Electronic Supplementary Information for

Hexagonal molecular "palladawheel"

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Single crystal X-ray diffraction study for 2·9.49CHCl$_3$

Gold single crystals of the CHCl$_3$ solvated [Pd(C$_{19}$H$_{13}$N$_3$O$_2$)]$_6$ hexamer (**2**) are, at 100(2) K, trigonal, space group P31c – C$_{3v}^4$(No. 159)[S1] with **a** = 16.5286(2) Å, **b** = 16.5286(2) Å, **c** = 30.1709(4) Å, α = 90.000°, β = 90.000°, γ = 120.000°, V = 7138.2(2) Å^3 and Z = 2 [Pd(C$_{19}$H$_{13}$N$_3$O$_2$)]$_6$•9.49CHCl$_3$ formula units {d$_{calcd}$ = 1.704 g/cm^3; μ_a(CuKα) =11..40 mm^{-1}}. A full set of unique diffracted intensities [4431 frames with counting times of 3 to 6 seconds and an ω- or ϕ-scan width of 0.50°] was measured[S2] for a single-domain specimen using monochromated CuKα radiation (λ= 1.54178 Å) on a Bruker Proteum Single Crystal Diffraction System equipped with Helios multilayer optics, an APEX II CCD detector and a Bruker MicroSTAR microfocus rotating anode X-ray source operating at 45kV and 60mA. Lattice constants were determined with the Bruker SAINT software package using peak centers for 9893 reflections. A total of 54020 integrated reflection intensities having 2θ(CuKα)< 137.86° were produced using the Bruker program SAINT[S3]; 8243 of these were unique and gave R$_{int}$ = 0.048. The data were corrected empirically for variable absorption effects using equivalent reflections; the relative transmission factors ranged from 0.702 to 1.000. The Bruker software package SHELXTL was used to solve the structure using "direct methods" techniques. All stages of weighted full-matrix least-squares refinement were conducted using F$_o^2$ data with the SHELXTL Version 2010.3-0 software package[S4].

The asymmetric unit contains portions of five different CHCl$_3$ solvent molecules of crystallization that readily leave the lattice. This solvent molecule loss presented serious problems with data collection and structure refinement. Many crystals were examined and several data sets were collected before a satisfactory data set was obtained. Two of these solvent molecules utilize separate crystallographic C$_3$ axes and three occupy general positions. Two of the general-position and one of the special-position CHCl$_3$ molecules are present only part of the time with occupancy factors of 0.84, 0.79 and 0.60. One of these partial occupancy general-position CHCl$_3$ molecules [containing Cl(8)] was eventually restrained to have bond lengths and angles close to those of the full occupancy general position CHCl$_3$ molecule [containing Cl(2)]. The six carbon atoms for each of the four crystallographically-independent phenyl rings in the asymmetric unit were also eventually constrained to be regular hexagons with a C-C bond length of 1.390 Å. Mild restraints were applied to the anisotropic thermal parameters for one oxygen atom and thirteen carbon atoms.

The final structural model incorporated anisotropic thermal parameters for all nonhydrogen atoms and isotropic thermal parameters for all hydrogen atoms. Hydrogen atoms were placed at idealized positions (sp^2- or sp^3-hybridized geometry and C-H bond lengths of 0.95–1.00 Å) with isotropic thermal parameters fixed at values equal to 1.20 times the equivalent isotropic thermal parameter of the carbon atom to which they were bonded. A total of 539 parameters were refined using 91 restraints and 8243 data. Final agreement factors at convergence for **2** are: R$_1$(unweighted, based on F) = 0.097 for 7970 independent absorption-corrected "observed" reflections having 2θ(CuKα)< 137.86° and I>2σ(I); R$_1$(unweighted, based on F) = 0.100 and wR$_2$(weighted, based on F^2) = 0.247 for all 8243 independent absorption-corrected reflections having 2θ(CuKα)< 137.86°. The largest shift/s.u. was 0.000 in the final refinement cycle. The final difference map had maxima and minima of 1.42 and -1.56 e$^-$/Å^3, respectively.

References

[S1] International Tables for Crystallography, Vol A, 4th ed., Kluwer: Boston (1996).

[S2] Data Collection: SMART Software in APEX2 v2010.3-0 Suite. Bruker-AXS, 5465 E. Cheryl Parkway,

Madison, WI 53711-5373 USA.

[S3] Data Reduction: SAINT Software in APEX2 v2010.3-0 Suite. Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373 USA.

[S4] Refinement: SHELXTL v2010.3-0. Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373 USA.

