Supplementary Material (ESI) for Chemical Communications
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An interdigitated functionally rigid [2]rotaxane

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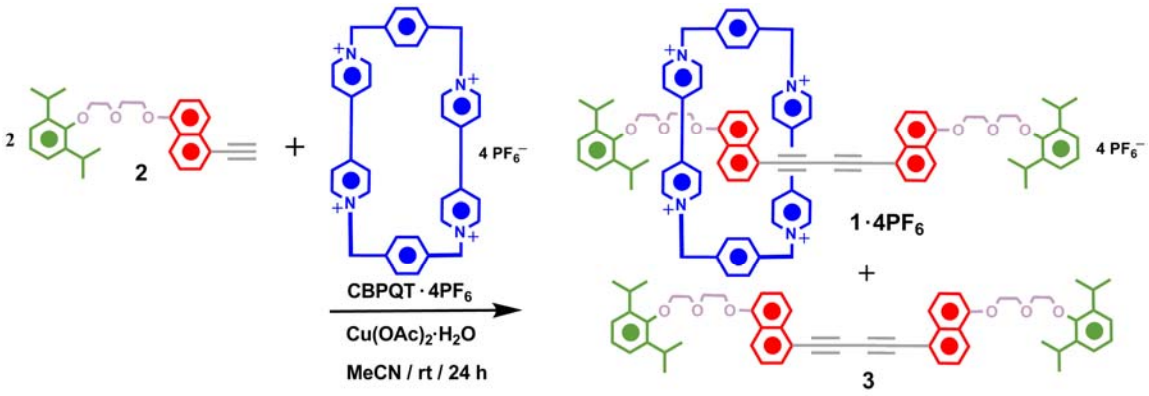
General Methods. All reagents were purchased from Aldrich and used without further purification. 1-(2-(2-(2,6-Diisopropylphenoxy)ethoxy)ethoxy)-5-ethynylnaphthalene (**2**),[S1] and cyclobis(paraquat-*p*-phenylene)hexafluorophosphate (**CBPQT**·4PF_6)[S2] were prepared according to literature procedures.

Synthesis of the Rigid [2]Rotaxane 1·4PF_6 by Cu^{2+}-Mediated Eglinton Coupling.



Scheme S1 Synthesis of a rigid [2]rotaxane **1**·4PF_6.

The NP half dumbbell **2** (100 mg, 0.24 mmol), and **CBPQT**·4PF_6 (264 mg, 0.24 mmol) were dissolved in anhydrous MeCN (20 mL), forming a reddish-orange solution. After 30 min stirring, solid $Cu(OAc)_2·H_2O$ (288 mg, 1.44 mmol) was added to the mixed solution, the solution changed to a dark green color. The mixture was stirred at 25 °C for 24 h. Filtration, followed by washing with MeCN afforded the crude reaction mixture. Free dumbbell **3** was eluted with Me_2CO, whereupon the eluent was changed to Me_2CO/NH_4PF_6 (100:1 v/w) and a red compound was collected. Removal of solvent in vacuo gave a red solid, which was washed with H_2O (25 mL). The resulting red solid gave the desired [2]rotaxane **1**·4PF_6 (42 mg, 18% yield). The spectroscopic data for this material were identical to those obtained for the product isolated from a previous template-directed clipping reaction.[S1] Selected data for [2]rotaxane **1**·4PF_6: MS(ESI): *m/z* = 1787 $[M - PF_6]^+$, 820 $[M - 2PF_6]^{2+}$, 499 $[M - 3PF_6]^{3+}$. HRMS Calcd for $C_{92}H_{94}F_{12}N_4O_6P_2$ ($[M - 2PF_6]^{2+}$): 820.3229. Found: 820.3629. Also spectroscopic data for 1,4-bis(5-(2-(2-(2,6-diisopropylphenoxy)ethoxy)ethoxy)naphthal-ene-1-yl)buta-1,3-diyne (**3**) were identical to those obtained from the previous result.[S1]

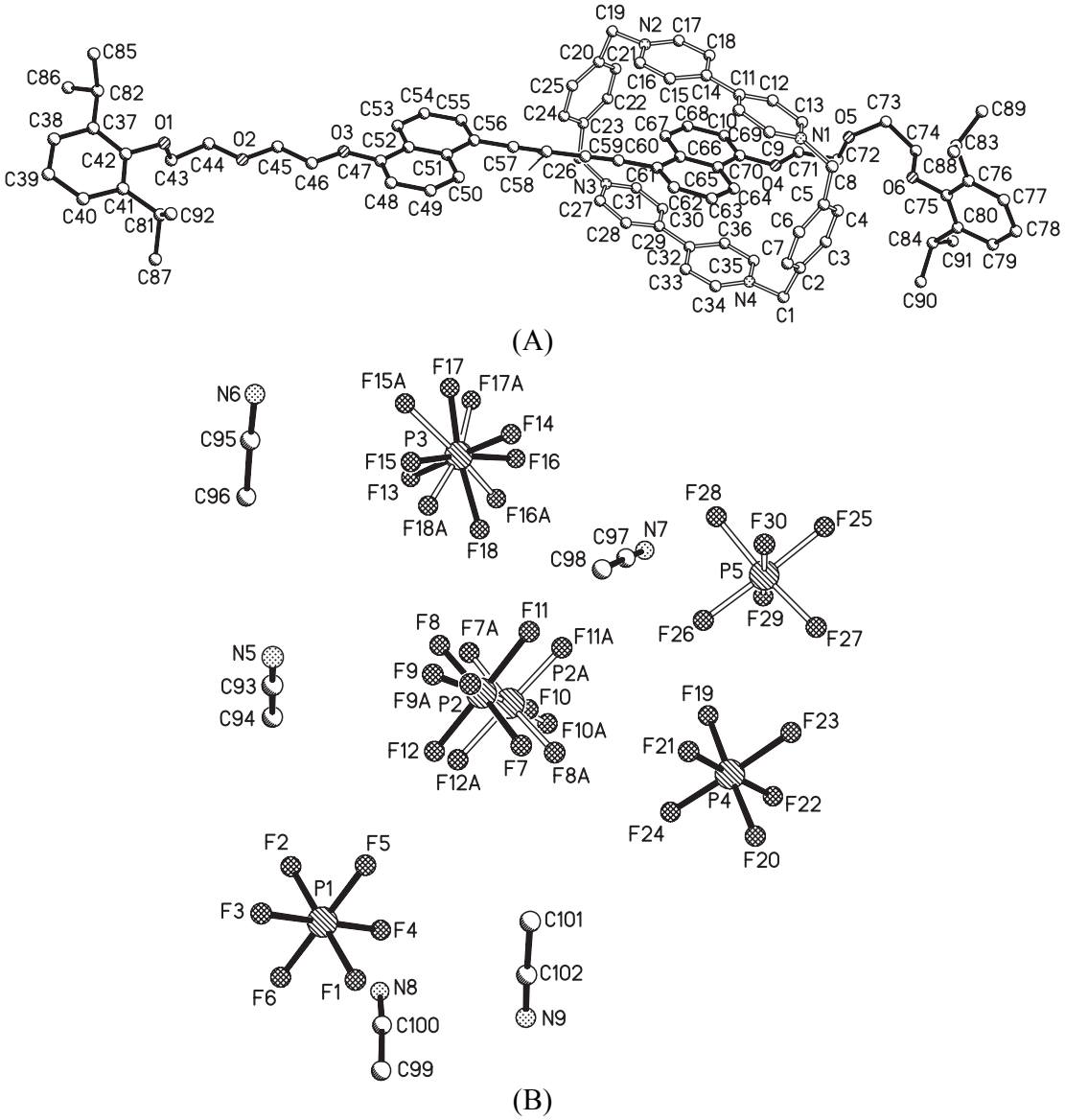


Fig. S1 Solid-state structure of rigid [2]rotaxane **1**·4PF_6. (A) The ball-and-stick representation of $\mathbf{1}^{4+}$ shows an encircled $CBPQT^{4+}$ ring located on one of the naphthalene stations of the dumbbell and its numbering scheme, and (B) Four ammonium hexafluorophosphate (PF_6^-) anions and five MeCN solvent molecules associated with $\mathbf{1}^{4+}$ and their numbering schemes. Three PF_6^- anions are disordered (63:37 for P2, 54:46 for P3, and 50:50 for P4 and P5) over two positions, respectively. All hydrogen atoms have been omitted for clarity.

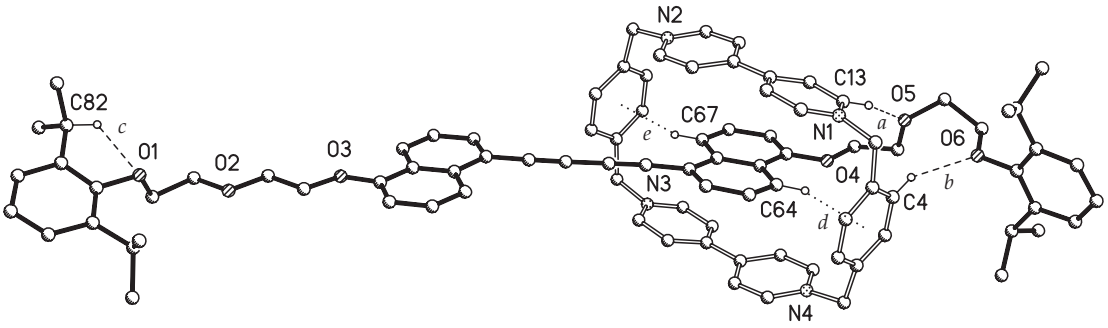


Fig. S2 A ball-and-stick representation of the intercomponent [C–H···O] and [C–H···π] interactions in $\mathbf{1}^{4+}$. [C–H···O] interactions geometries {[X···O], [H···O] distances (Å), and [X–H···O] angles (deg)}: a) 3.09, 2.24, 152; b) 3.21, 2.35, 154; c) 2.85, 2.37, 110. The [H···π] distances (Å) and [C–H···π] angles (deg) for the [C–H···π] interactions are d) 2.53, 146; e) 2.57, 148. All hydrogen atoms, except for those involved in [C–H···O] and [C–H···π] interactions, have been omitted for clarity.

