Supplementary Data

Asymmetric N-heteroacene Tetracene Analogues as Potential N-type Semiconductors

Max Attwood,¹ Dong Kuk Kim,¹ Joseph H. L. Hadden,¹ Anthony Maho,¹ Wern Ng,¹ Hao Wu,¹ Andrew White,² Hiroki Akutsu,³ Sandrine Heutz,¹ Mark Oxborrow¹

1/ Department of Materials, Imperial College London South Kensington Campus, Exhibition Road, London SW7 2AZ, UK; 2/ Department of Chemistry, Imperial College London White City Campus, 82 Wood Lane, London W12 0BZ, UK; 3/ Department of Chemistry, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan.

Instrument Information	S2
Synthesis of 5,12-dihydrobenzo[<i>b</i>]phenazine (H ₂ DAT)	S3
Synthesis of 5,12-dihydrobenzo[g]pyrido[2,3-b]quinoxaline (H ₂ TrAT1)	S3
Synthesis of 5,12-dihydrobenzo[g]pyrido[3,4-b]quinoxaline (H ₂ TrAT2)	S3
General Procedure for Synthesis of 5,12-diazatetracene (DAT), 1,5,12-triazatetracene (TrAT1) & 2,5,12-triazatetracene (TrAT2)	ι S3
NMR Spectroscopy	S5
¹ H NMR Spectrum and Crystal Structure of TrAT2:TCHQ	S11
Modelling EPR Spectroscopy Radical Signals	S12
Luminescence Spectroscopy	S13
Computational Electronic Calculations	S14
Cyclic Voltammetry	S15
Hirshfeld Fingerprint Plots	S16
Thin Film Characterisation Continued	S17
Powder X-ray Diffraction Indexing	S20
References	S22

Instrument Information

UV/Vis spectroscopy was performed using a sealed 1 cm quartz cuvette filled with samples diluted to 10^{-5} M. Data was measured using a Agilent Cary 5000 UV/Vis/NIR spectrophotometer. Fluorescence emission and excitation spectroscopy were performed using a Horiba Jobin-Yvon Spex Fluorolog-3 fluorimeter, with emission and excitation slit widths set to 2 nm.

Single crystal X-ray diffraction data were collected using Agilent Xcalibur 3 E (**DAT**, **TrAT1** and **TrAT2**:TCHQ) and Xcalibur PX Ultra A (**TrAT2**) diffractometers, and the structures were refined using the SHELXTL¹ and SHELX-2013² program systems.^[X1,X2] CCDC 2103753 to 2103756. Images of the crystal structures were captured using Mercury 4.3.1³ X-ray diffraction (XRD) scans in the Bragg-Brentano geometry were conducted on a Philips X'Pert Pro Panalytical diffractometer using a Cu-K α source ($\lambda = 1.5406$ Å) at a current of 40 A and voltage of 40 V.

EPR spectroscopy was performed using a Bruker ELEXSYS-II E500 spectrometer (X-band) at room temperature. Powder samples were decanted into a 4 mm O.D. Wilmad quartz (CFQ) EPR tube. The attenuation was set to 30 dB, with a modulation frequency of 100 kHz, and a modulation amplitude of 4 G.

Cyclic Voltammetry (CV) was performed using a Metrohm Autolab PGSTAT 12 at room temperature. Analysis was performed in a three-electrode cell configuration using a Pt Mesh counter electrode and a Radiometer Analytical saturated calomel reference electrode (SCE). The working electrode was a glassy carbon 3.0 mm diameter disc electrode which had been polished using 6 μ m, 3 μ m and 1 μ m diamond slurries sequentially. An external Fc/Fc⁺ vs. SCE reference was employed for estimation of LUMO energies.^{4,5}

The thin films were grown by organic molecular beam deposition (OMBD) in a Kurt J. Lesker Spectros 100 system at a base pressure of $3 \times 10-7$ mbar. All three materials were evaporated from separate Knudsen cells at deposition rates of 0.5 Å s-1 and 1.0 Å s-1 on silicon, quartz and glass substrates to a thickness of 100 nm. The film thicknesses and rates were monitored using quartz crystal microbalance sensors placed near the sources and substrates. The substrates were maintained at room temperature during deposition with the temperature monitored by a thermocouple placed near the substrate.

