ESI

A combined experimental and DFT investigation on the structure and CO-releasing properties of mono and binuclear *fac*-$Re^{I}(CO)_3$ complexes with 5-pyridin-2-ylmethylene-amino uracils†

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CONTENTS

Analytical data

DAAUPic (yellow)
Calc. for $C_{12}H_{13}N_5O_2$ (259.27): C, 55.59; H, 5.05; N, 27.01%.
Found: C, 55.36; H, 5.14; N, 27.56%.

FDUHzPic·H_2O (yellow)
Calc. for $C_{13}H_{16}N_6O_3$ (304.31): C, 51.31; H, 5.30; N, 27.62%.
Found: C, 51.27; H, 5.20; N, 27.66%.

[ReCl(CO)$_3$(DAAUPic)]·½C_7H_8 (1a)
Calc. for $C_{18.5}H_{17}ClN_5O_5Re$ (611.03): C, 36.37; H, 2.80; N, 11.46%;
found: C, 35.98; H, 2.68; N, 11.10%.

[ReCl(CO)$_3$(FDUHzPic)]·2H_2O (1b)
Calc. for $C_{16}H_{18}ClN_6O_7Re$ (628.01): C, 30.60; H, 2.89; N, 13.38%;
found: C, 30.90; H, 2.35; N, 13.49%.

[Re(CO)$_3$(DAAUPic)(CH_3CN)]ClO_4·2H_2O (2a)
Calc. for $C_{17}H_{20}ClN_6O_{11}Re$ (706.04): C, 28.92; H, 2.86; N, 11.90%;
found: C, 28.56; H, 2.48; N, 11.50%.

[Re(CO)$_3$(FDUHzPic)(CH_3CN)]ClO_4·4H_2O (2b)
Calc. for $C_{18}H_{25}ClN_7O_{13}Re$ (769.09): C, 28.11; H, 3.28; N, 12.75%;
found: C, 27.95; H, 3.06; N, 12.46%.

[Re(DAAUPic)(CO)$_3$py]ClO_4 (3a)
Calc. for $C_{20}H_{18}ClN_6O_9Re$ (708.06): C, 33.93; H, 2.56; N, 11.87%;
found: C, 34.15; H, 2.70; N, 11.45%.

[Re(FDUHzPic)(CO)$_3$py]ClO_4 (3b)
Calc. for $C_{21}H_{19}ClN_7O_9Re$ (735.08): C, 34.31; H, 2.61; N, 13.34%;
found: C, 34.13; H, 2.60; N, 13.52%.

[Re(CO)$_3$(DAAUPic)py]PF_6·2H_2O (4a)
Calc. for $C_{20}H_{22}PF_6N_6O_7Re$ (789.59): C, 30.42; H, 2.81; N, 10.64%;
found: C, 30.49; H, 2.47; N, 10.51%.

[Re(CO)$_3$(FDUHzPic)py]PF_6 (4b)
Calc. for $C_{21}H_{19}F_6N_7O_5PRe$ (780.59): C, 32.31; H, 2.45; N, 12.56%;
found: C, 32.01; H, 2.67; N, 12.54%.

[Re_2Cl_2(CO)$_6$(FDUHzPic)] (5b)
Calc. for $C_{19}H_{14}Cl_2N_6O_8Re_2$ (897.67): C, 25.42; H, 1.57; N, 9.36%;
found: C, 25.55; H, 1.64; N, 9.43%.

[Re_2(CO)$_6$(FDUHzPic)(CH_3CN)$_2$](ClO_4)$_2$·2H_2O (7b)
Calc. for $C_{23}H_{24}Cl_2N_8O_{18}Re_2$ (1143.81): C, 24.15; H, 2.11; N, 9.80%;
found: C, 24.62; H, 2.10; N, 9.21%.

Selected IR data (KBr, cm^{-1})

· **DAAUPic**
3399 (m), 3246 (w), 3089 (m), 1688 (s), 1625 (m), 1597 (s), 1542 (m), 1511(s), 1452 (m), 1429 (s), 1378 (m), 1288 (w), 1057 (m), 997 (m), 759 (m), 750 (m).