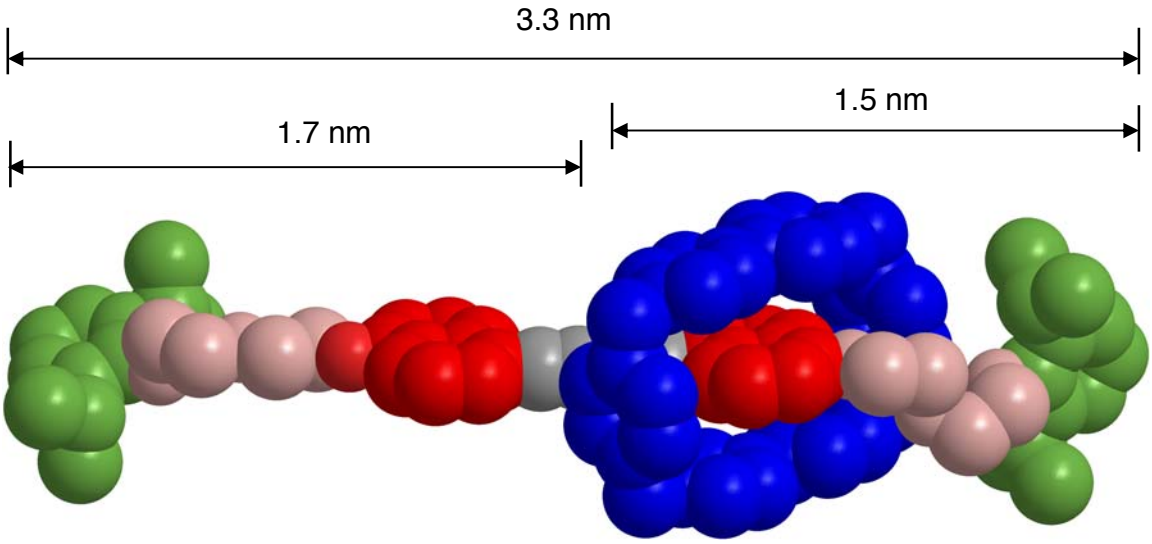


Fig. S3 Space-filling representation of $\mathbf{1}^{4+}$. The carbon atoms are colored gray; oxygen atoms, red; hydrogen atoms, white. The length of the molecule is 3.3 nm. The length of the half dumbbell is 1.5 nm with the $CBPQT^{4+}$ ring and 1.7 nm without the $CBPQT^{4+}$ ring, respectively. Counterions, solvent molecules and hydrogen atoms have been omitted for clarity.

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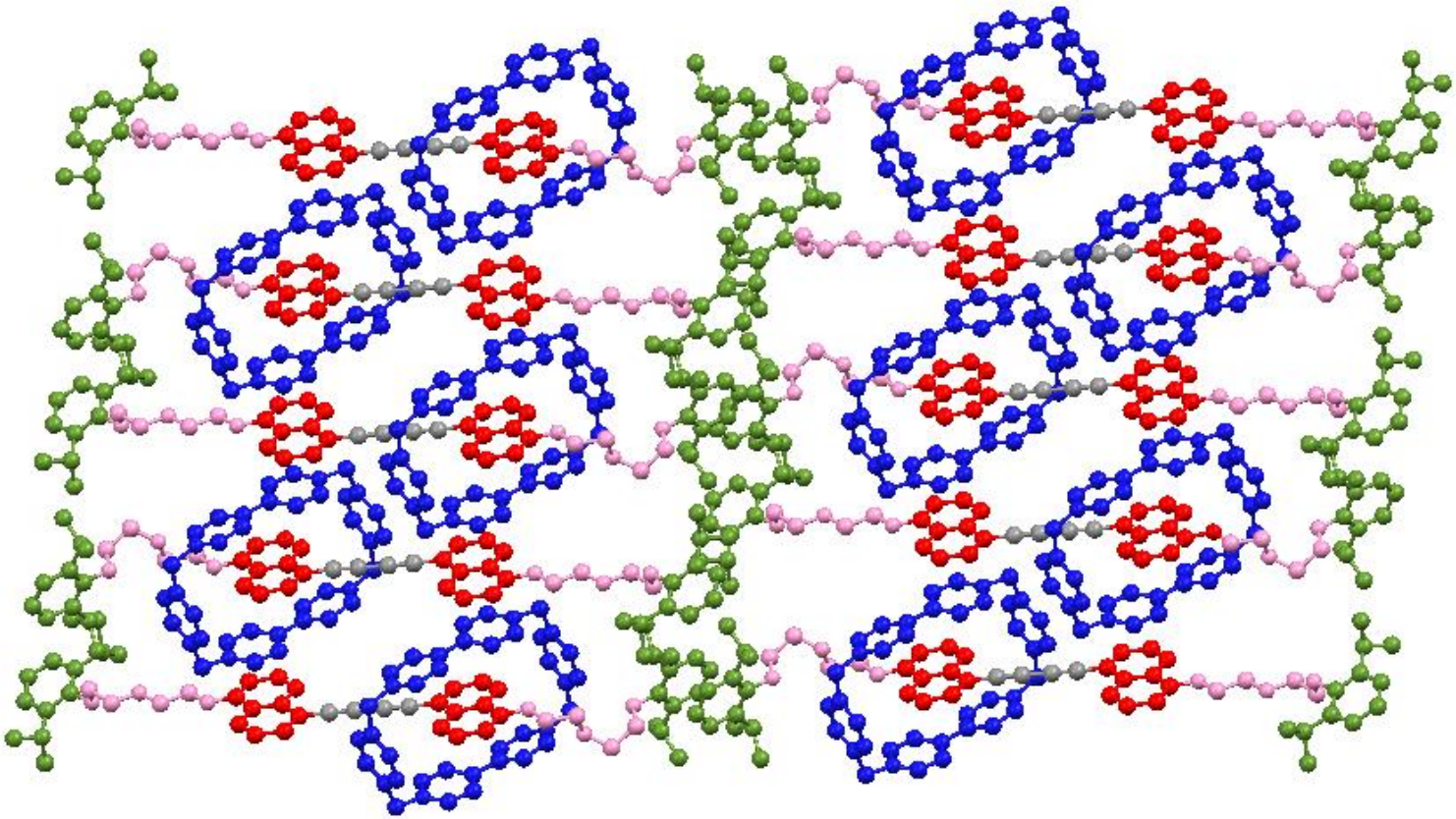

Fig. S4 A ball-and-stick presentation of the superstructure (packing diagram) of $\mathbf{1}^{4+}$. Colors show alternating π-π stacking columns between NP ring systems in the dumbbells and the $BIPY^{2+}$ units of the $CBPQT^{4+}$ ring as the [2]rotaxane molecules line up in the solid-state to form donor-acceptor arrays.

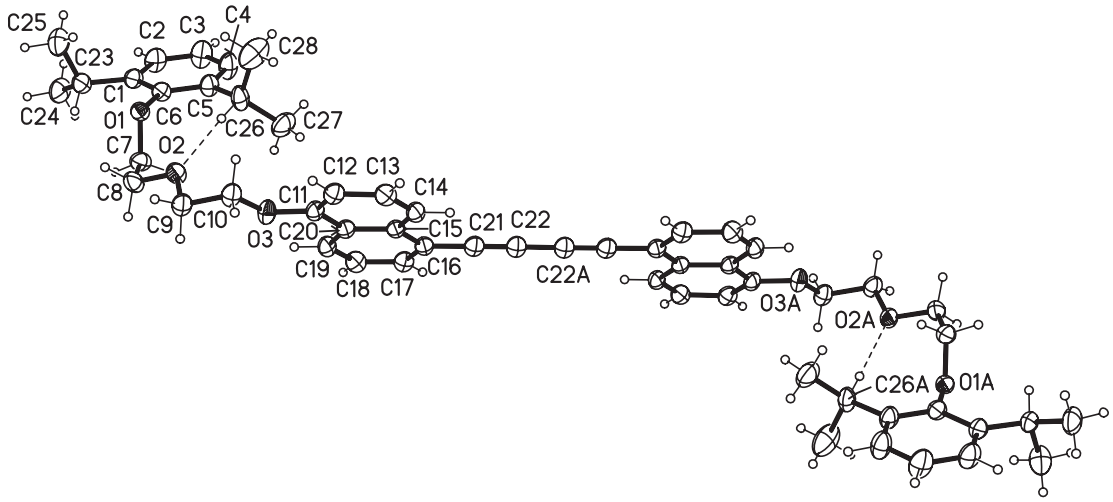

Fig. S5 A ball-and-stick representation of the solid-state structure of the rigid dumbbell **3** and its numbering scheme (ORTEP, 50% thermal probability ellipsoid). Dashed lines indicating a intramolecular [C–H···O] interactions, {[C···O], [H···O] distances (Å) and [C–H···O] angle (deg)}: 3.42, 2.42, 176.

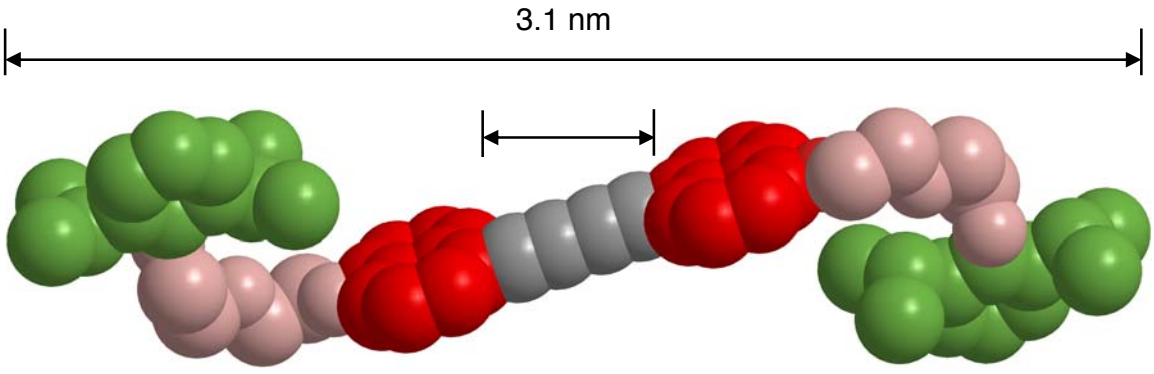

Fig. S6 Space-filling representation of **3**. The carbon atoms of the dumbbell are colored gray; oxygen atoms, red; hydrogen atoms, white. The length of the molecule is 3.1 nm. The length of the butadiyne unit as a spacer between two NP units is 3.8 Å.