Surface characterisation of the films was carried out using tapping mode atomic force microscopy (AFM) on the Asylum Research MFP-3D microscope and scanning electron microscopy (SEM) on the Zeiss LEO Gemini 1525 microscope. All roughness values were determined using the root mean square roughness (RRMS) of the total window of the AFM images, using the open-source software, Gwyddion.⁶ The reported RRMS is taken as the average over three separate areas of the image with the standard deviation quoted as an error. All samples for SEM were coated in a 10 nm conductive layer of chromium and grounded to the sample holder with carbon tape and silver paste.

Additional Experimental Information

2,3-dihydroxynapthalene (98%, TCI Europe), 1,2-diaminobenzene (98%, TCI Europe) and chloranil (99%, TCI Europe) were used as received without additional purification. Both 2,3- & 3,4-diaminopyridine (98%, Fluorochem) were first recrystallised from chloroform prior to use, and 2,3-diaminopyridine was also dissolved in chloroform and run through a short silica column to remove coloured impurities.



Scheme S1. Schematic for the synthesis of dihydrobenzophenazine and quinoxaline precursors (H₂DAT, H₂TrAT1 & H₂TrAT2) and their di- or triazatetracene derivatives (DAT, TrAT1 & TrAT2).

Synthesis of 5,12-dihydrobenzo[b]phenazine (H₂DAT)

2,3-dihydroxynaphthalene was ground in a pestle & mortar with 1,2-diaminobenzene (1:1 molar ratio) until a fine powder was obtained. The powder was decanted into a round bottomed flask equipped with a stirring bar and purged with argon for 30 minutes before being heated to 160°C. The temperature was then maintained for 1-2 hrs until the liquid mixture solidified into a yellow/brown mass. After cooling, the pellet was broken up with a glass rod before adding acetone and leaving the mixture to stir until a slurry formed. This solution was filtered and washed with DCM yielding a light brown powder, which was used as such without additional purification. Typical yields: %. ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.06 (s, 2H), 7.12 (dt, *J* = 5.9, 3.2 Hz, 2H), 6.86 (dd, *J* = 6.1, 3.2 Hz, 2H), 6.30 (dd, *J* = 5.7, 3.3 Hz, 2H), 6.18 (s, 2H), 6.12 (dd, *J* = 5.6, 3.4 Hz, 2H). ¹³C NMR (400 MHz, DMSO-*d*₆) δ 135.02, 132.16, 131.31, 125.31, 123.33, 120.72, 112.20, 104.78. ¹³C DEPT NMR (400 MHz, DMSO-*d*₆) δ 125.31, 123.33, 120.72, 112.20, 104.78. ¹³C DEPT NMR (400 MHz, DMSO-*d*₆) δ 125.31, 123.33, 120.72, 112.20, 104.78.

Synthesis of 5,12-dihydrobenzo[g]pyrido[2,3-b]quinoxaline (H₂TrAT1)

H₂TrAT1 was afforded as a green/brown powder using a 1:1 mixture of 2,3-dihydroxynaphthelene and 2,3-diaminopyridine following the same procedure as above. ¹H NMR (400 MHz, DMSO- d_6) δ 8.81 (s, 1H), 8.32 (s, 1H), 7.23 – 7.12 (m, 2H), 7.09 (dd, *J* = 4.7, 1.9 Hz, 1H), 6.94 – 6.88 (m, 2H), 6.40 (s, 1H), 6.34 – 6.22 (m, 3H). ¹³C NMR (400 MHz, DMSO- d_6) δ 146.28, 138.17, 134.10, 133.84, 131.41, 130.93, 128.52, 125.73, 125.61, 123.96, 123.75, 116.80, 116.02, 106.51, 105.36. ¹³C NMR (400 MHz, DMSO- d_6) δ 138.17, 125.73, 125.61, 123.96, 123.75, 116.02, 106.51, 105.37.

