Supporting Information

N-Acenoacenes

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S1. General Remarks

Reagents and solvents for synthesis
All reagents were obtained from commercial suppliers and were used without further purification if not otherwise stated. Deuterated solvents were purchased from Sigma-Aldrich Laborchemikalien GmbH (Seelze, Germany). All reactions requiring exclusion of oxygen and moisture were carried out in heat-gun dried glassware under a dry and oxygen free nitrogen or argon atmosphere using Schlenk and glovebox techniques.
**Column chromatography**

Column chromatography was performed using silica gel from Macherey, Nagel & Co. KG (Düren, Germany) (particle size: 0.040 - 0.063 mm). For TLC Polygram Sil G/UV 254 plates from Macherey, Nagel & Co. KG (Düren, Germany) were used and examined under UV-light irradiation (254 nm and 365 nm). Before column chromatography the crude product was mixed with Celite 545 and DCM to make a slurry. The solvent was removed by rotary evaporation to get a dry powder.

**Gel permeation chromatography**

Preparative GPC was performed on Bio-Beads® (S-X1 Beads, 200 - 400 Mesh, crosslinked polystyrene), purchased from Bio-Rad Laboratories, Inc.

**1H-NMR spectra and 13C-NMR spectra**

All spectra were recorded at room temperature on a Bruker Avance III 600 (1H: 600 MHz, 13C: 151 MHz) or Bruker Avance III 500 (1H: 500 MHz, 13C: 126 MHz). 13C-NMR spectra were measured proton decoupled if not stated otherwise. NMR spectra were integrated and processed using the Software TopSpin 3.5pl5 (Bruker). For calibration the residual solvent peaks were referenced. Chemical shifts δ are reported in ppm and coupling constants J in Hz. The following abbreviations describe the observed multiplicities: s = singlet, d = doublet, m = multiplet. Via 2D NMR methods, COSY, HSQC(me) and HMBC, and supported by DFT calculations (B3LYP/6–311++G** level) assignments of proton signals were performed.

**IR spectra**

All spectra were recorded neat at room temperature on a Jasco FT/IR-4100. Signals are reported in wavenumbers [cm⁻¹].

**Mass spectrometry**

The mass spectra were recorded using the following instruments: Bruker ApexQe hybrid 9.4 T FT-ICR (MALDI, ESI); Bruker AutoFlex Speed time-of-flight (MALDI).

**Melting points**

Melting points were determined in open glass capillaries with a Melting Point Apparatus MEL-TEMP (Electrothermal, Rochford, UK).
**X-ray single-crystal structure analysis**

X-ray single-crystal structure analyses were measured on a Bruker Smart APEX-II Quazar Area Detector diffractometer by Dr. F. Rominger (Heidelberg University). Diffraction intensities were corrected for Lorentz and polarization effects. An empirical absorption correction was applied using SADABS based on the Laue symmetry of reciprocal space. Heavy atom diffractions were solved by direct methods and refined against F2 with the full matrix least square algorithm. Hydrogen atoms were either isotropically refined or calculated. The structures were solved and refined using the SHELXTL software package.

**UV-Vis and fluorescence spectroscopy**

Absorption spectra were recorded on a Jasco UV-Vis V-660 or Jasco UV-Vis V-670. Fluorescence spectra were recorded on a Jasco FP-6500.

**Quantum yields**

Quantum yields were determined by an Ulbricht sphere (6 inch) using a PTI QuantaMaster 40 equipped with a Hamamatsu R928P Photomultiplier.

**Quantum lifetimes**

Quantum lifetimes were determined on a Horiba FluoroCube-01-NL lifetime spectrofluorometer with emission monochromator (Seya-Namioka type, 200 nm to 800 nm) and diode excitation (Nano-LED N-375L, 375 ± 10 nm, < 200 ps).

**Camera**

The photos were taken by a Canon EOS 7D under daylight or UV-light irradiation (\( \lambda = 365 \) nm).

**Computational studies**

Computational studies were carried out using DFT calculations on Turbomole 6.3.1 and Gaussian16. Geometry optimizations were performed using the B3LYP functional and def2-TZVP basis set. At this geometry, the absolute energy, NICS(1) values and FMO energies were assigned by a single-point approach at the B3LYP/6-311++G** level.[2]S2.