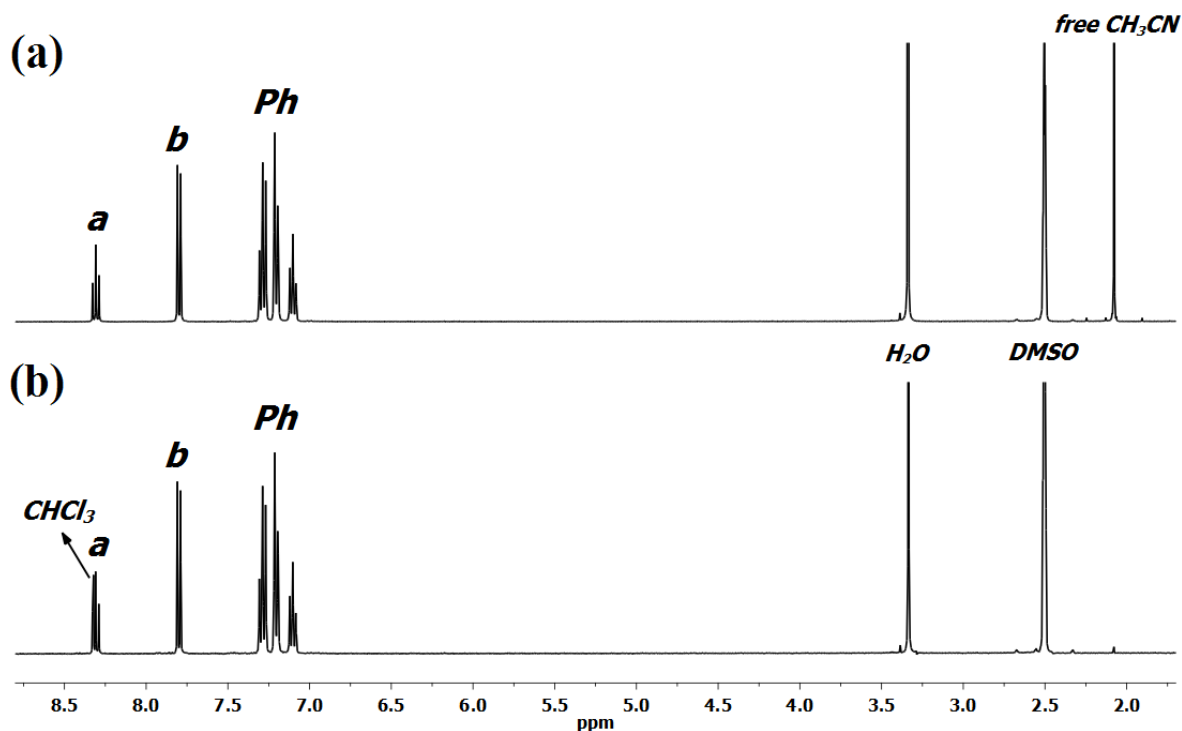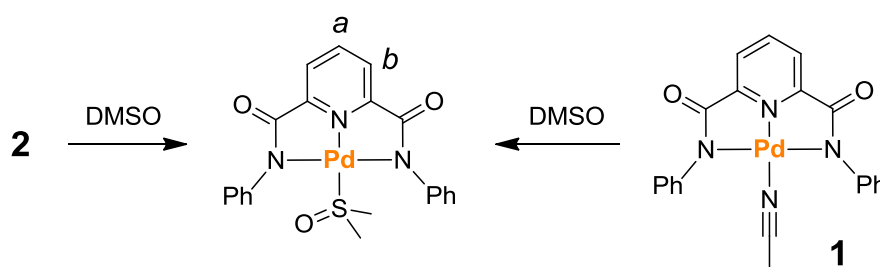**Transformation of 1 and 2 into the DMSO-bound complex in DMSO**