Synthesis of 5,12-dihydrobenzo[g]pyrido[3,4-b]quinoxaline (H₂TrAT2)

H₂TrAT2 was afforded as a yellow/brown powder using a 1:1 mixture of 2,3-dihydroxynaphthelene and 3,4diaminopyridine following the same procedure as above. ¹H NMR (400 MHz, DMSO- d_6) δ 8.57 (s, 1H), 8.19 (s, 1H), 7.39 (d, *J* = 5.1 Hz, 1H), 7.22 (s, 1H), 7.20 – 7.15 (m, 2H), 6.97 – 6.85 (m, 2H), 6.29 (s, 1H), 6.25 (s, 1H), 6.05 (d, *J* = 5.1 Hz, 1H). ¹³C NMR (400 MHz, DMSO- d_6) δ 143.38, 138.78, 134.59, 133.13, 132.32, 131.74, 130.92, 129.34, 125.85, 125.53, 124.21, 123.69, 106.82, 106.75, 105.85; ¹³C DEPT NMR (400 MHz, DMSO- d_6) δ 143.38, 132.33, 125.85, 125.53, 124.22, 123.69, 106.82, 106.76, 105.86.

General Procedure for Synthesis of 5,12-diazatetracene (DAT), 1,5,12-triazatetracene (TrAT1) & 2,5,12-triazatetracene (TrAT2)

The corresponding dihydro-precursor was suspended in toluene before adding chloranil (1:1 molar ratio), which quickly turned the mixture clear red. The solution was then refluxed for 1 hr before being filtered (hot) and diluted with additional toluene to prevent crystallisation of tetrachlorohydroquinone (TCHQ): heteroacene co-crystals.

The toluene filtrates were then washed repeatedly with 1 M NaOH solution until no further precipitation appeared, before being dried over Na_2SO_4 , filtered and then evaporated to dryness *in vacuo*.

DAT, ¹H NMR (400 MHz, DMSO- d_6) δ 9.01 (s, 2H), 8.25 (dd, J = 6.6, 3.3 Hz, 2H), 8.22 (dd, J = 6.9, 3.4 Hz, 2H), 7.92 (dd, 2H), 7.60 (dd, 2H). ¹³C NMR (400 MHz, DMSO- d_6) δ 144.55, 140.00, 134.65, 131.90, 130.09, 128.92, 127.91, 127.65. ¹³C NMR (400 MHz, DMSO- d_6) δ 131.89, 130.08, 128.91, 127.91, 127.65. Orange block crystals of **DAT** were obtained by recrystallisation from ethanol.

TrAT1, ¹H NMR (400 MHz, DMSO- d_6) δ 9.39 (dd, J = 3.7, 2.0 Hz, 1H), 9.08 (s, 2H), 8.66 (dd, J = 8.9, 1.9 Hz, 1H), 8.34 – 8.25 (m, 2H), 7.90 (dd, J = 8.8, 3.7 Hz, 1H), 7.69 – 7.59 (m, 2H).¹³C NMR (400 MHz, DMSO- d_6) δ 159.32, 149.35, 141.11, 140.86, 140.39, 138.91, 135.26, 129.02, 128.96, 128.37, 128.19, 128.03, 127.00. ¹³C DEPT NMR (400 MHz, DMSO- d_6) δ 159.33, 138.91, 129.02, 128.96, 128.38, 128.19, 128.03, 127.00. Red shard-like crystals of **TrAT1** were acquired by vacuum sublimination at 110°C for 24 hrs.

TrAT2, ¹H NMR (400 MHz, DMSO- d_6) δ 9.75 (d, J = 1.1 Hz, 1H), 9.13 (s, 1H), 9.03 (s, 1H), 8.75 (d, J = 6.4 Hz, 1H), 8.28 (ddd, J = 8.3, 5.6, 3.7 Hz, 2H), 8.08 (dd, J = 6.3, 1.0 Hz, 1H), 7.70 – 7.59 (m, 2H). ¹³C NMR (400 MHz, DMSO- d_6) δ 157.97, 145.48, 144.63, 142.00, 140.60, 139.00, 136.20, 135.21, 129.38, 129.15, 128.97, 128.83, 128.25, 127.99, 121.31. ¹³C NMR (400 MHz, DMSO- d_6) δ 157.97, 145.48, 129.39, 129.16, 128.97, 128.84, 128.25, 128.00, 121.31. Red needle crystals of **TrAT2** were acquired by vacuum sublimation at 110°C for 24 hrs.