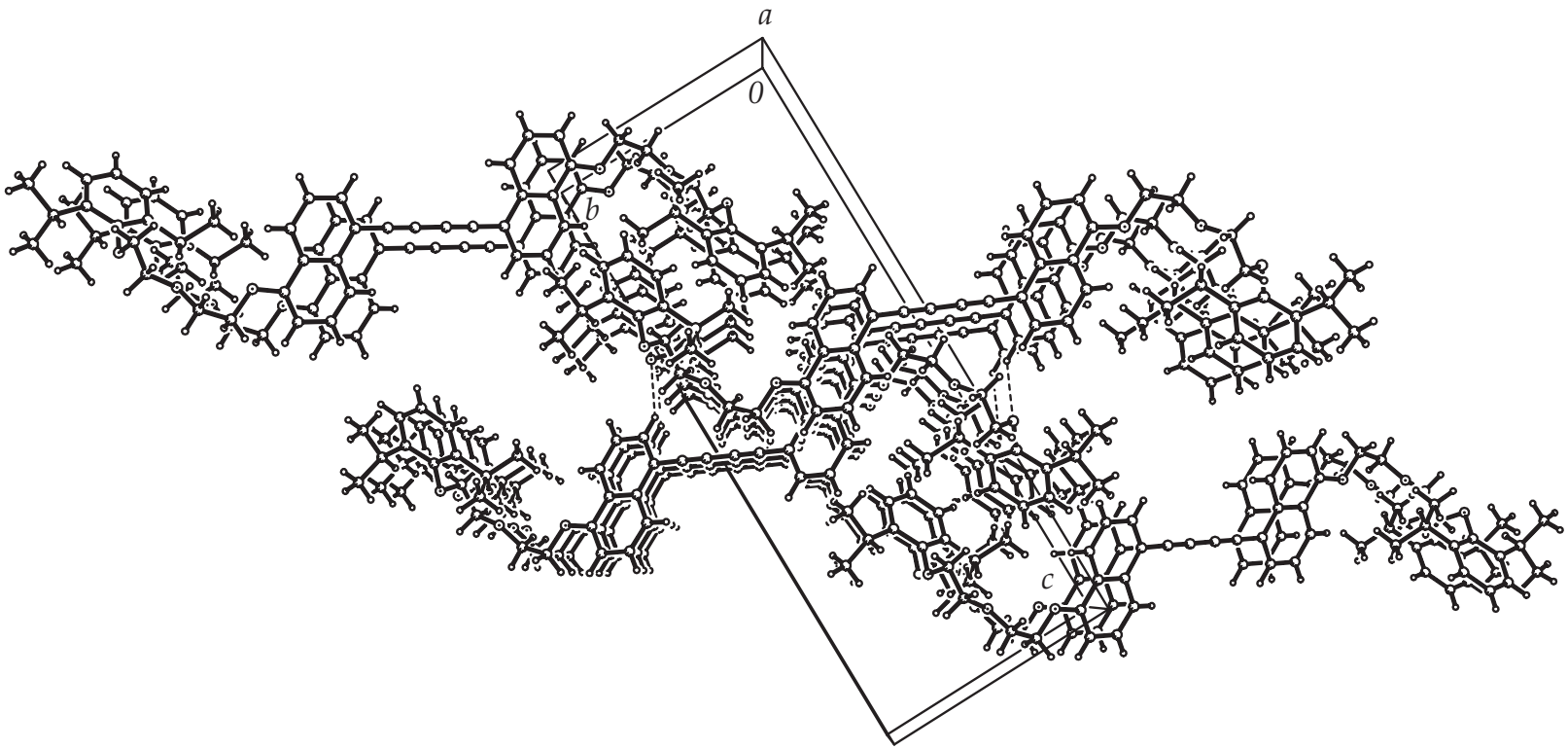

Fig. S7 The superstructure (packing diagram) for **3**. Dashed lines indicating intermolecular [C–H···O] interactions, {[C···O], [H···O] distances (Å) and [C–H···O] angle (deg)}: 3.35, 2.56, 140. Overlapping aromatic rings indicating intermolecular π–π stacking interactions with the distance of 3.36 Å.

X-Ray Crystal Data

Crystal data for **1**·4PF_6: $C_{102}H_{109}F_{24}N_9O_6P_4$, M_r = 2136.86, triclinic, space group $P\bar{1}$, a = 12.7352(2), b = 14.0183(3), c = 31.6155(6) Å, α = 90.064(2)°, β = 99.628(1)°, γ = 110.549(1)°, V = 5199.7(2) $Å^3$, Z = 2, ρ_{calcd} = 1.365 g cm^{-3}, μ(Cu Kα) = 1.542 mm^{-1}, $2\theta_{max}$ = 122.62°, 67667 reflections measured and 15208 were independent (R_{int} = 0.1499), T = 100(2) K, red needle, 0.10 × 0.10 × 0.02 mm, R_1 = 0.0911 [$I > 2\ \sigma(I)$], wR_2 = 0.2640 (all data), GOF = 0.841. The crystal size was very small and diffraction data at high angle are very weak or absent resulting in the higher R_{int} for redundant data.

Crystal data for **3**: $C_{56}H_{62}O_6$, M_r = 831.06, monoclinic, space group $P2_1/n$, a = 10.235(3), b = 8.654(2), c = 27.061(7) Å, β = 90.967(3)°, V = 2396.5(11) $Å^3$, Z = 2, ρ_{calcd} = 1.152 g cm^{-3}, μ(Mo Kα) = 0.073 mm^{-1}, $2\theta_{max}$ = 56.48°, 18014 reflections measured and 5864 were independent (R_{int} = 0.0445), T = 100(2) K, colorless cut-block, 0.60 × 0.40 × 0.40 mm, R_1 = 0.0457 [$I > 2\ \sigma(I)$], wR_2 = 0.1224 (all data), GOF = 1.056.

The data were processed using the program SAINT (Bruker Analytical X-Ray Instrument Inc., Madison, WI) to give the structure factors. The structures were solved by direct methods and refined by full-matrix least squares against |F2|. Absorption corrections were based on multiple and symmetry-equivalent reflections in the data sets using the SADABS program (G. M. Sheldrick, Göttingen University, Germany). All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were treated as idealized contributions. Scattering factors and anomalous dispersion coefficients are contained in the SHELXTL 6.12 program library (G. M. Sheldrick, Madison, WI). CCDC-661695 (**1**·4PF_6) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1 Bond lengths [Å] and angles [°] for **1**·4PF_6.

N(1)-C(9)	1.355(8)	N(1)-C(13)	1.361(8)
N(1)-C(8)	1.491(8)	N(2)-C(17)	1.346(8)
N(2)-C(16)	1.352(7)	N(2)-C(19)	1.507(8)
N(3)-C(31)	1.327(9)	N(3)-C(27)	1.336(8)
N(3)-C(26)	1.511(8)	N(4)-C(34)	1.342(8)
N(4)-C(35)	1.353(8)	N(4)-C(1)	1.496(8)
C(1)-C(2)	1.499(9)	C(2)-C(7)	1.397(9)

C(2)-C(3)	1.402(8)	C(3)-C(4)	1.384(8)
C(4)-C(5)	1.388(8)	C(5)-C(6)	1.399(9)
C(5)-C(8)	1.506(9)	C(6)-C(7)	1.371(9)
C(9)-C(10)	1.365(9)	C(10)-C(11)	1.404(8)
C(11)-C(12)	1.410(8)	C(11)-C(14)	1.480(9)
C(12)-C(13)	1.377(9)	C(14)-C(15)	1.393(9)
C(14)-C(18)	1.412(8)	C(15)-C(16)	1.363(9)
C(17)-C(18)	1.374(9)	C(19)-C(20)	1.504(9)
C(20)-C(25)	1.381(9)	C(20)-C(21)	1.416(9)
C(21)-C(22)	1.365(8)	C(22)-C(23)	1.389(9)
C(23)-C(24)	1.405(9)	C(23)-C(26)	1.506(9)
C(24)-C(25)	1.374(9)	C(27)-C(28)	1.378(9)
C(28)-C(29)	1.380(9)	C(29)-C(30)	1.386(9)
C(29)-C(32)	1.480(9)	C(30)-C(31)	1.379(10)
C(32)-C(33)	1.391(8)	C(32)-C(36)	1.403(9)
C(33)-C(34)	1.352(9)	C(35)-C(36)	1.372(9)
O(1)-C(42)	1.418(7)	O(1)-C(43)	1.428(7)
O(2)-C(45)	1.438(7)	O(2)-C(44)	1.443(7)
O(3)-C(47)	1.370(7)	O(3)-C(46)	1.442(7)
O(4)-C(70)	1.359(7)	O(4)-C(71)	1.446(6)
O(5)-C(72)	1.430(7)	O(5)-C(73)	1.442(7)
O(6)-C(75)	1.392(8)	O(6)-C(74)	1.430(7)
C(37)-C(42)	1.388(9)	C(37)-C(38)	1.415(9)
C(37)-C(82)	1.486(9)	C(38)-C(39)	1.371(10)
C(39)-C(40)	1.377(10)	C(40)-C(41)	1.404(9)
C(41)-C(42)	1.361(9)	C(41)-C(81)	1.503(11)
C(43)-C(44)	1.504(8)	C(45)-C(46)	1.492(9)
C(47)-C(48)	1.357(8)	C(47)-C(52)	1.437(8)
C(48)-C(49)	1.392(9)	C(49)-C(50)	1.379(8)
C(50)-C(51)	1.435(9)	C(51)-C(52)	1.398(8)
C(51)-C(56)	1.447(8)	C(52)-C(53)	1.431(8)
C(53)-C(54)	1.374(8)	C(54)-C(55)	1.384(9)
C(55)-C(56)	1.387(9)	C(56)-C(57)	1.419(10)
C(57)-C(58)	1.198(10)	C(58)-C(59)	1.397(11)
C(59)-C(60)	1.189(9)	C(60)-C(61)	1.410(9)
C(61)-C(62)	1.375(9)	C(61)-C(66)	1.448(8)
C(62)-C(63)	1.391(9)	C(63)-C(64)	1.385(8)
C(64)-C(65)	1.424(8)	C(65)-C(66)	1.423(8)
C(65)-C(70)	1.434(8)	C(66)-C(67)	1.420(8)