**S2. Synthesis**

2,6-Dibromonaphthalene-1,5-diyl bis(trifluoromethanesulfonate) (1a),[3] 3,6-bis((triisopropylsilyl)ethynyl)benzene-1,2-diamine (2a),[4] 1,4-bis((triisopropylsilyl)ethynyl)naphthalene-2,3-diamine (2b),[5b] 1,4-bis((triisopropylsilyl)ethynyl)anthracene-2,3-diamine (2c),[6] 1,4-bis-
((triisopropylsilyl)ethynyl)phenazine (4a),\textsuperscript{[5]} 6,11-bis((triisopropylsilyl)ethynyl)benzo[\textit{b}]-phenazine (4b),\textsuperscript{[5]} and 6,13-bis((triisopropylsilyl)ethynyl)naphtho[2,3-\textit{b}]phenazine (4c)\textsuperscript{[5]} were synthesized according to literature procedures.

**General procedure:**

In a heatgun dried Schlenk tube under an atmosphere of argon was added 1 (1.0 equiv.), the \textit{ortho}-diamine 2 (2.00 equiv.), caesium carbonate (6.0 equiv.) and RuPhos Pd G1 (10 mol%). Then anhydrous, degassed toluene was added, and the reaction mixture stirred at 110 °C for 24 h. The mixture was cooled to room temperature and diluted with water (10 mL). The phases were separated, and the aqueous layer was extracted with dichloromethane (3\times10 mL). The combined organic phases were washed with brine (10 mL), dried over magnesium sulfate and filtrated. The solvent was removed under reduced pressure and the crude product was isolated.

\[
\begin{array}{c}
\text{2,6-Dibromonaphthalene-1,5-diyl bis(1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate) (1b)}
\end{array}
\]

In a heatgun dried Schlenk tube under an atmosphere of argon was dissolved 2,6-dibromonaphthalene-1,5-diol (200 mg, 629 \(\mu\text{mol}, 1.00\) equiv.), \(N,N\)-dimethylpyridin-4-amine (7.68 mg, 62.9 \(\mu\text{mol}, 0.10\) equiv.) and diisopropylamine (153 mg, 212 \(\mu\text{L}, 1.51\) mmol, 2.40 equiv.) in 10 mL anhydrous dichloromethane and the mixture cooled to 0 °C.

Nonafluorobutanesulfonic acid fluoride (440 mg, 262 \(\mu\text{L}, 1.38\) mmol, 2.20 equiv.) was added dropwise, and the reaction mixture stirred at room temperature for 48 h. The mixture was poured in water (20 mL), the phases were separated, and the aqueous layer was extracted with dichloromethane (3\times20 mL). The combined organic phases were washed with brine (10 mL), dried over magnesium sulfate and filtrated. The solvent was removed under reduced pressure and the crude product was absorbed on Celite\textsuperscript{®}. After flash column chromatography
(petroleum ether/ethyl acetate 100:1 v/v) the product 1b was isolated as a colorless solid (466 mg, 528 μmol, 84%).

Rf = 0.80 (SiO2; petroleum ether/ethyl acetate 10:1 v/v). Mp: 108 °C. 1H-NMR (CDCl3, 600.24 MHz, RT): δ = 8.04 (d, J = 9.05 Hz, 2H, H2), 7.88 (d, J = 9.05 Hz, 2H, H1) ppm. 13C-NMR (CDCl3, 150.93 MHz, RT): δ = 142.5, 133.3, 128.8, 123.2, 118.1, 116.9, 116.2, 115.0, 110.1 ppm. IR (ATR): ν̃ = 3089, 1586, 1413, 1408, 1194, 1171, 1140, 1028, 937, 858, 815, 731, 687, 579, 497 cm⁻¹. HRMS (ESI⁺) m/z: [M-H]+: calcd. for [C18H37Br8Si4O2S2]: 880.7424; found 880.7459; correct isotope distribution.

1,4,9,12-Tetrakis((triisopropylsilyl)ethynyl)phenazino[2,1-a]phenazine (3a)

The GP was applied to 1a (50.0 mg, 85.9 μmol, 1.00 equiv.) and 2a (80.6 mg, 172 μmol, 2.00 equiv.) in 1 mL anhydrous, degassed toluene. Flash column chromatography (SiO2; petroleum ether/diethyl ether 250:1 v/v) and gel permeation chromatography (toluene) yielded a yellow solid 3a (31.1 mg, 29.5 μmol, 34%).

