Supplementary information for:

# From Structure to Function: A One-Dimensional Palladium(II) Hybrid for Real-Sample Hydroquinone Detection

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**Table S1.** Crystal data and refinement parameters of $(C_4H_7N_2)[PdCl_3(H_2O)]$.

| Formula | $(C_4H_7N_2)[PdCl_3(H_2O)]$ |
|---|---|
| $D_{calc.}$/ g cm$^{-3}$ | 2.126 |
| $\mu$/mm$^{-1}$ | 2.658 |
| Formula Weight | 313.88 |
| Colour | colourless |
| Shape | Block-shaped |
| Size/mm$^3$ | 0.59×0.23×0.18 |
| $T$/K | 100.00(10) |
| Crystal System | monoclinic |
| Space Group | $P2_1/c$ |
| $a$/Å | 9.0007(2) |
| $b$/Å | 14.7508(4) |
| $c$/Å | 7.4059(2) |
| $\alpha^\circ$ | 90 |
| $\beta^\circ$ | 94.084(2) |
| $\gamma^\circ$ | 90 |
| $V$/Å$^3$ | 980.77(4) |
| $Z$ | 4 |
| $Z'$ | 1 |
| Wavelength/Å | 0.71073 |
| Radiation type | Mo K$_\alpha$ |
| $\Theta_{min}$ $^\circ$ | 5.393 |
| $\Theta_{max}$ $^\circ$ | 30.208 |
| Measured Refl's. | 14007 |
| Indep't Refl's | 2517 |
| Refl's I$\geq$2 $\sigma$(I) | 2320 |
| $R_{int}$ | 0.0916 |
| Parameters | 103 |
| Restraints | 0 |
| Largest Peak | 0.872 |
| Deepest Hole | -0.894 |
| GooF | 1.044 |
| $wR_2$ | 0.1063 |
| $R_1$ | 0.0389 |

**Table S2.** Molecular geometric parameters (Å, °) of $(C_4H_7N_2)[PdCl_3(H_2O)]$.

| Bond length (Å) | | | |
|---|---|---|---|
| Pd1—Cl3 | 2.6143 (8) | N2—H2 | 0.8800 |
| Pd1—Cl3i | 2.6508 (9) | N2—C2 | 1.387 (4) |
| Pd1—Cl2 | 2.5762 (8) | N2—C1 | 1.327 (4) |
| Pd1—Cl2ii | 2.5886 (9) | C2—H2A | 0.9500 |
| Pd1—Cl1 | 2.5984 (8) | C2—C3 | 1.348 (5) |
| Pd1—O1 | 2.391 (2) | C4—H4A | 0.9800 |
| O1—H1A | 0.8514 | C4—H4B | 0.9800 |
| O1—H1B | 0.8516 | C4—H4C | 0.9800 |
| N1—H1 | 0.8800 | C4—C1 | 1.478 (5) |
| N1—C1 | 1.335 (4) | C3—H3 | 0.9500 |
| N1—C3 | 1.375 (4) | | |
| **Bond angles (°)** | | | |
| Cl3—Pd1—Cl3i | 89.62 (3) | C1—N1—C3 | 110.6 (3) |
| Cl2ii—Pd1—Cl3i | 172.16 (3) | C3—N1—H1 | 124.7 |
| Cl2—Pd1—Cl3 | 169.09 (3) | C2—N2—H2 | 124.8 |
| Cl2—Pd1—Cl3i | 88.10 (3) | C1—N2—H2 | 124.8 |
| Cl2ii—Pd1—Cl3 | 88.62 (3) | C1—N2—C2 | 110.4 (3) |
| Cl2—Pd1—Cl2ii | 92.21 (3) | N2—C2—H2A | 126.9 |
| Cl2—Pd1—Cl1 | 96.01 (3) | C3—C2—N2 | 106.3 (3) |
| Cl2ii—Pd1—Cl1 | 97.67 (3) | C3—C2—H2A | 126.9 |
| Cl1—Pd1—Cl3 | 94.66 (2) | H4A—C4—H4B | 109.5 |
| Cl1—Pd1—Cl3i | 90.09 (3) | H4A—C4—H4C | 109.5 |
| O1—Pd1—Cl3 | 81.11 (6) | H4B—C4—H4C | 109.5 |
| O1—Pd1—Cl3i | 84.79 (6) | C1—C4—H4A | 109.5 |
| O1—Pd1—Cl2 | 88.06 (6) | C1—C4—H4B | 109.5 |
| O1—Pd1—Cl2ii | 87.40 (6) | C1—C4—H4C | 109.5 |
| O1—Pd1—Cl1 | 173.36 (6) | N1—C1—C4 | 126.8 (3) |
| Pd1—Cl3—Pd1ii | 90.12 (3) | N2—C1—N1 | 106.2 (3) |
| Pd1—Cl2—Pd1i | 92.37 (3) | N2—C1—C4 | 127.0 (3) |
| Pd1—O1—H1A | 109.5 | N1—C3—H3 | 126.7 |
| Pd1—O1—H1B | 109.3 | C2—C3—N1 | 106.5 (3) |
| H1A—O1—H1B | 104.4 | C2—C3—H3 | 126.7 |
| C1—N1—H1 | 124.7 | | |
| N2—C2—C3—N1 | 0.3 (4) | C1—N2—C2—C3 | 0.0 (4) |
| C2—N2—C1—N1 | −0.3 (4) | C3—N1—C1—N2 | 0.5 (4) |
| C2—N2—C1—C4 | 179.8 (3) | C3—N1—C1—C4 | −179.7 (3) |
| C1—N1—C3—C2 | −0.5 (4) | | |
| Symmetry codes : (i) x, −y+1/2, z−1/2; (ii) x, −y+1/2, z+1/2. | | | |

**Table S3.** Hydrogen-bond geometry (Å, °) of $(C_4H_7N_2)[PdCl_3(H_2O)]$.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| O1—H1$A\cdots$Cl1[i] | 0.85 | 2.36 | 3.194 (3) | 165 |
| O1—H1$B\cdots$Cl1[iii] | 0.85 | 2.40 | 3.146 (2) | 147 |
| N1—H1$\cdots$Cl3[ii] | 0.88 | 2.89 | 3.452 (3) | 124 |
| N1—H1$\cdots$O1 | 0.88 | 2.05 | 2.845 (4) | 150 |
| N2—H2$\cdots$Cl1[iv] | 0.88 | 2.28 | 3.144 (3) | 166 |
| C3—H3$\cdots$Cl2[v] | 0.95 | 2.87 | 3.550 (4) | 129 |
| C3—H3$\cdots$Cl1[iii] | 0.95 | 2.89 | 3.713 (3) | 145 |
| **Symmetry codes:** (i) $x$, $-y+1/2$, $z+1/2$; (ii) $x$, $-y+1/2$, $z-1/2$; (iii) $-x+1$, $y+1/2$, $-z+1/2$; (iv) $-x+2$, $y+1/2$, $-z+1/2$; (v) $-x+1$, $-y+1$, $-z$. | | | | |