C(67)-C(68)	1.365(8)	C(68)-C(69)	1.404(8)
C(69)-C(70)	1.378(8)	C(71)-C(72)	1.493(8)
C(73)-C(74)	1.512(9)	C(75)-C(76)	1.391(9)
C(75)-C(80)	1.401(9)	C(76)-C(77)	1.398(10)
C(76)-C(83)	1.499(10)	C(77)-C(78)	1.361(11)
C(78)-C(79)	1.365(11)	C(79)-C(80)	1.399(10)
C(80)-C(84)	1.542(10)	C(81)-C(92)	1.512(12)
C(81)-C(87)	1.554(12)	C(82)-C(86)	1.508(10)
C(82)-C(85)	1.532(10)	C(83)-C(89)	1.512(9)
C(83)-C(88)	1.533(9)	C(84)-C(90)	1.505(10)
C(84)-C(91)	1.537(9)	P(1)-F(1)	1.5881(17)
P(1)-F(6)	1.5882(17)	P(1)-F(3)	1.5889(17)
P(1)-F(5)	1.5891(17)	P(1)-F(4)	1.5892(17)
P(1)-F(2)	1.5896(17)	P(2)-F(8)	1.577(9)
P(2)-F(12)	1.580(8)	P(2)-F(7)	1.584(9)
P(2)-F(9)	1.597(9)	P(2)-F(11)	1.597(8)
P(2)-F(10)	1.599(8)	P(2A)-F(11A)	1.557(12)
P(2A)-F(12A)	1.564(12)	P(2A)-F(8A)	1.584(13)
P(2A)-F(9A)	1.596(12)	P(2A)-F(7A)	1.599(13)
P(2A)-F(10A)	1.602(12)	P(3)-F(16A)	1.462(11)
P(3)-F(17)	1.481(8)	P(3)-F(18A)	1.538(12)
P(3)-F(15)	1.560(8)	P(3)-F(13)	1.588(5)
P(3)-F(14)	1.597(5)	P(3)-F(16)	1.639(8)
P(3)-F(17A)	1.643(12)	P(3)-F(18)	1.659(8)
P(3)-F(15A)	1.679(11)	P(4)-F(19)	1.528(9)
P(4)-F(24)	1.532(8)	P(4)-F(21)	1.576(8)
P(4)-F(20)	1.577(8)	P(4)-F(23)	1.592(8)
P(4)-F(22)	1.596(8)	P(5)-F(29)	1.523(9)
P(5)-F(27)	1.551(9)	P(5)-F(30)	1.554(10)
P(5)-F(26)	1.571(9)	P(5)-F(25)	1.586(9)
P(5)-F(28)	1.614(10)	N(5)-C(93)	1.152(9)
C(93)-C(94)	1.429(10)	N(6)-C(95)	1.145(8)
C(95)-C(96)	1.459(10)	N(7)-C(97)	1.097(10)
C(97)-C(98)	1.473(11)	N(8)-C(100)	1.140(12)
C(99)-C(100)	1.461(14)	N(9)-C(102)	1.189(13)
C(101)-C(102)	1.443(14)		

C(9)-N(1)-C(13)	120.5(6)	C(9)-N(1)-C(8)	121.0(6)
C(13)-N(1)-C(8)	118.1(6)	C(17)-N(2)-C(16)	120.2(6)

C(17)-N(2)-C(19)	119.1(6)	C(16)-N(2)-C(19)	120.5(6)
C(31)-N(3)-C(27)	121.0(7)	C(31)-N(3)-C(26)	119.6(7)
C(27)-N(3)-C(26)	119.1(7)	C(34)-N(4)-C(35)	120.3(6)
C(34)-N(4)-C(1)	120.4(6)	C(35)-N(4)-C(1)	119.0(6)
N(4)-C(1)-C(2)	109.1(5)	C(7)-C(2)-C(3)	118.2(7)
C(7)-C(2)-C(1)	121.6(6)	C(3)-C(2)-C(1)	120.0(6)
C(4)-C(3)-C(2)	120.6(6)	C(3)-C(4)-C(5)	120.3(6)
C(4)-C(5)-C(6)	119.1(7)	C(4)-C(5)-C(8)	120.5(6)
C(6)-C(5)-C(8)	120.1(6)	C(7)-C(6)-C(5)	120.4(7)
C(6)-C(7)-C(2)	121.0(7)	N(1)-C(8)-C(5)	109.4(5)
N(1)-C(9)-C(10)	120.0(7)	C(9)-C(10)-C(11)	121.5(7)
C(10)-C(11)-C(12)	117.1(6)	C(10)-C(11)-C(14)	122.8(6)
C(12)-C(11)-C(14)	120.0(6)	C(13)-C(12)-C(11)	119.6(7)
N(1)-C(13)-C(12)	121.1(6)	C(15)-C(14)-C(18)	116.1(7)
C(15)-C(14)-C(11)	121.4(6)	C(18)-C(14)-C(11)	122.3(6)
C(16)-C(15)-C(14)	121.0(7)	N(2)-C(16)-C(15)	121.3(6)
N(2)-C(17)-C(18)	120.2(7)	C(17)-C(18)-C(14)	121.2(6)
C(20)-C(19)-N(2)	109.1(5)	C(25)-C(20)-C(21)	118.3(7)
C(25)-C(20)-C(19)	121.0(6)	C(21)-C(20)-C(19)	120.4(6)
C(22)-C(21)-C(20)	120.4(6)	C(21)-C(22)-C(23)	120.6(7)
C(22)-C(23)-C(24)	119.2(7)	C(22)-C(23)-C(26)	120.4(7)
C(24)-C(23)-C(26)	120.1(7)	C(25)-C(24)-C(23)	119.6(7)
C(24)-C(25)-C(20)	121.5(7)	C(23)-C(26)-N(3)	109.6(6)
N(3)-C(27)-C(28)	120.9(7)	C(27)-C(28)-C(29)	120.4(7)
C(28)-C(29)-C(30)	116.1(7)	C(28)-C(29)-C(32)	122.0(7)
C(30)-C(29)-C(32)	121.8(7)	C(31)-C(30)-C(29)	122.0(7)
N(3)-C(31)-C(30)	119.3(7)	C(33)-C(32)-C(36)	116.5(6)
C(33)-C(32)-C(29)	122.6(6)	C(36)-C(32)-C(29)	120.8(7)
C(34)-C(33)-C(32)	121.3(7)	N(4)-C(34)-C(33)	121.0(7)
N(4)-C(35)-C(36)	120.3(6)	C(35)-C(36)-C(32)	120.5(7)
C(42)-O(1)-C(43)	113.0(5)	C(45)-O(2)-C(44)	109.8(5)
C(47)-O(3)-C(46)	118.7(5)	C(70)-O(4)-C(71)	116.9(5)
C(72)-O(5)-C(73)	114.2(5)	C(75)-O(6)-C(74)	114.2(5)
C(42)-C(37)-C(38)	115.5(7)	C(42)-C(37)-C(82)	123.7(6)
C(38)-C(37)-C(82)	120.8(7)	C(39)-C(38)-C(37)	122.4(7)
C(38)-C(39)-C(40)	118.8(7)	C(39)-C(40)-C(41)	121.7(7)
C(42)-C(41)-C(40)	117.1(7)	C(42)-C(41)-C(81)	122.4(7)
C(40)-C(41)-C(81)	120.5(7)	C(41)-C(42)-C(37)	124.6(6)
C(41)-C(42)-O(1)	118.5(6)	C(37)-C(42)-O(1)	116.9(6)