· **FDUHzPic·H_2O**
3316 (s), 3075 (s), 2948 (m), 1700 (s), 1645 (s), 1617 (s), 1595 (s), 1540 (s), 1452 (s), 1384 (m), 1297(m), 1178 (m), 1032 (m), 768 (m), 752 (m).

· **[ReCl(CO)$_3$(DAAUPic)]·½C_7H_8 (1a)**
3369 (m), 3206 (m), 3077 (w), 2024 (s), 1902 (s), 1693 (s), 1645 (s), 1625 (s), 1586 (s), 1542 (m), 1506(s), 1456 (m), 1429 (m), 1382 (m), 1230 (m), 1064 (m), 776 (m), 762 (m).

· **[ReCl(CO)$_3$(FDUHzPic)]·2H_2O (1b)**
3455 (m), 3318 (m), 2028 (s), 1979 (m), 1911 (s), 1709 (s), 1650 (s), 1625 (s), 1543 (s), 1451 (s), 1384 (m), 1275 (w), 770 (w).

· **[Re(CO)$_3$(DAAUPic)(CH_3CN)]ClO_4·2H_2O (2a)**
3416 (s), 2320(vw), 2302 (w), 2036 (s), 1930 (s), 1695 (s), 1628 (s), 1510 (m), 1449 (m), 1382 (w), 1230 (w), 1119 (m), 1084 (m), 776 (m), 628 (m).

· **[Re(CO)$_3$(FDUHzPic)(CH_3CN)]ClO_4·4H_2O (2b)**
3422 (b), 2324 (vw), 2296 (w), 2040 (s), 1930 (s), 1709 (m), 1651 (s), 1590 (m), 1537 (m), 1108 (s), 1090(s), 772 (m), 752 (m), 625 (m).

· **[Re(DAAUPic)(CO)$_3$py]ClO_4 (3a)**
3413 (m), 2935 (w), 2029 (s), 1913 (s), 1693 (s), 1637 (s), 1608 (m), 1587 (m), 1530 (s), 1447 (m), 1287 (w), 1090 (s), 760 (m), 703 (m), 625 (m).

· **[Re(FDUHzPic)(CO)$_3$py]ClO_4 (3b)**
3412 (m), 2922 (w), 2032 (s), 1914 (s), 1708 (s), 1650 (s), 1607 (m), 1536 (s), 1094 (s), 1068 (s), 764 (m), 701 (m), 623 (m).

· **[Re(CO)$_3$(DAAUPic)py]PF_6·2H_2O (4a)**
3467 (m), 3218 (w), 2031 (s), 1937 (s), 1918 (s), 1697 (m), 1628 (m), 1602 (m), 1512 (s), 1449 (m), 1288 (w), 1069 (w), 844 (s), 762(m), 703 (m), 559 (m).

· **[Re(CO)$_3$(FDUHzPic)py]PF_6 (4b)**
3441 (m), 2034 (s), 1942 (s), 1918 (s), 1708 (m), 1649 (s), 1588 (m), 1538 (m), 1450 (m), 1281 (w), 843 (s), 775 (w), 753 (w), 558 (m).

· **[Re_2Cl_2(CO)$_6$(FDUHzPic)] (5b)**
3468 (m), 3318 (m), 2121(m), 2026 (s), 2000(m), 1932(s), 1911 (s), 1709 (m), 1661(m), 1615 (s), 1543 (s), 1451 (m), 769 (w), 752 (w).

· **[Re_2Cl(CO)$_6$(FDUH$_z$PicH$_{-1}$)(H_2O)]·2DMSO (6b)**
3462 (m), 2028 (s), 1979 (m), 1928 (s), 1910 (s), 1880 (s), 1714 (m), 1662 (s), 1630 (m), 1541 (m), 1450 (m), 772 (w).

· **[Re_2(CO)$_6$(FDUHzPic)(CH_3CN)$_2$](ClO_4)$_2$·2H_2O (7b)**
3415 (m), 3003(w), 2937 (w), 2327 (vw), 2298 (w), 2061 (s), 2040 (m), 1953 (s), 1931 (s), 1922 (s), 1709 (m), 1647 (m), 1590 (w), 1538 (m), 1455 (m), 1091 (s), 1031 (m), 769 (w), 752 (w), 625 (m).