Applying the GP to 1b (150 mg, 170 μmol, 1.00 equiv.) and 2a (159 mg, 340 μmol, 2.00 equiv.) in 2 mL anhydrous, degassed toluene, flash column chromatography (SiO2; petroleum ether/diethyl ether 250:1 v/v) and gel permeation chromatography (toluene) yielded a yellow solid 3a (64.8 mg, 61.5 μmol, 36%).

Rf = 0.85 (SiO2; petroleum ether/dichloromethane 2:1, v/v). Mp: ≥326 °C (decomposition). 1H-NMR (CDCl3, 600.24 MHz, RT): δ = 9.92 (d, J = 9.26 Hz, 2H, H2), 8.39 (d, J = 9.26 Hz, 2H, H1), 8.03 - 8.07 (m, 4H, H3/H4), 1.32 - 1.36 (m, 42H, H5/H6), 1.28 - 1.31 (m, 42H, H7/H8) ppm. 13C-NMR (CDCl3, 150.93 MHz, RT): δ = 144.5, 143.8, 142.5, 141.1, 134.1, 134.3, 132.3, 129.1, 129.0, 124.7, 124.6, 103.7, 103.6, 101.3, 100.6, 19.0, 19.0, 11.73, 11.7 ppm. IR (ATR): ν̃ = 2941, 2862, 2358, 2147, 1461, 1354, 1239, 995, 881, 849, 793, 677, 661, 627, 589, 582, 460, 415 cm⁻¹. HRMS (MALDI⁺) m/z: [M]+: calcd. for [C66H32N4Si4]: 1052.6405; found 1052.6408; correct isotope distribution. Single crystalline specimen was obtained by slow diffusion of methanol into a chloroform solution of 3a.
5,10,15,20-Tetrakis((triisopropylsilyl)ethynyl)benzo[\textit{i}]benzo[7,8]phenazino[2,1-\textit{a}]phenazine (3b)

The GP was applied to \textit{1a} (150 mg, 258 \textmu mol, 1.00 equiv.) and \textit{2b} (281 mg, 541 \textmu mol, 2.10 equiv.) in 1 mL anhydrous, degassed toluene. Flash column chromatography (SiO$_2$; petroleum ether/diethyl ether 250:1 v/v) and gel permeation chromatography (toluene) yielded a green solid \textit{3b} (140 mg, 121 \textmu mol, 48%).

Applying the GP to \textit{1b} (50.0 mg, 56.7 \textmu mol, 1.00 equiv.) and \textit{2b} (58.8 mg, 113 \textmu mol, 2.00 equiv.) in 1 mL anhydrous, degassed toluene, flash column chromatography (SiO$_2$; petroleum ether/diethyl ether 250:1 v/v) and gel permeation chromatography (toluene) yielded a green solid \textit{3b} (33.4 mg, 28.9 \textmu mol, 51%).

R$_f$ = 0.60 (SiO$_2$; petroleum ether/dichloromethane 2:1, v/v). Mp: ≥400°C (decomposition). $^1$H-NMR (CDCl$_3$, 600.24 MHz, RT): δ = 9.95 (d, J = 9.32 Hz, 2H, H$_2$), 8.81 - 8.87 (m, 4H, H$^7$/H$^8$), 8.38 (d, J = 9.32 Hz, 2H, H$^1$), 7.71 - 7.75 (m, 4H, H$^4$/H$^5$), 1.40 - 1.43 (m, 2H, H$^7$/H$^8$), 1.36 - 1.40 (m, 2H, H$^9$/H$^{10}$) ppm. $^{13}$C-NMR (CDCl$_3$, 150.93 MHz, RT): δ = 145.4, 142.1, 141.5, 140.4, 135.6, 135.5, 132.6, 129.4, 129.4, 128.4, 128.4, 127.9, 127.8, 121.3, 121.1, 108.6, 108.1, 103.0, 102.9, 11.2, 19.1, 11.9, 11.8 ppm. IR (ATR): $\tilde{\nu}$ = 2941, 2862, 1461, 1386, 1239, 1044, 994, 881, 871, 757, 674, 663, 622, 595, 482, 457 cm$^{-1}$. HRMS (MALDI$^+$) m/z: [M+2H]$^+$: calcld. for [C$_{78}$H$_{88}$N$_4$Si$_4$]: 1154.6863; found 1154.6901; correct isotope distribution. Single crystalline specimen was obtained by slow diffusion of methanol into a chloroform solution of 3b.