O(1)-C(43)-C(44)	108.7(5)	O(2)-C(44)-C(43)	109.1(6)
O(2)-C(45)-C(46)	108.3(5)	O(3)-C(46)-C(45)	103.1(5)
C(48)-C(47)-O(3)	125.4(6)	C(48)-C(47)-C(52)	121.4(7)
O(3)-C(47)-C(52)	113.1(6)	C(47)-C(48)-C(49)	119.5(6)
C(50)-C(49)-C(48)	122.2(7)	C(49)-C(50)-C(51)	118.6(7)
C(52)-C(51)-C(50)	120.0(6)	C(52)-C(51)-C(56)	118.9(6)
C(50)-C(51)-C(56)	121.1(6)	C(51)-C(52)-C(53)	120.3(6)
C(51)-C(52)-C(47)	118.2(6)	C(53)-C(52)-C(47)	121.4(6)
C(54)-C(53)-C(52)	119.7(6)	C(53)-C(54)-C(55)	120.5(6)
C(54)-C(55)-C(56)	122.1(6)	C(55)-C(56)-C(57)	119.7(6)
C(55)-C(56)-C(51)	118.5(7)	C(57)-C(56)-C(51)	121.8(6)
C(58)-C(57)-C(56)	176.3(7)	C(57)-C(58)-C(59)	178.2(7)
C(60)-C(59)-C(58)	179.0(8)	C(59)-C(60)-C(61)	174.5(7)
C(62)-C(61)-C(60)	119.1(6)	C(62)-C(61)-C(66)	119.4(6)
C(60)-C(61)-C(66)	121.5(6)	C(61)-C(62)-C(63)	122.0(6)
C(64)-C(63)-C(62)	120.5(7)	C(63)-C(64)-C(65)	119.6(7)
C(66)-C(65)-C(64)	120.2(6)	C(66)-C(65)-C(70)	118.5(6)
C(64)-C(65)-C(70)	121.3(6)	C(67)-C(66)-C(65)	119.7(6)
C(67)-C(66)-C(61)	122.1(6)	C(65)-C(66)-C(61)	118.2(6)
C(68)-C(67)-C(66)	119.5(6)	C(67)-C(68)-C(69)	122.1(6)
C(70)-C(69)-C(68)	119.6(6)	O(4)-C(70)-C(69)	125.0(6)
O(4)-C(70)-C(65)	114.5(6)	C(69)-C(70)-C(65)	120.4(6)
O(4)-C(71)-C(72)	108.7(5)	O(5)-C(72)-C(71)	109.2(5)
O(5)-C(73)-C(74)	113.0(6)	O(6)-C(74)-C(73)	109.2(5)
C(76)-C(75)-O(6)	117.6(7)	C(76)-C(75)-C(80)	122.2(7)
O(6)-C(75)-C(80)	120.1(7)	C(75)-C(76)-C(77)	117.2(8)
C(75)-C(76)-C(83)	122.3(7)	C(77)-C(76)-C(83)	120.5(8)
C(78)-C(77)-C(76)	122.1(8)	C(77)-C(78)-C(79)	119.5(9)
C(78)-C(79)-C(80)	122.1(8)	C(79)-C(80)-C(75)	116.9(7)
C(79)-C(80)-C(84)	122.3(8)	C(75)-C(80)-C(84)	120.8(7)
C(41)-C(81)-C(92)	110.2(8)	C(41)-C(81)-C(87)	113.8(8)
C(92)-C(81)-C(87)	110.2(8)	C(37)-C(82)-C(86)	113.6(6)
C(37)-C(82)-C(85)	109.4(6)	C(86)-C(82)-C(85)	110.5(7)
C(76)-C(83)-C(89)	111.9(7)	C(76)-C(83)-C(88)	113.2(6)
C(89)-C(83)-C(88)	110.8(7)	C(90)-C(84)-C(91)	110.5(7)
C(90)-C(84)-C(80)	110.6(7)	C(91)-C(84)-C(80)	111.0(6)
F(1)-P(1)-F(6)	90.06(6)	F(1)-P(1)-F(3)	90.03(6)
F(6)-P(1)-F(3)	90.02(6)	F(1)-P(1)-F(5)	90.02(6)
F(6)-P(1)-F(5)	179.92(8)	F(3)-P(1)-F(5)	89.98(6)

F(1)-P(1)-F(4)	90.01(6)	F(6)-P(1)-F(4)	90.04(6)
F(3)-P(1)-F(4)	179.93(9)	F(5)-P(1)-F(4)	89.96(6)
F(1)-P(1)-F(2)	179.95(9)	F(6)-P(1)-F(2)	89.97(6)
F(3)-P(1)-F(2)	90.00(6)	F(5)-P(1)-F(2)	89.95(6)
F(4)-P(1)-F(2)	89.96(6)	F(8)-P(2)-F(12)	88.4(6)
F(8)-P(2)-F(7)	176.7(7)	F(12)-P(2)-F(7)	88.7(5)
F(8)-P(2)-F(9)	88.7(7)	F(12)-P(2)-F(9)	91.7(6)
F(7)-P(2)-F(9)	89.7(6)	F(8)-P(2)-F(11)	89.7(6)
F(12)-P(2)-F(11)	178.0(7)	F(7)-P(2)-F(11)	93.1(6)
F(9)-P(2)-F(11)	88.9(6)	F(8)-P(2)-F(10)	91.0(7)
F(12)-P(2)-F(10)	89.3(6)	F(7)-P(2)-F(10)	90.6(8)
F(9)-P(2)-F(10)	178.9(8)	F(11)-P(2)-F(10)	90.0(6)
F(11A)-P(2A)-F(12A)	178.1(13)	F(11A)-P(2A)-F(8A)	86.7(10)
F(12A)-P(2A)-F(8A)	91.6(11)	F(11A)-P(2A)-F(9A)	88.9(10)
F(12A)-P(2A)-F(9A)	90.0(11)	F(8A)-P(2A)-F(9A)	86.5(11)
F(11A)-P(2A)-F(7A)	89.6(11)	F(12A)-P(2A)-F(7A)	92.0(11)
F(8A)-P(2A)-F(7A)	176.3(13)	F(9A)-P(2A)-F(7A)	94.3(12)
F(11A)-P(2A)-F(10A)	91.2(11)	F(12A)-P(2A)-F(10A)	89.9(11)
F(8A)-P(2A)-F(10A)	91.8(12)	F(9A)-P(2A)-F(10A)	178.3(16)
F(7A)-P(2A)-F(10A)	87.4(12)	F(16A)-P(3)-F(18A)	96.6(7)
F(17)-P(3)-F(15)	97.8(7)	F(17)-P(3)-F(13)	95.2(5)
F(15)-P(3)-F(13)	93.5(5)	F(17)-P(3)-F(14)	86.0(5)
F(15)-P(3)-F(14)	87.7(5)	F(13)-P(3)-F(14)	178.2(4)
F(17)-P(3)-F(16)	91.3(7)	F(15)-P(3)-F(16)	167.9(7)
F(13)-P(3)-F(16)	93.6(5)	F(14)-P(3)-F(16)	85.0(5)
F(16A)-P(3)-F(17A)	91.4(6)	F(18A)-P(3)-F(17A)	164.7(8)
F(17)-P(3)-F(18)	171.7(6)	F(15)-P(3)-F(18)	87.1(6)
F(13)-P(3)-F(18)	91.2(4)	F(14)-P(3)-F(18)	87.5(4)
F(16)-P(3)-F(18)	83.0(6)	F(16A)-P(3)-F(15A)	167.7(7)
F(18A)-P(3)-F(15A)	87.3(6)	F(17A)-P(3)-F(15A)	82.3(6)
F(19)-P(4)-F(24)	90.1(5)	F(19)-P(4)-F(21)	92.4(5)
F(24)-P(4)-F(21)	89.4(5)	F(19)-P(4)-F(20)	178.2(6)
F(24)-P(4)-F(20)	91.7(5)	F(21)-P(4)-F(20)	87.7(5)
F(19)-P(4)-F(23)	89.7(5)	F(24)-P(4)-F(23)	176.9(6)
F(21)-P(4)-F(23)	87.5(4)	F(20)-P(4)-F(23)	88.5(5)
F(19)-P(4)-F(22)	89.2(5)	F(24)-P(4)-F(22)	93.0(5)
F(21)-P(4)-F(22)	177.1(4)	F(20)-P(4)-F(22)	90.6(5)
F(23)-P(4)-F(22)	90.1(5)	F(29)-P(5)-F(27)	96.0(7)
F(29)-P(5)-F(30)	174.0(9)	F(27)-P(5)-F(30)	88.9(7)

F(29)-P(5)-F(26)	93.3(7)	F(27)-P(5)-F(26)	93.4(7)
F(30)-P(5)-F(26)	89.9(7)	F(29)-P(5)-F(25)	91.1(7)
F(27)-P(5)-F(25)	87.3(7)	F(30)-P(5)-F(25)	85.6(8)
F(26)-P(5)-F(25)	175.4(8)	F(29)-P(5)-F(28)	86.7(7)
F(27)-P(5)-F(28)	174.4(9)	F(30)-P(5)-F(28)	88.1(8)
F(26)-P(5)-F(28)	91.3(7)	F(25)-P(5)-F(28)	87.7(7)
N(5)-C(93)-C(94)	178.9(9)	N(6)-C(95)-C(96)	178.5(10)
N(7)-C(97)-C(98)	177.6(15)	N(8)-C(100)-C(99)	176.7(16)
N(9)-C(102)-C(101)	178.2(13)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z

Table S2 Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1**·4PF_6.
The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
N(1)	47(4)	42(4)	73(4)	0(3)	16(3)	9(3)
N(2)	63(4)	29(3)	65(4)	3(3)	13(3)	17(3)
N(3)	59(4)	33(3)	74(5)	10(3)	6(3)	8(3)
N(4)	62(4)	32(3)	49(4)	-2(3)	9(3)	6(3)
C(1)	67(5)	39(4)	61(5)	-8(4)	12(4)	7(4)
C(2)	45(4)	41(4)	60(5)	3(4)	11(3)	5(4)
C(3)	47(4)	47(5)	53(5)	-3(4)	10(3)	7(4)
C(4)	39(4)	50(5)	53(5)	-4(4)	10(3)	2(4)
C(5)	41(4)	49(5)	53(5)	2(4)	10(3)	4(4)
C(6)	42(5)	51(5)	77(6)	-4(4)	12(4)	3(4)
C(7)	46(5)	50(5)	67(5)	-7(4)	18(4)	-3(4)
C(8)	50(5)	66(5)	54(5)	0(4)	9(3)	19(4)
C(9)	49(5)	49(5)	72(6)	5(4)	20(4)	16(4)
C(10)	41(5)	50(5)	76(6)	6(4)	25(4)	8(4)
C(11)	62(5)	30(4)	56(5)	11(3)	20(4)	16(4)
C(12)	55(5)	50(5)	60(5)	8(4)	17(4)	21(4)
C(13)	55(5)	52(5)	65(5)	4(4)	26(4)	18(4)
C(14)	53(5)	32(4)	65(5)	10(4)	18(4)	21(4)
C(15)	55(5)	34(4)	68(5)	-1(4)	14(4)	14(4)
C(16)	51(5)	29(4)	83(6)	11(4)	35(4)	9(4)