NMR data (DMSO-d_6, δ, ppm):

· **DAAUPic**
^{13}C NMR: 157.14 (C6), 156.86 (C2F), 153.98 (C4), 149.72 (C2), 149.15 (C51), 148.80 (C6F), 136.35 (C5F), 123.32 (C4F), 119.96 (C3F), 98.76 (C5), 30.38 (C3), 27.09 (C1). ^{1}H NMR: 9.69 (s, 1H, H51), 8.55 (d, 1H, H6F), 8.40 (d, 1H, H3F), 7.80 (t, 1H, H5F), 7.47 (s, 2H, N6-H_2), 7.31 (t, 1H, H4F), 3.40 (s, 3H, N3-CH_3), 3.17 (s, 3H, N1-CH_3).

· **FDUHzPic·H_2O**
^{13}C NMR: 161.34 (C51), 161.15 (C6), 158.02 (C52), 154.92 (C4), 153.09 (C2F), 150.23 (C6F), 149.73 (C2), 136.91 (C5F), 124.85 (C4F), 120.93 (C3F), 83.39 (C5), 29.59 (C3), 27.66 (C1). ^{1}H NMR: 10.02 (s, 1H, N6-H_2), 8.92 (s, 1H, H51), 8.65 (d, 1H, H6F), 8.54 (s, 1H, H52), 8.43 (s, 1H, N6-H_2), 8.06 (d, 1H, H3F), 7.88 (t, 1H, H5F), 7.44 (t, 1H, H4F), 3.36 (s, 3H, N3-CH_3), 3.17 (s, 3H, N1-CH_3).

· **[ReCl(CO)$_3$(DAAUPic)]·½C_7H_8 (1a)**
^{13}C NMR: 196.74, 196.66, 187.50 (CO), 174.52 (C51), 155.58 (C6), 154.34 (C4), 153.18 (C6F), 149.61 (C2), 148.74 (C2F), 140.73 (C5F), 137.31 (Ci-T), 129.78 (C4F), 129.77 (C3F), 128.86 (CH-T(o)), 128.16 (CH-T(m)), 125.02 (CH-T(p)), 105.90 (C5), 30.11 (C3), 28.16 (C1), 21.00 (CH_3-T). ^{1}H NMR: 9.33 (s, 1H, H51), 9.05 (d, 1H, H6F), 8.35 (d, 1H, H3F), 8.30 (t, 1H, H5F), 7.85 (t, 1H, H4F), 7.52 (s, 2H, N6-H_2), 7.25 (m, CH-T(m)), 7.15 (m, CH-T(o/p)), 3.38 (s, 3H, N3-CH_3), 3.23 (s, 3H, N1-CH_3), 2.29 (s, 3H, CH_3-T).

· **[ReCl(CO)$_3$(FDUHzPic)]·2H_2O (1b)**
^{13}C NMR: 188.3, 187.63, 187.01 (CO), 162.53 (C52), 161.33 (C51), 160.91 (C6), 155.40 (C4), 154.26 (C2F), 153.10 (C6F), 150.09 (C2), 140.35 (C5F), 128.84 (C4F), 128.57 (C3F), 83.40 (C5), 29.91 (C3), 27.77 (C1). ^{1}H NMR: 9.50 (s, 1H, N6-H_2), 9.38 (s, 1H, H52), 9.25 (s, 1H, H51), 9.02 (d, 1H, H6F), 8.73 (s, 1H, N6-H_2), 8.29 (t, 1H, H5F), 8.20 (d, 1H, H3F), 7.74 (t, 1H, H4F), 3.40 (s, 3H, N3-CH_3), 3.20 (s, 3H, N1-CH_3).

· **[Re(CO)$_3$(DAAUPic)(CH_3CN)]ClO_4·2H_2O (2a)**
^{13}C NMR: 196.10, 196.02, 189.50 (CO), 175.32 (C51), 156.04 (C6), 155.72 (C4), 153.36 (C6F), 149.77 (C2F), 148.68 (C2), 141.46 (C5F), 130.27 (C4F), 129.46 (C3F), 118.02 (CN-(CH_3)), 105.34 (C5), 30.25 (C3), 28.07 (C1), 1.07 (CH_3(-CN)). ^{1}H NMR: 9.38 (s, 1H, H51), 9.15 (d, 1H, H6F), 9.12 (d, 1H, H3F), 8.43 (m, 1H, H5F), 7.88 (m, 1H, H4F), 7.25 (s, 2H, N6-H_2), 3.41 (s, 3H, N3-CH_3), 3.23 (s, 3H, N1-CH_3), 2.06 (s, 3H, CH_3-CN).

