Crystal Structure Analysis of:

TA22

(Shown below)

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Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 618859. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 618859."
Table 1. Crystal data and structure refinement for TA22 (CCDC 618859).

Empirical formula  $\text{C}_{40}\text{H}_{50}\text{NO}_{2}\text{F}_{2}\text{Ta} \cdot \text{C}_{6}\text{H}_{6}$
Formula weight  873.87
Crystallization Solvent  Benzene
Crystal Habit  Blade
Crystal size  0.33 x 0.23 x 0.07 mm$^3$
Crystal color  Pale yellow

**Data Collection**

Type of diffractometer  Bruker SMART 1000
Wavelength  0.71073 Å MoKα
Data Collection Temperature  100(2) K
θ range for 35940 reflections used in lattice determination  2.42 to 39.55°
Unit cell dimensions  $a = 13.6879(4)$ Å $b = 28.6266(7)$ Å $c = 11.3658(3)$ Å $\beta = 113.9350(10)^\circ$
Volume  4070.57(19) Å$^3$
Z  4
Crystal system  Monoclinic
Space group  P2$_1$/c
Density (calculated)  1.426 Mg/m$^3$
F(000)  1784
Data collection program  Bruker SMART v5.630
θ range for data collection  1.63 to 40.73°
Completeness to θ = 40.73°  95.4 %
Index ranges  -25 ≤ h ≤ 24, -52 ≤ k ≤ 48, -20 ≤ l ≤ 20
Data collection scan type  ω scans at 7 φ settings
Data reduction program  Bruker SAINT v6.45A
Reflections collected  109242
Independent reflections  25167 [R$_{int}$ = 0.0668]
Absorption coefficient  2.747 mm$^{-1}$
Absorption correction  SADABES
Max. and min. transmission  0.7294 and 0.0000
### Table 1 (cont.)

#### Structure solution and Refinement

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#### Special Refinement Details

Refinement of F² against ALL reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F², conventional R-factors (R) are based on F, with F set to zero for negative F². The threshold expression of F² > 2σ(F²) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F² are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for TA22 (CCDC 618859). U(eq) is defined as the trace of the orthogonalized U_ij tensor.

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Table 3. Selected bond lengths [Å] and angles [°] for TA22 (CCDC 618859).

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Table 4. Bond lengths [Å] and angles [°] for TA22 (CCDC 618859).

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