C(17)	52(5)	43(4)	61(5)	4(4)	13(4)	15(4)
C(18)	61(5)	37(4)	62(5)	8(4)	24(4)	20(4)
C(19)	60(5)	43(4)	59(5)	-8(4)	14(4)	10(4)
C(20)	52(5)	36(4)	54(5)	-2(3)	9(3)	2(4)
C(21)	50(4)	35(4)	54(5)	0(3)	11(3)	-2(4)
C(22)	53(5)	42(4)	59(5)	2(4)	5(3)	11(4)
C(23)	60(5)	32(4)	57(5)	-2(4)	2(4)	6(4)
C(24)	63(5)	54(5)	51(5)	5(4)	10(4)	8(4)
C(25)	59(5)	50(5)	60(5)	-4(4)	10(4)	12(4)
C(26)	76(6)	53(5)	61(5)	4(4)	0(4)	8(4)
C(27)	81(6)	55(5)	48(5)	10(4)	10(4)	8(5)
C(28)	57(5)	51(5)	53(5)	6(4)	14(4)	4(4)
C(29)	55(5)	36(4)	61(5)	8(4)	14(4)	10(4)
C(30)	66(6)	50(5)	68(6)	0(4)	11(4)	21(4)
C(31)	65(5)	54(5)	79(6)	0(5)	12(5)	26(5)
C(32)	69(5)	36(4)	57(5)	8(4)	13(4)	21(4)
C(33)	59(5)	45(4)	56(5)	11(4)	22(4)	18(4)
C(34)	63(5)	48(5)	50(5)	1(4)	11(4)	18(4)
C(35)	67(5)	40(4)	58(5)	7(4)	19(4)	14(4)
C(36)	57(5)	40(4)	62(5)	10(4)	16(4)	18(4)
O(1)	51(3)	59(3)	52(3)	4(2)	14(2)	17(3)
O(2)	63(3)	60(3)	55(3)	2(3)	22(2)	16(3)
O(3)	56(3)	63(3)	51(3)	6(3)	20(2)	13(3)
O(4)	43(3)	56(3)	49(3)	5(2)	15(2)	12(2)
O(5)	54(3)	63(3)	47(3)	2(2)	11(2)	22(3)
O(6)	52(3)	51(3)	51(3)	1(2)	14(2)	6(3)
C(37)	48(5)	52(5)	63(5)	3(4)	19(4)	14(4)
C(38)	59(5)	70(6)	65(5)	-1(4)	23(4)	21(5)
C(39)	57(5)	90(7)	64(6)	12(5)	25(4)	17(5)
C(40)	43(5)	96(7)	67(6)	14(5)	10(4)	6(5)
C(41)	54(5)	59(5)	47(5)	-1(4)	8(4)	-4(4)
C(42)	48(5)	54(5)	47(5)	3(4)	14(3)	12(4)
C(43)	58(5)	67(5)	51(5)	4(4)	17(3)	21(4)
C(44)	58(5)	81(6)	42(5)	-8(4)	4(3)	22(4)
C(45)	54(5)	63(5)	58(5)	5(4)	19(4)	7(4)
C(46)	56(5)	55(5)	61(5)	7(4)	28(4)	17(4)
C(47)	47(5)	38(4)	58(5)	9(4)	19(4)	13(4)
C(48)	57(5)	44(4)	61(5)	15(4)	28(4)	18(4)
C(49)	51(5)	47(5)	74(6)	19(4)	23(4)	13(4)

C(50)	55(5)	41(4)	58(5)	9(4)	16(4)	14(4)
C(51)	48(5)	34(4)	61(5)	8(3)	15(4)	15(4)
C(52)	48(4)	32(4)	49(5)	9(3)	10(3)	15(4)
C(53)	49(5)	40(4)	55(5)	2(3)	9(3)	14(4)
C(54)	40(4)	49(5)	67(5)	9(4)	10(4)	8(4)
C(55)	47(5)	47(5)	75(6)	12(4)	27(4)	16(4)
C(56)	51(5)	43(4)	62(5)	10(4)	21(4)	14(4)
C(57)	63(5)	51(5)	57(5)	9(4)	22(4)	18(4)
C(58)	47(5)	42(4)	76(6)	5(4)	17(4)	9(4)
C(59)	56(5)	49(5)	74(6)	3(4)	20(4)	8(4)
C(60)	62(5)	39(4)	59(5)	0(4)	17(4)	11(4)
C(61)	53(5)	43(4)	52(5)	2(4)	19(4)	13(4)
C(62)	55(5)	44(4)	71(6)	7(4)	23(4)	16(4)
C(63)	53(5)	38(4)	66(5)	5(4)	21(4)	12(4)
C(64)	56(5)	35(4)	55(5)	-1(3)	12(4)	11(4)
C(65)	45(4)	39(4)	52(5)	8(3)	8(3)	15(4)
C(66)	54(5)	34(4)	51(5)	7(3)	12(3)	19(4)
C(67)	45(4)	38(4)	54(5)	3(3)	9(3)	10(4)
C(68)	42(4)	44(4)	63(5)	3(4)	10(3)	9(4)
C(69)	53(5)	47(4)	58(5)	8(4)	16(4)	17(4)
C(70)	49(5)	39(4)	51(5)	3(3)	14(3)	13(4)
C(71)	46(4)	53(5)	58(5)	1(4)	19(3)	15(4)
C(72)	47(4)	57(5)	59(5)	-4(4)	16(3)	17(4)
C(73)	53(5)	67(5)	55(5)	5(4)	6(4)	16(4)
C(74)	60(5)	61(5)	58(5)	0(4)	14(4)	7(4)
C(75)	54(5)	49(5)	54(5)	8(4)	22(4)	9(4)
C(76)	60(5)	56(5)	52(5)	10(4)	16(4)	11(4)
C(77)	71(6)	85(7)	58(6)	11(5)	12(4)	18(5)
C(78)	63(6)	104(8)	64(6)	-5(6)	8(4)	6(6)
C(79)	75(6)	57(5)	78(6)	-25(5)	32(5)	-2(5)
C(80)	58(5)	60(5)	58(5)	5(4)	18(4)	16(4)
C(81)	90(4)	117(4)	82(4)	-10(4)	18(3)	-12(4)
C(82)	72(6)	59(5)	67(6)	-5(4)	25(4)	12(5)
C(83)	63(5)	62(5)	72(6)	18(4)	10(4)	18(4)
C(84)	81(6)	56(5)	84(6)	4(4)	28(5)	28(5)
C(85)	108(7)	67(6)	112(8)	17(5)	49(6)	18(6)
C(86)	71(6)	76(6)	111(8)	-8(5)	2(5)	2(5)
C(87)	90(4)	117(4)	82(4)	-10(4)	18(3)	-12(4)
C(88)	81(7)	83(7)	132(8)	16(6)	38(5)	36(6)

C(89)	95(7)	76(6)	153(9)	43(6)	59(6)	32(6)
C(90)	107(7)	70(6)	104(7)	17(5)	40(6)	40(6)
C(91)	84(7)	114(8)	138(9)	24(7)	53(6)	52(6)
C(92)	90(4)	117(4)	82(4)	-10(4)	18(3)	-12(4)
P(1)	66(1)	80(2)	64(1)	15(1)	17(1)	31(1)
F(1)	160(5)	106(4)	111(4)	9(3)	22(3)	97(4)
F(2)	91(3)	65(3)	117(4)	3(3)	16(3)	36(3)
F(3)	60(3)	150(5)	69(3)	0(3)	-1(2)	36(3)
F(4)	58(3)	84(3)	109(4)	6(3)	1(2)	14(3)
F(5)	86(3)	134(4)	61(3)	27(3)	25(2)	28(3)
F(6)	109(4)	120(4)	82(3)	38(3)	51(3)	37(3)
P(2)	51(3)	73(4)	74(4)	25(3)	23(3)	26(3)
F(7)	137(7)	72(4)	123(8)	8(4)	52(6)	60(5)
F(8)	137(7)	72(4)	123(8)	8(4)	52(6)	60(5)
F(9)	46(5)	127(9)	82(7)	16(6)	16(4)	1(5)
F(10)	35(6)	122(9)	94(7)	44(6)	10(5)	15(6)
F(11)	63(4)	89(4)	73(4)	42(4)	35(3)	31(3)
F(12)	63(4)	89(4)	73(4)	42(4)	35(3)	31(3)
P(2A)	59(8)	123(13)	100(10)	49(8)	37(7)	40(8)
F(7A)	116(9)	197(17)	120(12)	65(10)	54(8)	84(10)
F(8A)	116(9)	197(17)	120(12)	65(10)	54(8)	84(10)
F(9A)	31(8)	170(18)	173(17)	29(12)	36(9)	21(9)
F(10A)	31(8)	170(18)	173(17)	29(12)	36(9)	21(9)
F(11A)	116(9)	197(17)	120(12)	65(10)	54(8)	84(10)
F(12A)	116(9)	197(17)	120(12)	65(10)	54(8)	84(10)
P(3)	72(2)	133(3)	126(2)	53(2)	50(2)	50(2)
F(13)	87(3)	165(4)	141(3)	45(3)	70(2)	50(3)
F(14)	87(3)	165(4)	141(3)	45(3)	70(2)	50(3)
F(15)	62(5)	186(10)	116(6)	16(7)	3(4)	51(6)
F(16)	62(5)	186(10)	116(6)	16(7)	3(4)	51(6)
F(17)	152(9)	73(5)	153(8)	57(5)	70(7)	50(6)
F(18)	152(9)	73(5)	153(8)	57(5)	70(7)	50(6)
F(15A)	60(7)	143(9)	221(13)	-9(9)	63(7)	1(7)
F(16A)	60(7)	143(9)	221(13)	-9(9)	63(7)	1(7)
F(17A)	127(11)	194(12)	150(9)	53(9)	33(8)	92(10)
F(18A)	127(11)	194(12)	150(9)	53(9)	33(8)	92(10)
P(4)	82(3)	49(3)	89(3)	-10(2)	50(3)	10(3)
F(19)	90(5)	105(6)	146(7)	-10(5)	49(4)	24(5)
F(20)	90(5)	105(6)	146(7)	-10(5)	49(4)	24(5)