6,11,18,23-Tetrakis((triisopropylsilyl)ethynyl)naphtho[2,3-\textit{i}]naphtho[2',3':7,8]phenazino[2,1-\textit{a}]phenazine (3c)
The GP was applied to 1a (60.0 mg, 103 μmol, 1.00 equiv.) and 2c (117 mg, 206 μmol, 2.00 equiv.) in 1 mL anhydrous, degassed toluene. Flash column chromatography (SiO₂; petroleum ether/diethyl ether 250:1 v/v) and gel permeation chromatography (toluene) yielded a brown solid 3c (10.7 mg, 8.53 μmol, 8%).

Applying the GP to 1b (100 mg, 113 μmol, 1.00 equiv.) and 2c (129 mg, 227 μmol, 2.00 equiv.) in 1 mL anhydrous, degassed toluene, flash column chromatography (SiO₂; petroleum ether/diethyl ether 250:1 v/v) and gel permeation chromatography (toluene) yielded a brown solid 3c (13.1 mg, 10.5 μmol, 9%).

Rf = 0.60 (SiO₂; petroleum ether/dichloromethane 2:1, v/v). Mp: ≥400°C (decomposition). ¹H-NMR (CDCl₃, 600.24 MHz, RT): δ = 9.89 (d, J = 9.28 Hz, 2H, H²), 9.54 (s, 2H, H⁹/H⁸), 9.50 (s, 2H, H⁹/H⁸), 8.23 (d, J = 9.28 Hz, 2H, H¹), 8.06-8.10 (m, 4H, H⁴/H⁷), 7.52 - 7.55 (m, 4H, H⁵/H⁶), 1.46 - 1.49 (m, 42H, H⁸/H¹⁰), 1.41 - 1.44 (s, 42H, H¹¹/H¹²) ppm. IR (ATR): ʋ = 2940, 2862, 1462, 1374, 996, 880, 848, 740, 673, 585 cm⁻¹. HRMS (MALDI⁺) m/z: [M+2H]⁺: calcd. for [C₈₂H₁₀₂N₄Si₄]⁺: 1254.7176; found 1254.7215; correct isotope distribution.

S3. Catalyst screening
**Table S1.** Screening of reaction conditions for the Buchwald-Hartwig coupling reaction of 1 with 2b yielding 3b.

| Compd | Catalyst     | Base       | Solvent   | Temperature | Reaction Time | Yield     |
|-------|--------------|------------|-----------|-------------|---------------|-----------|
| 1a    | Pd(dba)$_2$/dppf | NaO'Bu   | toluene   | 85 °C       | 24 h          | decomposition |
| 1a    | Pd(dba)$_2$/BINAP | K$_3$PO$_4$ | toluene   | 85 °C       | 24 h          | decomposition |
| 1a    | Pd(dba)$_2$/dppf | Cs$_2$CO$_3$  | toluene   | 85 °C       | 24 h          | 5%        |
| 1a    | RuPhos G1     | Cs$_2$CO$_3$  | toluene   | 85 °C       | 24 h          | 30%       |
| 1a    | RuPhos G1     | Cs$_2$CO$_3$  | 1,4-dioxane | 120 °C/ microwave | 16 h          | 33%       |
| 1a    | RuPhos G1     | Cs$_2$CO$_3$  | toluene   | 120 °C/ microwave | 16 h          | 37%       |
| 1a    | RuPhos G1     | Cs$_2$CO$_3$  | toluene   | 110 °C      | 24 h          | 48%       |
| 1a    | RuPhos G1     | Cs$_2$CO$_3$  | toluene   | 110 °C      | 72 h          | 23%       |
| 1b    | RuPhos G1     | Cs$_2$CO$_3$  | toluene   | 110 °C      | 24 h          | 51%       |

S4. **UV-Vis spectra**
Figure S1: Absorption (left) and emission (right) spectrum of 4a (green), 3a (red), 5a (blue) in DCM.

Figure S2: Absorption (left) and emission (right) spectrum of 4b (green), 3b (red), 5b (blue) in DCM.

Figure S3: Absorption (left) and emission (right) spectrum of 4c (green), 3c (red), 5c (blue) in DCM. 3c is nonfluorescent.
Figure S4: Photographs of 3b in different concentrations in hexane. Already at relatively low concentrations the strong fluorescence of 3b starts to overwhelm the true color (green) of the solution even in daylight.