NMR Spectroscopy



138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112 111 110 109 108 107 106 105 104 103

Figure S1: (A) ¹H, (B) ¹³C & (C) DEPT NMR spectrum of 5,12-dihydrobenzo[*b*]phenazine (H₂DAT) in DMSO (400 MHz, 25°C). ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.06 (s, 2H), 7.12 (dt, *J* = 5.9, 3.2 Hz, 2H), 6.86 (dd, *J* = 6.1, 3.2 Hz, 2H), 6.30 (dd, *J* = 5.7, 3.3 Hz, 2H), 6.18 (s, 2H), 6.12 (dd, *J* = 5.6, 3.4 Hz, 2H). ¹³C NMR (400 MHz, DMSO-*d*₆) δ 135.02, 132.16, 131.31, 125.31, 123.33, 120.72, 112.20, 104.78. ¹³C DEPT NMR (400 MHz, DMSO-*d*₆) δ 125.31, 123.33, 120.72, 112.20, 104.79.



Figure S2: (A) ¹H, (B) ¹³C & (C) DEPT NMR spectrum of 5,12-dihydrobenzo[g]pyrido[2,3-b]quinoxaline (H₂TrAT1) in DMSO (400 MHz, 25°C). ¹H NMR (400 MHz, DMSO- d_6) δ 8.81 (s, 1H), 8.32 (s, 1H), 7.23 – 7.12 (m, 2H), 7.09 (dd, *J* = 4.7, 1.9 Hz, 1H), 6.94 – 6.88 (m, 2H), 6.40 (s, 1H), 6.34 – 6.22 (m, 3H). ¹³C NMR (400 MHz, DMSO- d_6) δ 146.28, 138.17, 134.10, 133.84, 131.41, 130.93, 128.52, 125.73, 125.61, 123.96, 123.75, 116.80, 116.02, 106.51, 105.36. ¹³C NMR (400 MHz, DMSO- d_6) δ 138.17, 125.73, 125.61, 123.96, 123.75, 116.80, 116.02, 106.51, 105.37.



Figure S3. (A) ¹H, (B) ¹³C & (C) DEPT NMR spectrum 5,12-dihydrobenzo[g]pyrido[3,4-b]quinoxaline (H₂TrAT2) in DMSO (400 MHz, 25°C). ¹H NMR (400 MHz, DMSO- d_6) δ 8.57 (s, 1H), 8.19 (s, 1H), 7.39 (d, *J* = 5.1 Hz, 1H), 7.22 (s, 1H), 7.20 – 7.15 (m, 2H), 6.97 – 6.85 (m, 2H), 6.29 (s, 1H), 6.25 (s, 1H), 6.05 (d, *J* = 5.1 Hz, 1H). ¹³C NMR (400 MHz, DMSO- d_6) δ 143.38, 138.78, 134.59, 133.13, 132.32, 131.74, 130.92, 129.34, 125.85, 125.53, 124.21, 123.69, 106.82, 106.75, 105.85; ¹³C DEPT NMR (400 MHz, DMSO- d_6) δ 143.38, 132.33, 125.85, 125.53, 124.22, 123.69, 106.82, 106.76, 105.86.



Figure S4. (A) ¹**H**, **(B)** ¹³**C & (C) DEPT NMR spectrum of 5,12-diazatetracene (DAT) in DMSO (400 MHz, 25°C).** ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.01 (s, 2H), 8.25 (dd, *J* = 6.6, 3.3 Hz, 2H), 8.22 (dd, *J* = 6.9, 3.4 Hz, 2H), 7.92 (dd, 2H), 7.60 (dd, 2H). ¹³C NMR (400 MHz, DMSO-*d*₆) δ 144.55, 140.00, 134.65, 131.90, 130.09, 128.92, 127.91, 127.65. ¹³C NMR (400 MHz, DMSO-*d*₆) δ 131.89, 130.08, 128.91, 127.91, 127.65.



Figure S5. (A) ¹H, (B) ¹³C & (C) DEPT NMR spectrum of 1,5,12-triazatetracene (TrAT1) in DMSO (400 MHz, 25°C). ¹H NMR (400 MHz, DMSO- d_6) δ 9.39 (dd, *J* = 3.7, 2.0 Hz, 1H), 9.08 (s, 2H), 8.66 (dd, *J* = 8.9, 1.9 Hz, 1H), 8.34 – 8.25 (m, 2H), 7.90 (dd, *J* = 8.8, 3.7 Hz, 1H), 7.69 – 7.59 (m, 2H).¹³C NMR (400 MHz, DMSO- d_6) δ 159.32, 149.35, 141.11, 140.86, 140.39, 138.91, 135.26, 129.02, 128.96, 128.37, 128.19, 128.03, 127.00. ¹³C DEPT NMR (400 MHz, DMSO- d_6) δ 159.33, 138.91, 129.02, 128.96, 128.37, 128.19, 128.03, 127.00. ¹³C DEPT NMR (400 MHz, DMSO- d_6) δ 159.33, 138.91, 129.02, 128.96, 128.38, 128.19, 128.03, 127.00.



