuO_2$ (520.1): calcd. C 60.04, H 5.43, N 16.16; found: C 59.88, H 5.55, N 16.02%. FAB$^+$-MS, *m/z*: 520 $[M]^+$. IR (KBr): 3204 [(vs) *ν*(NH)],

2968 and 2924 [(m-w) ν_{as}(CH)], 2870 [(m) ν_{s}(CH)], 1698 [(vs) ν(C=O)], 1603 [(vs) ν(C=N)], 1548 [(vs) δ(NH)], 760 [(s) δ(CH from Ar)] cm^{-1}.

[Cu{H*N*=C(Et)N=C($C_6H_2Cl_2CO$)*N*}$_2$] (**10**). $C_{22}H_{16}N_6CuO_2Cl_4$ (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) ν(NH)], 2975 [(w) ν_{as}(CH)], 2937 [(w) ν_{s}(CH)], 1696 [(vs) ν(C=O)], 1612 (vs) and 1598 [(vs) ν(C=N)], 1558 [(vs) δ(NH)] cm^{-1}.

[Cu{H*N*=C(Et)N=C(C_6F_4CO)*N*}$_2$] (**11**). $C_{22}H_{12}N_6CuO_2F_8$ (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) ν(NH)], 2989 [(w) ν_{as}(CH)], 2921 [(w) ν_{s}(CH)], 1708 [(s) ν(C=O)], 1609 [(vs) ν(C=N)], 1568 [(s) δ(NH)] cm^{-1}.