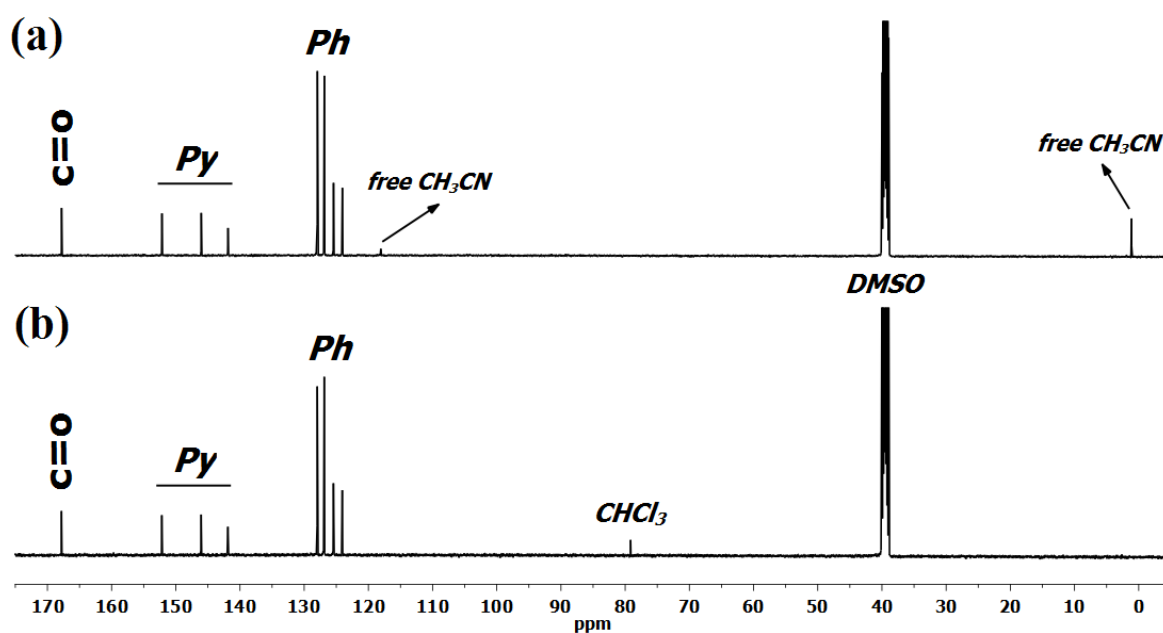Fig. S1. ^{1}H NMR (400 MHz) of (a) **1** and (b) **2** in DMSO-d_6 at 298K.