S5. UV-Vis absorption stability study

Figure S5: Change in absorption intensity of a solution of 3a (10^{-6}M) after irradiation with a handheld UV lamp (\(\lambda = 365\) nm) in DCM at room temperature under ambient conditions.
Figure S6: Change in absorption intensity of a solution of 3a (10^{-6} M) after irradiation with a handheld UV lamp (\lambda = 365 nm) in DCM at room temperature under nitrogen atmosphere.

Figure 7: Change in absorption intensity of a solution of 3b (10^{-6} M) after irradiation with a handheld UV lamp (\lambda = 365 nm) in DCM at room temperature under ambient conditions.
Figure 8: Change in absorption intensity of a solution of 3b (10⁻⁶M) after irradiation with a handheld UV lamp (λ = 365 nm) in DCM at room temperature under nitrogen atmosphere.

S6. Electrochemistry/cyclic voltammetry

The cyclic voltammetry (CV) experiments were carried out using a platinum working electrode, a platinum/titanium wire auxiliary electrode, a silver wire reference electrode, a 0.1 molL⁻¹ NBut4PF6 solution in degassed dry THF, and ferrocene/ferrocnium as the reference redox system and internal standard (~4.8 eV) at room temperature and 0.2 mVs⁻¹. To determine the first reduction potentials (E_red(0/-)) of 3a-c and the first oxidation potential of ferrocene, the half-wave potentials were used.⁷

Figure S9: CV spectrum of 1,4,9,12-tetrakis((triisopropylsilyl)ethynyl)phenazino[2,1-a]phenazine (3a).
**Figure S10**: CV spectrum of 5,10,15,20-tetrakis((triisopropylsilyl)ethynyl)benzo[\(\text{[7,8]}\) phenazine-(2,1-\(\text{a}\)])phenazine (3b).

**S7. Quantum-chemical calculations of the FMOs**

**Figure S11**: Quantum chemical calculations (TURBOMOLE B3LYP/d6/TZVP//Gaussian09 B3LYP/6-311++G**) of the FMOs (LUMOs top, HOMOs bottom) for compounds 3a, 4a, and 5a. TMS groups were used instead of TIPS.
Figure S12: Quantum chemical calculations (TURBOMOLE B3LYP/def2-TZVP//Gaussian09 B3LYP/6-311++G**) of the FMOs (LUMOs top, HOMOs bottom) for compounds 3b, 4b, and 5b. TMS groups were used instead of TIPS.

Figure S13: Quantum chemical calculations (TURBOMOLE B3LYP/def2-TZVP//Gaussian09 B3LYP/6-311++G**) of the FMOs (LUMOs top, HOMOs bottom) for compounds 3c, 4c, and 5c. TMS groups were used instead of TIPS.
S8. NMR spectra

Figure S14: $^1$H-NMR spectrum (600 MHz) of 1b in CDCl$_3$.

Figure S15: $^{13}$C($^1$H)-NMR spectrum (151 MHz) of 1b in CDCl$_3$. 
Figure S16: $^1$H,$^1$H-COSY-NMR spectrum (500 MHz) of 1b in CDCl$_3$.

Figure S17: $^1$H,$^{13}$C-HSQC-NMR spectrum (500 MHz/126 MHz) of 1b in CDCl$_3$. 
**Figure S18:** $^{1}H^{13}C$-HMBC-NMR spectrum (500 MHz/126 MHz) of 1b in CDCl$_3$.

**Figure S19:** $^{1}H$-NMR spectrum (600 MHz) of 3a in CDCl$_3$. 
Figure S20: $^{13}$C{$^{1}$H}-NMR spectrum (151 MHz) of 3a in CDCl$_3$.

Figure S21: $^1$H,$^1$H-COSY-NMR spectrum (600 MHz) of 3a in CDCl$_3$. 

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Figure S22: $^1$H, $^{13}$C-HSQC-NMR spectrum (600 MHz/151 MHz) of 3a in CDCl$_3$.

Figure S23: $^1$H, $^{13}$C-HMBC-NMR spectrum (600 MHz/151 MHz) of 3a in CDCl$_3$. 
Figure S24: $^1$H-NMR spectrum (600 MHz) of 3b in CDCl$_3$.

Figure S25: $^{13}$C($^1$H)-NMR spectrum (151 MHz) of 3b in CDCl$_3$. 
Figure S26: $^1$H, $^1$H-COSY-NMR spectrum (600 MHz) of 3b in CDCl$_3$.