F(21)	56(4)	69(4)	104(5)	-8(3)	50(3)	10(3)
F(22)	56(4)	69(4)	104(5)	-8(3)	50(3)	10(3)
F(23)	87(5)	100(5)	103(5)	-25(4)	44(4)	6(4)
F(24)	87(5)	100(5)	103(5)	-25(4)	44(4)	6(4)
P(5)	147(6)	113(5)	94(4)	-1(4)	-2(4)	78(5)
F(25)	242(11)	178(8)	87(6)	-2(6)	-31(6)	122(8)
F(26)	242(11)	178(8)	87(6)	-2(6)	-31(6)	122(8)
F(27)	167(8)	90(6)	197(10)	-41(6)	-25(6)	90(6)
F(28)	167(8)	90(6)	197(10)	-41(6)	-25(6)	90(6)
F(29)	101(7)	209(11)	193(10)	-20(8)	7(6)	81(8)
F(30)	101(7)	209(11)	193(10)	-20(8)	7(6)	81(8)
N(5)	96(6)	105(6)	86(5)	30(4)	29(4)	59(5)
C(93)	86(7)	63(6)	88(7)	22(5)	32(5)	30(6)
C(94)	94(7)	74(6)	140(9)	-1(6)	73(6)	0(6)
N(6)	71(5)	74(5)	125(7)	9(4)	45(5)	13(4)
C(95)	57(6)	59(5)	93(7)	3(5)	19(5)	19(5)
C(96)	64(6)	128(8)	89(7)	46(6)	28(5)	30(6)
N(7)	77(4)	183(5)	122(5)	94(4)	31(3)	47(4)
C(97)	77(4)	183(5)	122(5)	94(4)	31(3)	47(4)
C(98)	77(4)	183(5)	122(5)	94(4)	31(3)	47(4)
N(8)	131(9)	106(8)	136(8)	4(7)	32(6)	24(6)
C(99)	156(11)	108(9)	145(11)	32(8)	57(8)	35(9)
C(100)	116(10)	75(9)	142(10)	20(7)	47(8)	26(7)
N(9)	108(9)	163(10)	141(9)	-42(7)	13(7)	20(7)
C(101)	78(7)	65(6)	190(11)	10(7)	45(7)	1(6)
C(102)	91(9)	115(10)	129(10)	-8(8)	-4(7)	46(8)

Table S3 Hydrogen atom coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **1**·4PF_6.

	x	*y*	*z*	U_{eq}
H(1A)	1454	7257	2680	65
H(1B)	2426	7521	2404	65
H(3)	1036	5736	3090	57
H(4)	1454	4338	3335	56
H(6)	3923	4970	2625	66

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H(7)	3509	6358	2381	65
H(8A)	3655	3570	3113	63
H(8B)	2665	3306	3381	63
H(9)	3320	2688	2432	61
H(10)	2120	1585	1880	62
H(12)	-533	1311	2469	59
H(13)	718	2439	3012	61
H(15)	895	1069	1290	58
H(16)	-402	206	704	58
H(17)	-2843	-689	1395	58
H(18)	-1580	161	1998	56
H(19A)	-2257	-1058	398	62
H(19B)	-3230	-1360	675	62
H(21)	-4329	-213	733	56
H(22)	-4789	1162	504	59
H(24)	-2459	1782	-272	65
H(25)	-1972	425	-28	64
H(26A)	-4580	2576	24	76
H(26B)	-3635	2840	-264	76
H(27)	-1661	3742	78	73
H(28)	-386	4904	604	63
H(30)	-2903	4516	1256	68
H(31)	-4155	3402	710	72
H(33)	715	6015	1089	57
H(34)	1989	6857	1678	59
H(35)	-398	6022	2393	61
H(36)	-1721	5124	1811	57
H(38)	3529	194	-5215	70
H(39)	5117	1642	-5177	79
H(40)	5626	2809	-4597	81
H(43A)	1378	1263	-4359	64
H(43B)	2183	2227	-4059	64
H(44A)	419	1328	-3816	68
H(44B)	868	426	-3718	68
H(45A)	718	699	-2985	67
H(45B)	372	1655	-3094	67
H(46A)	2293	1690	-2488	61
H(46B)	2049	2690	-2618	61
H(48)	2879	2887	-1875	57

H(49)	3303	3394	-1152	63
H(50)	1917	2964	-729	57
H(53)	-991	982	-2127	53
H(54)	-2404	542	-1717	60
H(55)	-1982	1021	-996	60
H(62)	2045	3741	1173	61
H(63)	2410	4431	1867	58
H(64)	946	4146	2253	55
H(67)	-1884	2002	870	52
H(68)	-3305	1662	1265	56
H(69)	-2949	2287	1975	57
H(71A)	-2226	2387	2660	57
H(71B)	-2365	3454	2605	57
H(72A)	-791	4150	3179	59
H(72B)	-1849	3338	3328	59
H(73A)	-202	2086	3795	66
H(73B)	-1444	2095	3739	66
H(74A)	-800	3744	4031	69
H(74B)	-199	3148	4346	69
H(77)	3533	4633	5132	82
H(78)	3368	6111	5357	92
H(79)	2084	6710	4963	82
H(81)	4111	2607	-3723	120
H(82)	1593	-412	-4469	74
H(83)	1930	3070	4187	74
H(84)	195	5515	3963	78
H(85A)	2861	-1420	-4816	105
H(85B)	1756	-1993	-4630	105
H(85C)	2854	-1275	-4325	105
H(86A)	908	-114	-5159	103
H(86B)	572	-1294	-5119	103
H(86C)	1588	-699	-5349	103
H(87A)	5370	4183	-4203	120
H(87B)	5059	4378	-3759	120
H(87C)	4094	3951	-4163	120
H(88A)	3857	3884	4197	104
H(88B)	3652	2769	4336	104
H(88C)	4144	3688	4683	104
H(89A)	2406	2686	5055	113

H(89B)	2055	1856	4674	113
H(89C)	1187	2353	4772	113
H(90A)	1607	7494	4300	98
H(90B)	674	7256	3883	98
H(90C)	1748	6949	3891	98
H(91A)	-774	5399	4531	114
H(91B)	-795	6378	4297	114
H(91C)	54	6480	4729	114
H(92A)	5726	2128	-3592	120
H(92B)	5962	3209	-3377	120
H(92C)	6405	3113	-3803	120
H(94A)	6995	6182	3410	115
H(94B)	7146	5184	3585	115
H(94C)	6557	5181	3108	115
H(96A)	5774	9730	3219	103
H(96B)	6238	8831	3233	103
H(96C)	5360	8902	2834	103
H(98A)	3995	5564	1319	138
H(98B)	4557	6093	934	138
H(98C)	3949	4904	911	138
H(99A)	3461	414	3885	150
H(99B)	2839	-209	3447	150
H(99C)	2376	-571	3871	150
H(10A)	5132	1667	2540	127
H(10B)	4458	1282	2073	127
H(10C)	5285	758	2300	127

Table S4 Torsion angles [°] for **1**·4PF_6.

C(34)-N(4)-C(1)-C(2)	-91.2(7)
C(35)-N(4)-C(1)-C(2)	82.9(7)
N(4)-C(1)-C(2)-C(7)	86.7(8)
N(4)-C(1)-C(2)-C(3)	-88.2(8)
C(7)-C(2)-C(3)-C(4)	-4.3(10)
C(1)-C(2)-C(3)-C(4)	170.8(6)
C(2)-C(3)-C(4)-C(5)	0.5(10)
C(3)-C(4)-C(5)-C(6)	3.4(10)
C(3)-C(4)-C(5)-C(8)	-171.2(6)

C(4)-C(5)-C(6)-C(7)	-3.4(10)
C(8)-C(5)-C(6)-C(7)	171.2(6)
C(5)-C(6)-C(7)-C(2)	-0.5(10)
C(3)-C(2)-C(7)-C(6)	4.3(10)
C(1)-C(2)-C(7)-C(6)	-170.7(6)
C(9)-N(1)-C(8)-C(5)	96.5(7)
C(13)-N(1)-C(8)-C(5)	-76.5(7)
C(4)-C(5)-C(8)-N(1)	88.7(7)
C(6)-C(5)-C(8)-N(1)	-85.8(7)
C(13)-N(1)-C(9)-C(10)	1.4(10)
C(8)-N(1)-C(9)-C(10)	-171.4(6)
N(1)-C(9)-C(10)-C(11)	1.2(10)
C(9)-C(10)-C(11)-C(12)	-3.9(10)
C(9)-C(10)-C(11)-C(14)	173.1(6)
C(10)-C(11)-C(12)-C(13)	4.2(9)
C(14)-C(11)-C(12)-C(13)	-172.9(6)
C(9)-N(1)-C(13)-C(12)	-1.1(10)
C(8)-N(1)-C(13)-C(12)	172.0(6)
C(11)-C(12)-C(13)-N(1)	-1.8(10)
C(10)-C(11)-C(14)-C(15)	-15.2(9)
C(12)-C(11)-C(14)-C(15)	161.6(6)
C(10)-C(11)-C(14)-C(18)	168.5(6)
C(12)-C(11)-C(14)-C(18)	-14.6(9)
C(18)-C(14)-C(15)-C(16)	0.9(9)
C(11)-C(14)-C(15)-C(16)	-175.6(6)
C(17)-N(2)-C(16)-C(15)	-0.6(9)
C(19)-N(2)-C(16)-C(15)	174.3(6)
C(14)-C(15)-C(16)-N(2)	-0.1(10)
C(16)-N(2)-C(17)-C(18)	0.5(9)
C(19)-N(2)-C(17)-C(18)	-174.4(6)
N(2)-C(17)-C(18)-C(14)	0.3(9)
C(15)-C(14)-C(18)-C(17)	-0.9(9)
C(11)-C(14)-C(18)-C(17)	175.5(6)
C(17)-N(2)-C(19)-C(20)	90.3(7)
C(16)-N(2)-C(19)-C(20)	-84.7(7)
N(2)-C(19)-C(20)-C(25)	90.8(8)
N(2)-C(19)-C(20)-C(21)	-83.6(7)
C(25)-C(20)-C(21)-C(22)	-4.8(10)
C(19)-C(20)-C(21)-C(22)	169.7(6)