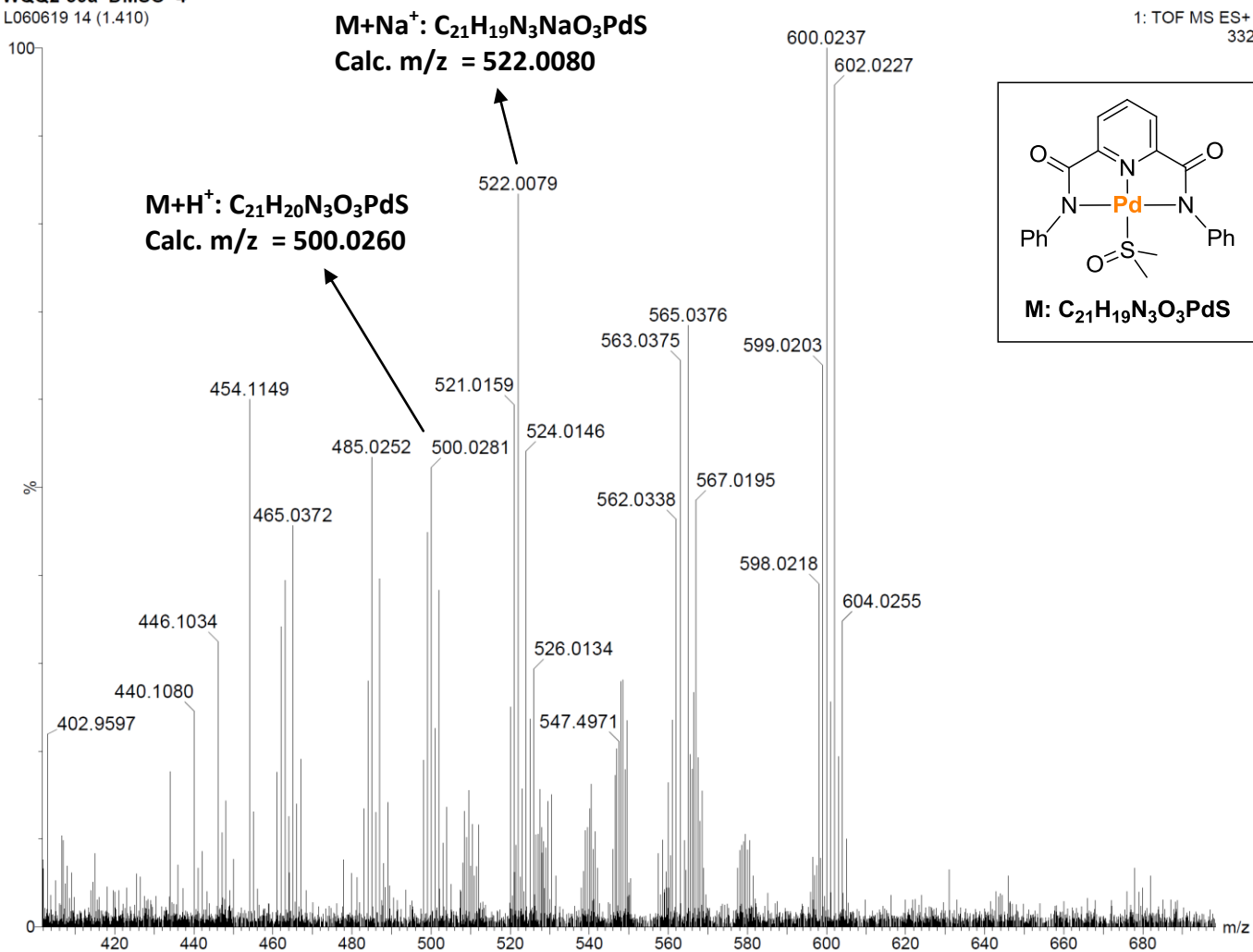Fig. S2. ^{13}C NMR (125 MHz) of (a) **1** and (b) **2** in DMSO-d_6 at 298K.
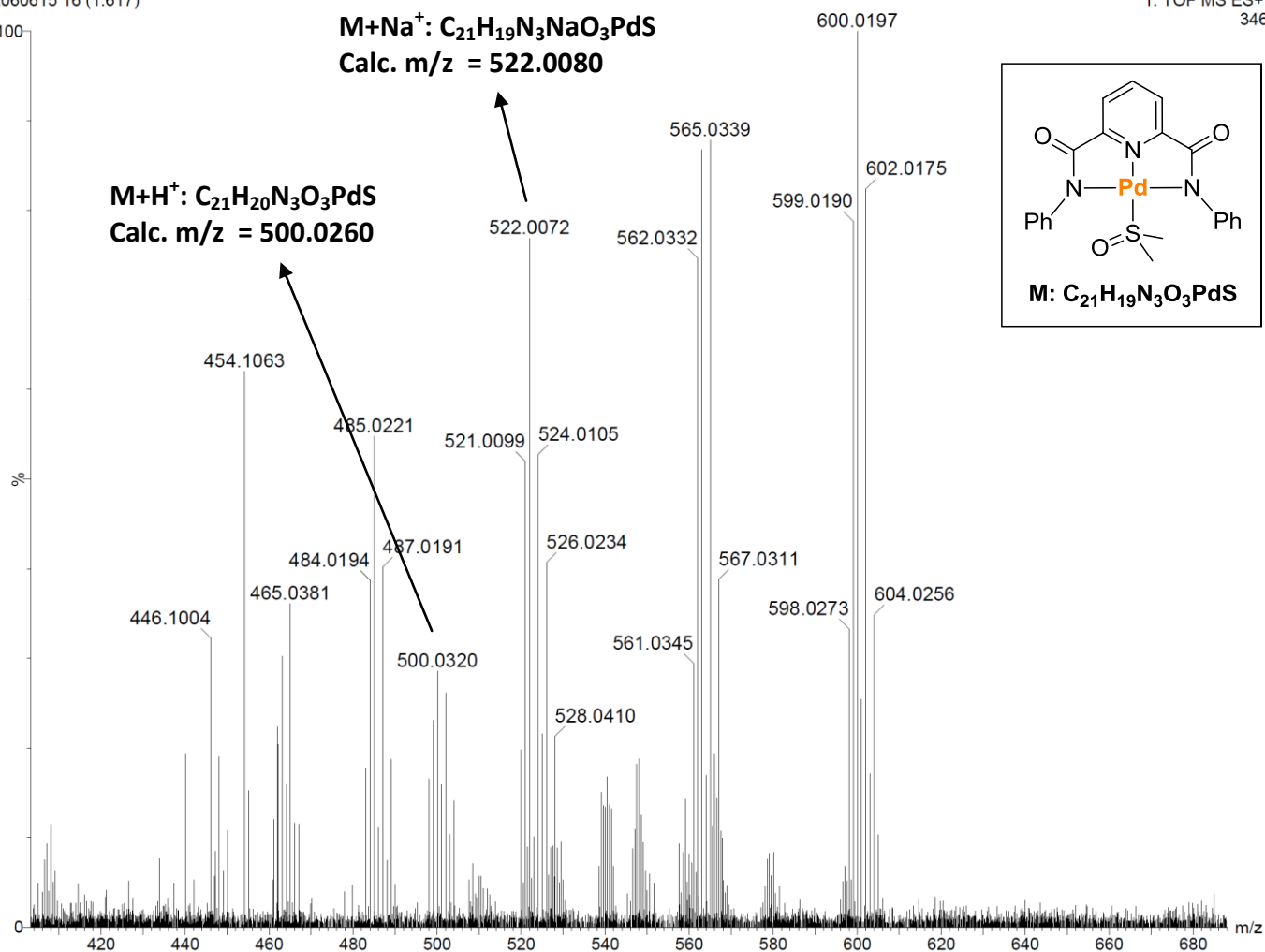
Fig. S3. High-resolution ESI-MS (positive) of the solution of **1** in DMSO.

Fig. S4. High-resolution ESI-MS (positive) of the solution of **2** in DMSO.