Figure S27: $^1$H, $^{13}$C-HSQC-NMR spectrum (600 MHz/151 MHz) of 3b in CDCl$_3$. 
Figure S28: $^1$H,$^{13}$C-HMBC-NMR spectrum (600 MHz/151 MHz) of 3b in CDCl$_3$.

Figure S29: $^1$H-NMR spectrum (600 MHz) of 3c in CDCl$_3$. 
Figure S30: $^1$H-1H-COSY-NMR spectrum (600 MHz) of 3c in CDCl₃.
S9. X-ray single-crystal structure analysis

Figure S31: Left: ORTEP structure of 3a (CCDC 1946373); right: bond lengths, measured in black, calculated (TURBOMOLE B3LYP/def2-TZVP) in red.

Empirical formula: $\text{C}_{66}\text{H}_{92}\text{N}_{4}\text{Si}_{4}$

Formula weight: 1053.79

Temperature: 200(2) K

Wavelength: 1.54178 Å

Crystal system: triclinic

Space group: $P\overline{1}$

$Z$: 1

Unit cell dimensions:

\[ a = 10.7023(6) \text{ Å} \quad \alpha = 108.434(5) \text{ deg.} \]
\[ b = 12.3000(8) \text{ Å} \quad \beta = 91.691(4) \text{ deg.} \]
\[ c = 12.8404(7) \text{ Å} \quad \gamma = 98.192(5) \text{ deg.} \]

Volume: 1582.18(17) Å$^3$

Density (calculated): 1.11 g/cm$^3$

Absorption coefficient: 1.17 mm$^{-1}$

Crystal shape: plank

Crystal size: 0.203 x 0.044 x 0.019 mm$^3$

Crystal colour: brown
Theta range for data collection 3.8 to 62.2 deg.

Index ranges 
-12≤h≤10, -13≤k≤14, -14≤l≤11

Reflections collected 12488

Independent reflections 4792 (R(int) = 0.0440)

Observed reflections 2909 (I > 2σ(I))

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 1.42 and 0.63

Refinement method Full-matrix least-squares on F^2

Data/restraints/parameters 4792 / 1989 / 483

Goodness-of-fit on F^2 1.07

Final R indices (I>2sigma(I)) R1 = 0.089, wR2 = 0.168

Largest diff. peak and hole 0.43 and -0.25 eÅ⁻³

Figure S32: Left: ORTEP structure of 3b (CCDC 1946372); right: bond lengths, measured in black, calculated (TURBOMOLE B3LYP/def2-TZVP) in red.

Empirical formula C₇₄H₉₆N₄Si₄

Formula weight 1153.90

Temperature 110(2) K

Wavelength 1.54178 Å

Crystal system triclinic

S25
Space group $\text{P}\overline{1}$

$Z = 2$

Unit cell dimensions

\begin{align*}
  a &= 12.2249(8) \ \text{Å} \quad \alpha = 71.693(5) \ \text{deg.} \\
  b &= 16.5676(10) \ \text{Å} \quad \beta = 86.957(5) \ \text{deg.} \\
  c &= 17.9511(11) \ \text{Å} \quad \gamma = 87.140(5) \ \text{deg.}
\end{align*}

Volume $3444.8(4) \ \text{Å}^3$

Density (calculated) $1.11 \ \text{g/cm}^3$

Absorption coefficient $1.12 \ \text{mm}^{-1}$

Crystal shape cubic

Crystal size $0.089 \times 0.053 \times 0.046 \ \text{mm}^3$

Crystal colour violet

Theta range for data collection $2.8$ to $67.1$ deg.

Index ranges $-14 \leq h \leq 13$, $-19 \leq k \leq 13$, $-20 \leq l \leq 21$

Reflections collected $28544$

Independent reflections $11684 \ (R(\text{int}) = 0.0523)$

Observed reflections $6610 \ (I > 2\sigma(I))$

Absorption correction Semi-empirical from equivalents

Max. and min. transmission $1.87$ and $0.56$

Refinement method Full-matrix least-squares on $F^2$

Data/restraints/parameters $11684 / 1304 / 791$

Goodness-of-fit on $F^2$ $1.04$

Final $R$ indices ($I>2\sigma(I)$) $R1 = 0.085$, $wR2 = 0.177$

Largest diff. peak and hole $0.49$ and $-0.49 \ \text{eÅ}^{-3}$
S27

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