· **[Re(CO)$_3$(FDUHzPic)(CH_3CN)]ClO_4·4H_2O (2b)**
^{13}C NMR: 190.92, 189.57, 189.15 (CO), 164.20 (C52), 160.98 (C51), 159.88 (C6), 155.47 (C4), 154.19 (C2F), 153.83 (C6F), 150.03 (C2), 141.69 (C5F), 129.40 (C4F), 129.18 (C3F), 118.06 (CN-(CH_3)), 83.38 (C5), 29.98 (C3), 27.82 (C1), 1.12 (CH_3-(CN)). ^{1}H NMR: 9.46 (s, 1H, H52), 9.39 (s, 1H, N6-H_2), 9.22 (s, 1H, H51), 9.15 (d, 1H, H6F), 8.78, (s, 2H, N6-H_2), 8.40 (t, 1H, H5F), 8.23 (d, 1H, H3F), 7.84 (t, 1H, H4F), 3.40 (s, 3H, N3-CH_3), 3.20 (s, 3H, N1-CH_3), 2.06 (s, 3H, CH_3-CN).

· **[Re(DAAUPic)(CO)$_3$py]ClO_4 (3a)**
^{13}C NMR: 194.10, 192.22, 190.50 (CO), 174.23 (C51), 156.74 (C6), 153.17 (C6F), 152.66 (C4), 152.59 (CH(2)-py), 151.90 (C2F), 147.12 (C2), 140.46 (CH(4)-py), 141.41 (C5F), 130.67 (C4F), 127.22 (C3F), 126.79 (CH(3)-py), 105.04 (C5), 30.51 (C3), 28.62 (C1). ^{1}H NMR: 9.31 (s, 1H, H51), 9.22 (d, 1H, H6F), 9.08 (d, 1H, H3F), 8.39 (m, CH(2)-py), 8.12

(m, 1H, H5F), 7.95 (m, CH(4)-py), 7.65 (m, 1H, H4F), 7.52 (s, 2H, N6-H_2), 7.39 (m, CH(3)-py), 3.44 (s, 3H, N3-CH_3), 3.12 (s, 3H, N1-CH_3).

· **[Re(FDUHzPic)(CO)$_3$py]ClO_4 (3b)**
^{13}C NMR: 190.72, 189.52, 189.45 (CO), 164.22 (C52), 161.36 (C51), 161.01 (C6), 155.54 (C4), 154.36 (C2F), 153.99 (C6F), 152.47 (CH(2)-py), 150.03 (C2), 141.56 (C5F), 136.51 (CH(4)-py), 129.94 (C4F), 129.59 (C3F), 127.31 (CH(3)-py), 83.77 (C5), 30.04 (C3), 27.85 (C1). ^{1}H NMR: 9.43 (s, 1H, H52), 9.32 (s, 1H, H51), 9.29 (d, 1H, H6F), 8.84, (s, 2H, N6-H_2), 8.57 (m, CH(2)-py), 8.36 (t, 1H, H5F), 8.14 (d, 1H, H3F), 7.89 (m, CH(4)-py), 7.78 (t, 1H, H4F), 7.39 (m, CH(3)-py), 3.43 (s, 3H, N3-CH_3), 3.22 (s, 3H, N1-CH_3).

· **[Re(CO)$_3$(DAAUPic)py]$PF_6\cdot 2H_2O$ (4a)**
^{13}C NMR: 196.23, 195.77, 190.68 (CO), 174.54 (C51), 156.38 (C6), 154.35 (C4), 152.29 (CH(2)-py),153.19 (C6F), 149.77 (C2F), 148.74 (C2), 141.46 (C5F), 138.42 (CH(4)-py), 130.10 (C4F), 129.80 (C3F), 126.50 (CH(3)-py), 105.37 (C5), 30.25 (C3), 28.16 (C1). ^{1}H NMR: 9.35 (s, 1H, H51), 9.15 (d, 1H, H6F), 8.52 (m, CH(2)-py), 8.40 (m, 1H, H3F), 8.18 (m, 1H, H5F), 7.85 (m, 1H, H4F), 7.95(m, CH(4)-py), 7.55 (s, 2H, N6-H_2), 7.38 (m, CH(3)-py), 3.45 (s, 3H, N3-CH_3), 3.13 (s, 3H, N1-CH_3).