Figure S6. (A) ¹H, (B) ¹³C & (C) DEPT NMR spectrum of 2,5,12-triazatetracene (TrAT2) in DMSO (400 MHz, 25°C). ¹H NMR (400 MHz, DMSO- d_6) δ 9.75 (d, J = 1.1 Hz, 1H), 9.13 (s, 1H), 9.03 (s, 1H), 8.75 (d, J = 6.4 Hz, 1H), 8.28 (ddd, J = 8.3, 5.6, 3.7 Hz, 2H), 8.08 (dd, J = 6.3, 1.0 Hz, 1H), 7.70 – 7.59 (m, 2H). ¹³C NMR (400 MHz, DMSO- d_6) δ 157.97, 145.48, 144.63, 142.00, 140.60, 139.00, 136.20, 135.21, 129.38, 129.15, 128.97, 128.83, 128.25, 127.99, 121.31. ¹³C NMR (400 MHz, DMSO- d_6) δ 157.97, 145.48, 129.39, 129.16, 128.97, 128.84, 128.25, 128.00, 121.31.

¹H NMR Spectrum and Crystal Structure of TrAT2:TCHQ



Figure S7. ¹H NMR spectrum of TrAT2:tetrachloroquinone (TCHQ) showing the characteristic OH-signal associated with TCHQ.



Figure S8. Crystal packing of TrAT2:TCHQ revealing layers of TrAT2 and TCHQ interacting via OH...N and Cl...CH hydrogen bonds. (A) Unit cell viewed along the *b*-axis with labelled atoms; (B) molecular packing viewed along the *a*-axis. Hydrogen atoms have been omitted for clarity.

Modelling EPR Spectroscopy Radical Signals

All data was processed using the EasySpin 6.1 package for Matlab 2020b. The spectra were first baseline corrected using CorrSpec function and then fitted "as is" using the Nelder/Mead simplex algorithm. All signals were best modelled using two radicals ($S = 0.5 \ 0.5$) with ¹⁴N as the coupling nuclei. It was found that modelling a single radical was unable to reproduce the shape of the signal, regardless of whether 1H or 14N was adopted as the coupling atom. The least squares fitting was performing using the esfit function, and was initiated by changing the g-factors, linewidth (Iw) and, where applicable, coupling (J) parameters, before switching to the hyperfine (A) parameters. This cycle was repeated until the root mean squared deviation (RSMD) was minimised (Table S1).

Table S1. Fitting parameters used for EPR simulations.												
	ç	Nuc	g-	lw	A1	A2	A3	A4	A5	A6	J	DMCD
	3		factor	/mT		/MHz					/MHz	
DAT	0.5		1.9945 1.9980 1.9980	0.66 1.29	11.92	0.081	0.003	-	-	-	-	0.046
TrAT1	- 0.5	14N	2.0022 2.0000 2.0031	0.07 1.77	0.455	10.77	0.368	-	-	-	-	0.017
TrAT2	0.5 0.5		2.0026 2.0017	0.53 0.66	2.528	8.51	0.430	21.02	36.01	11.56	17.11	0.018
DAT Crystal Spectrum	0.5		2.0045 2.0023 2.0041	0.52 1.33	0.032	25.12	0.012	_	-	_	-	0.027



Figure S9. EPR spectrum of DAT crystals with fitting.

Luminescence Spectroscopy



Figure S10. Luminescence spectroscopy of (A) DAT, (B) TrAT1 and (C) TrAT2. Illumination wavelengths were set to correspond to each of the absorbance peaks.

Computational Electronic Calculations

Density functional theory (DFT) calculations were performed in Gaussian09 software⁷ at the B3LYP⁸ 6-311G++(d,p) level of theory. In each case, the compounds were first optimised in their ground state prior to single point energy calculations that were performed to determine the HOMO-LUMO levels. Excited state UV/Vis spectra were obtained from TD-DFT calculations at the same level of theory.



Figure S11. UV/Vis spectrum calculated by DFT at the B3LYP 6-311G++(d,p) level.