· **[Re(CO)$_3$(FDUHzPic)py]PF_6 (4b)**
^{13}C NMR: 194.46, 192.15, 189.99 (CO), 164.24 (C52), 161.36 (C51), 161.95 (C6), 155.50 (C4), 154.33 (C6F), 153.96 (C2F), 152.44 (CH(2)-py), 149.98 (C2), 141.52 (C5F), 140.42 (CH(4)-py), 129.90 (C4F), 129.55 (C3F), 127.17 (CH(3)-py), 83.73 (C5), 30.01 (C3), 27.80 (C1). ^{1}H NMR: 9.44 (s, 1H, H52), 9.36 (s, 1H, H51), 9.24 (d, 1H, H6F), 8.84 (s, 1H, N6-H_2), 8.34 (m, CH(2)-py), 8.14 (t, 1H, H5F), 8.14 (d, 1H, H3F), 8.08 (m, CH(4)-py), 7.82 (t, 1H, H4F), 7.45 (m, CH(3)-py), 3.42 (s, 3H, N3-CH_3), 3.21 (s, 3H, N1-CH_3).

· **[Re_2Cl_2(CO)$_6$(FDUHzPic)] (5b)**
^{13}C NMR: 195.10, 193.82, 189.57 (CO), 162.53 (C52), 161.32 (C51), 160.90 (C6), 155.40 (C4), 154.23 (C2F), 153.09 (C6F), 150.08 (C2), 140.34 (C5F), 128.83 (C4F), 128.55 (C3F), 83.39 (C5), 29.90 (C3), 27.76 (C1). ^{1}H NMR: 9.50 (s, 1H, N6-H_2), 9.38 (s, 1H, H52), 9.25 (s, 1H, H51), 9.01 (d, 1H, H6F), 8.73 (s, 2H, N6-H_2), 8.29 (t, 1H, H5F), 8.20 (d, 1H, H3F), 7.74 (t, 1H, H4F), 3.40 (s, 3H, N3-CH_3), 3.20 (s, 3H, N1-CH_3).

· **[Re_2(CO)$_6$(FDUHzPic)(CH_3CN)$_2$]$(ClO_4)_2\cdot 2H_2O$ (7b)**
^{13}C NMR: 192.01, 191.95, 189.56 (CO), 164.18 (C52), 160.92 (C51), 155.44 (C4), 154.18 (C2F), 153.81 (C6F), 150.01 (C2), 141.67 (C5F), 129.43 (C4F), 129.36 (C3F), 118.05 (CN-(CH_3)), 83.36 (C5), 29.96 (C3), 27.78 (C1), 1.10 (CH_3-(CN)). ^{1}H NMR: 9.50 (s, 1H, H52), 9.41 (s, 2H, N6-H_2), 9.15 (s, 1H, H51), 9.09 (d, 1H, H6F), 8.80 (s, 2H, N6-H_2), 8.40 (t, 1H, H5F), 8.28 (d, 1H, H3F), 7.85 (t, 1H, H4F), 3.41 (s, 3H, N3-CH_3), 3.21 (s, 3H, N1-CH_3), 2.07 (s, 3H, CH_3-CN).

MS data

· **DAAUPic**
MS (m/z): 260 $[L-H]^+$, 181 $[C_7H_9N_4O_2]^+$, 79 $[C_5H_5N]^+$.

· **FDUHzPic·H_2O**
MS (m/z): 287 $[L+H]^+$, 181 $[C_7H_9N_4O_2]^+$, 106 $[C_6H_5N_2+H]^+$.

· **$[ReCl(CO)_3(DAAUPic)]\cdot\frac{1}{2}C_7H_8$ (1a)**
ESI-MS (m/z, CH_3CN/H_2O): 565 $[ReCl(CO)_3L]H^+$, 501 $[Re(CO)_2L]^+$.

· **$[ReCl(CO)_3(FDUHzPic)]\cdot 2H_2O$ (1b)**
ESI-MS (m/z, CH_3CN/H_2O): 592 $[ReCl(CO)_3L]H^+$, 556 $[Re(CO)_3L]^+$.

· **$[Re(CO)_3(DAAUPic)(CH_3CN)]ClO_4\cdot 2H_2O$ (2a)**
ESI-MS (m/z, CH_3CN/H_2O): 571 $[Re(CO)_3L(CH_3CN)]^+$, 530 $[Re(CO)_3L]^+$, 502 $[Re(CO)_2L]^+$.

· **$[Re(CO)_3(FDUHzPic)(CH_3CN)]ClO_4\cdot 4H_2O$ (2b)**
ESI-MS (m/z, CH_3CN/H_2O): 598 $[Re(CO)_3L(CH_3CN)]^+$, 556 $[Re(CO)_3L]^+$.

· **$[Re(DAAUPic)(CO)_3py]ClO_4$ (3a)**
ESI-MS (m/z, CH_3CN/H_2O): 609 $[Re(CO)_3Lpy]^+$, 530 $[Re(CO)_3L]^+$, 502 $[Re(CO)_2L]^+$.

· **$[Re(FDUHzPic)(CO)_3py]ClO_4$ (3b)**
ESI-MS (m/z, CH_3CN/H_2O): 636 $[Re(CO)_3Lpy]^+$, 556 $[Re(CO)_3L]^+$.

· **$[Re(CO)_3(DAAUPic)py]PF_6\cdot 2H_2O$ (4a)**
ESI-MS (m/z, CH_3CN/H_2O): 609 $[Re(CO)_3Lpy]^+$, 530 $[Re(CO)_3L]^+$, 502 $[Re(CO)_2L]^+$.

· **$[Re(CO)_3(FDUHzPic)py]PF_6$ (4b)**
ESI-MS (m/z, CH_3CN/H_2O): 636 $[Re(CO)_3Lpy]^+$, 556 $[Re(CO)_3L]^+$.

· **$[Re_2Cl_2(CO)_6(FDUHzPic)]$ (5b).**
ESI-MS (m/z, CH_3CN/H_2O): 904 $[Re_2Cl(CO)_6L(CH_3CN)]^+$, 863 $[Re_2Cl(CO)_3L]^+$.

· **$[Re_2(CO)_6(FDUHzPic)(CH_3CN)_2](ClO_4)_2\cdot 2H_2O$ (7b)**
ESI-MS (m/z, CH_3CN/H_2O): 867 $[Re_2(CO)_6L(CH_3CN)]^{2+}$, 827 $[Re_2(CO)_6L]^{2+}$, 771 $[Re_2(CO)_4L]^{2+}$.

Table S1
Mulliken charges for the atoms of the coordination sphere in complexes **6b**, **4b** and **1a**.

Atom/Method	M06L	ωB97XD	B3LYP
$[Re_2Cl(CO)_6(FDUHzPicH_{-1})(H_2O)]$ (**6b**)			
Re1	0.59	0.26	0.32
C7X	0.34	0.35	0.30
C8X	0.33	0.35	0.30
C9X	0.36	0.37	0.30
N1F	-0.81	-0.72	-0.67
N52	-0.53	-0.50	-0.44
Cl	-0.57	-0.51	-0.54
Re2	0.54	0.27	0.38
C7Y	0.37	0.38	0.33
C8Y	0.31	0.32	0.26
C9Y	0.32	0.33	0.27
O1W	-0.78	-0.74	-0.72
N6	-0.96	-0.87	-0.70
N51	-0.61	-0.56	-0.53
Balance	-1.10	-1.27	-1.14
$[Re(CO)_3(FDUHzPic)py]^+$ (**4b**)			
Re	0.69	0.36	0.39
C7X	0.32	0.34	0.31
C8X	0.28	0.30	0.25
C9X	0.31	0.32	0.28
N1F	-0.84	-0.73	-0.69
N52	-0.56	-0.50	-0.48
N1P	-0.78	-0.70	-0.66
Balance	-0.58	-0.61	-0.60
$[ReCl(CO)_3(DAAUPic)]$ (**1a**)			
Re	0.52		
C7X	0.33		
C8X	0.32		
C9X	0.33		
Cl	-0.58		
N1F	-0.99		
N52	-0.85		
Balance	-0.92		