Figure S12. Mulliken charge densities for the DAT radical cation (left) and radical anion (right). The radical cation exhibits a high electron density on N-atoms compared to benzene and naphthalene carbon atoms, relative to the radical anion. Calculated by DFT at the B3LYP 6-311G level.

Band structure calculations were performed on crystal structures using Caesar 1.0 and Caesar 2.0 software.⁹ Calculations began by calculating the molecular orbitals to determine the energies of HOMO and LUMO bands using the "MC" sub-program of Caesar 1.0. Note: It was found that equivalent molecules would erroneously return unequal energies if calculated using Caesar 2.0. Next, the band structures for our chosen k-points were calculated using the "BC" sub-program and finally dispersion relations calculated using the "PC" sub-program. Frontier molecular orbitals could also be visualised using the "MC" sub-program, as shown in **Fig. S13**.



Figure S13. Frontier molecular orbital calculated using extended Hückle method provided with Caesar 2.0 software.

Cyclic Voltammetry



Figure S14. Cyclic voltammetry of DAT, TrAT1 and TrAT2 in THF (0.1 M NBu_4PF_6) vs. SCE reference.

Hirshfeld Fingerprint Plots



Figure S15. Hirshfeld fingerprint plots derived from the crystal structures of (A) DAT, (B) TrAT1 and (C) TrAT2. Data plots were generated using CrystalExplorer 17.5.¹⁰ Red/yellow/green regions correspond to C-C interactions. Extrusions towards the lower left corners correspond to N...C-H interactions for DAT and TrAT1, and C-H...C-H interactions for TrAT2.

Thin Film Characterisation Continued



Figure S16. UV/Vis absorptance of thin films measured between 200 – 800 nm.



Figure S17. High resolution SEM images of (A & B) DAT, (C & D) TrAT1, (E & F) TrAT2 crystallites. Scale bars are given for each image.



Figure S18. Atomic force microscopy (AFM) imaging (A & C) DAT, (B & D) TrAT1 thin films on a silicon substrate. Films were grown at rate of 0.5 Å/s up to a thickness 100 nm. AFM imaging, scale bar = 5 μ m. AFM images of TrAT2 could not be obtained due to excessive roughness.



Figure S19. SEM side-view of thin films of (A & B) DAT; (C) TrAT1 and (D) TrAT2. Scale bar = $2 \mu m$.



Figure S20. Optical micrographs of (A & B) DAT; (C & D) TrAT1 and (E & F) TrAT2. Scale bar = $10 \ \mu m$.

Powder X-ray Diffraction Indexing



Figure S21. Indexing of DAT single crystal structure corresponding to the thin-film X-ray diffraction measurements.



Figure S22. Indexing of TrAT1 single crystal structure corresponding to the thin-film X-ray diffraction measurements.





References

- 1 SHELXTL v5.1, Madison, WI, 53711, 1997.
- 2 G. M. Sheldrick, Acta Crystallogr. Sect. C Struct. Chem., 2015, **71**, 3–8.
- 3 C. F. Macrae, I. Sovago, S. J. Cottrell, P. T. A. Galek, P. McCabe, E. Pidcock, M. Platings, G. P. Shields, J. S. Stevens, M. Towler and P. A. Wood, *J. Appl. Crystallogr.*, 2020, **53**, 226–235.
- 4 J. R. Aranzaes, M. C. Daniel and D. Astruc, Can. J. Chem., 2006, 84, 288–299.
- 5 C. M. Cardona, W. Li, A. E. Kaifer, D. Stockdale and G. C. Bazan, *Adv. Mater.*, 2011, **23**, 2367–2371.
- 6 D. Nečas and P. Klapetek, Cent. Eur. J. Phys., 2012, **10**, 181–188.
- M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, G. Z. J. Bloino, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, C. J. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09*, Gaussian, Inc., Wallingford CT, 2009.
- 8 J. Tirado-Rives and W. L. Jorgensen, J. Chem. Theory Comput., 2008, 4, 297–306.
- J. Ren, W. Liang and W.-H. Whangbo, *Caesar 2.0*, PrimeColor Software, Inc., Cary, North Carolina, USA, 2005.
- 10 P. R. Spackman, M. J. Turner, J. J. McKinnon, S. K. Wolff, D. J. Grimwood, D. Jayatilaka and M. A. Spackman, *J. Appl. Crystallogr.*, 2021, **54**, 1006–1011.