C(20)-C(21)-C(22)-C(23)	0.6(10)
C(21)-C(22)-C(23)-C(24)	4.5(10)
C(21)-C(22)-C(23)-C(26)	-169.6(6)
C(22)-C(23)-C(24)-C(25)	-5.3(10)
C(26)-C(23)-C(24)-C(25)	168.8(6)
C(23)-C(24)-C(25)-C(20)	1.0(10)
C(21)-C(20)-C(25)-C(24)	3.9(10)
C(19)-C(20)-C(25)-C(24)	-170.5(6)
C(22)-C(23)-C(26)-N(3)	85.0(8)
C(24)-C(23)-C(26)-N(3)	-89.0(8)
C(31)-N(3)-C(26)-C(23)	-95.5(8)
C(27)-N(3)-C(26)-C(23)	78.8(7)
C(31)-N(3)-C(27)-C(28)	0.4(10)
C(26)-N(3)-C(27)-C(28)	-173.8(6)
N(3)-C(27)-C(28)-C(29)	3.1(11)
C(27)-C(28)-C(29)-C(30)	-5.0(10)
C(27)-C(28)-C(29)-C(32)	173.4(6)
C(28)-C(29)-C(30)-C(31)	3.9(10)
C(32)-C(29)-C(30)-C(31)	-174.5(6)
C(27)-N(3)-C(31)-C(30)	-1.6(10)
C(26)-N(3)-C(31)-C(30)	172.6(6)
C(29)-C(30)-C(31)-N(3)	-0.7(11)
C(28)-C(29)-C(32)-C(33)	10.0(10)
C(30)-C(29)-C(32)-C(33)	-171.6(6)
C(28)-C(29)-C(32)-C(36)	-166.2(6)
C(30)-C(29)-C(32)-C(36)	12.2(10)
C(36)-C(32)-C(33)-C(34)	2.2(9)
C(29)-C(32)-C(33)-C(34)	-174.2(6)
C(35)-N(4)-C(34)-C(33)	-0.7(10)
C(1)-N(4)-C(34)-C(33)	173.3(6)
C(32)-C(33)-C(34)-N(4)	-1.2(10)
C(34)-N(4)-C(35)-C(36)	1.5(9)
C(1)-N(4)-C(35)-C(36)	-172.6(6)
N(4)-C(35)-C(36)-C(32)	-0.4(10)
C(33)-C(32)-C(36)-C(35)	-1.4(9)
C(29)-C(32)-C(36)-C(35)	175.0(6)
C(42)-C(37)-C(38)-C(39)	-0.9(10)
C(82)-C(37)-C(38)-C(39)	-178.2(7)
C(37)-C(38)-C(39)-C(40)	1.3(11)

C(38)-C(39)-C(40)-C(41)	-0.8(12)
C(39)-C(40)-C(41)-C(42)	0.0(11)
C(39)-C(40)-C(41)-C(81)	176.9(8)
C(40)-C(41)-C(42)-C(37)	0.3(11)
C(81)-C(41)-C(42)-C(37)	-176.5(8)
C(40)-C(41)-C(42)-O(1)	178.6(6)
C(81)-C(41)-C(42)-O(1)	1.7(11)
C(38)-C(37)-C(42)-C(41)	0.1(11)
C(82)-C(37)-C(42)-C(41)	177.3(7)
C(38)-C(37)-C(42)-O(1)	-178.2(5)
C(82)-C(37)-C(42)-O(1)	-1.0(10)
C(43)-O(1)-C(42)-C(41)	89.1(7)
C(43)-O(1)-C(42)-C(37)	-92.5(7)
C(42)-O(1)-C(43)-C(44)	173.8(6)
C(45)-O(2)-C(44)-C(43)	175.4(5)
O(1)-C(43)-C(44)-O(2)	71.4(7)
C(44)-O(2)-C(45)-C(46)	179.1(6)
C(47)-O(3)-C(46)-C(45)	177.5(5)
O(2)-C(45)-C(46)-O(3)	174.6(5)
C(46)-O(3)-C(47)-C(48)	4.2(9)
C(46)-O(3)-C(47)-C(52)	-178.9(5)
O(3)-C(47)-C(48)-C(49)	179.3(6)
C(52)-C(47)-C(48)-C(49)	2.6(9)
C(47)-C(48)-C(49)-C(50)	-1.3(10)
C(48)-C(49)-C(50)-C(51)	1.0(9)
C(49)-C(50)-C(51)-C(52)	-2.0(9)
C(49)-C(50)-C(51)-C(56)	179.9(6)
C(50)-C(51)-C(52)-C(53)	-179.4(5)
C(56)-C(51)-C(52)-C(53)	-1.2(9)
C(50)-C(51)-C(52)-C(47)	3.2(9)
C(56)-C(51)-C(52)-C(47)	-178.6(5)
C(48)-C(47)-C(52)-C(51)	-3.6(9)
O(3)-C(47)-C(52)-C(51)	179.3(5)
C(48)-C(47)-C(52)-C(53)	179.0(6)
O(3)-C(47)-C(52)-C(53)	2.0(8)
C(51)-C(52)-C(53)-C(54)	1.5(9)
C(47)-C(52)-C(53)-C(54)	178.8(6)
C(52)-C(53)-C(54)-C(55)	-1.5(9)
C(53)-C(54)-C(55)-C(56)	1.3(10)

C(54)-C(55)-C(56)-C(57)	179.5(6)
C(54)-C(55)-C(56)-C(51)	-1.0(9)
C(52)-C(51)-C(56)-C(55)	0.9(9)
C(50)-C(51)-C(56)-C(55)	179.1(6)
C(52)-C(51)-C(56)-C(57)	-179.5(6)
C(50)-C(51)-C(56)-C(57)	-1.4(9)
C(55)-C(56)-C(57)-C(58)	-10(12)
C(51)-C(56)-C(57)-C(58)	171(12)
C(56)-C(57)-C(58)-C(59)	8(35)
C(57)-C(58)-C(59)-C(60)	-22(63)
C(58)-C(59)-C(60)-C(61)	-148(40)
C(59)-C(60)-C(61)-C(62)	-12(9)
C(59)-C(60)-C(61)-C(66)	165(8)
C(60)-C(61)-C(62)-C(63)	174.1(6)
C(66)-C(61)-C(62)-C(63)	-3.3(10)
C(61)-C(62)-C(63)-C(64)	2.3(10)
C(62)-C(63)-C(64)-C(65)	0.5(9)
C(63)-C(64)-C(65)-C(66)	-2.2(9)
C(63)-C(64)-C(65)-C(70)	177.0(6)
C(64)-C(65)-C(66)-C(67)	179.5(5)
C(70)-C(65)-C(66)-C(67)	0.2(9)
C(64)-C(65)-C(66)-C(61)	1.2(9)
C(70)-C(65)-C(66)-C(61)	-178.1(5)
C(62)-C(61)-C(66)-C(67)	-176.7(6)
C(60)-C(61)-C(66)-C(67)	6.0(9)
C(62)-C(61)-C(66)-C(65)	1.5(9)
C(60)-C(61)-C(66)-C(65)	-175.8(6)
C(65)-C(66)-C(67)-C(68)	-0.1(9)
C(61)-C(66)-C(67)-C(68)	178.1(6)
C(66)-C(67)-C(68)-C(69)	0.0(9)
C(67)-C(68)-C(69)-C(70)	0.0(10)
C(71)-O(4)-C(70)-C(69)	3.0(9)
C(71)-O(4)-C(70)-C(65)	-174.9(5)
C(68)-C(69)-C(70)-O(4)	-177.6(6)
C(68)-C(69)-C(70)-C(65)	0.2(9)
C(66)-C(65)-C(70)-O(4)	177.7(5)
C(64)-C(65)-C(70)-O(4)	-1.5(8)
C(66)-C(65)-C(70)-C(69)	-0.2(9)
C(64)-C(65)-C(70)-C(69)	-179.5(6)

C(70)-O(4)-C(71)-C(72)	169.2(5)
C(73)-O(5)-C(72)-C(71)	-139.7(5)
O(4)-C(71)-C(72)-O(5)	-67.7(6)
C(72)-O(5)-C(73)-C(74)	-60.5(7)
C(75)-O(6)-C(74)-C(73)	-152.4(6)
O(5)-C(73)-C(74)-O(6)	-50.2(8)
C(74)-O(6)-C(75)-C(76)	95.7(7)
C(74)-O(6)-C(75)-C(80)	-88.2(7)
O(6)-C(75)-C(76)-C(77)	179.0(6)
C(80)-C(75)-C(76)-C(77)	3.0(10)
O(6)-C(75)-C(76)-C(83)	-2.3(9)
C(80)-C(75)-C(76)-C(83)	-178.4(6)
C(75)-C(76)-C(77)-C(78)	-0.2(11)
C(83)-C(76)-C(77)-C(78)	-178.9(7)
C(76)-C(77)-C(78)-C(79)	-1.3(12)
C(77)-C(78)-C(79)-C(80)	0.1(12)
C(78)-C(79)-C(80)-C(75)	2.5(11)
C(78)-C(79)-C(80)-C(84)	-178.0(7)
C(76)-C(75)-C(80)-C(79)	-4.1(10)
O(6)-C(75)-C(80)-C(79)	180.0(6)
C(76)-C(75)-C(80)-C(84)	176.5(6)
O(6)-C(75)-C(80)-C(84)	0.5(9)
C(42)-C(41)-C(81)-C(92)	112.1(9)
C(40)-C(41)-C(81)-C(92)	-64.7(10)
C(42)-C(41)-C(81)-C(87)	-123.6(8)
C(40)-C(41)-C(81)-C(87)	59.7(11)
C(42)-C(37)-C(82)-C(86)	128.7(8)
C(38)-C(37)-C(82)-C(86)	-54.3(10)
C(42)-C(37)-C(82)-C(85)	-107.4(8)
C(38)-C(37)-C(82)-C(85)	69.7(9)
C(75)-C(76)-C(83)-C(89)	-108.3(8)
C(77)-C(76)-C(83)-C(89)	70.4(9)
C(75)-C(76)-C(83)-C(88)	125.7(7)
C(77)-C(76)-C(83)-C(88)	-55.7(9)
C(79)-C(80)-C(84)-C(90)	60.4(9)
C(75)-C(80)-C(84)-C(90)	-120.2(7)
C(79)-C(80)-C(84)-C(91)	-62.7(10)
C(75)-C(80)-C(84)-C(91)	116.8(8)

Table S5 Bond lengths [Å] and angles [°] for **3**.

O(1)-C(6)	1.3975(16)	O(1)-C(7)	1.4372(16)
O(2)-C(9)	1.4133(16)	O(2)-C(8)	1.4154(16)
O(3)-C(11)	1.3675(15)	O(3)-C(10)	1.4252(17)
C(1)-C(2)	1.396(2)	C(1)-C(6)	1.4038(18)
C(1)-C(23)	1.516(2)	C(2)-C(3)	1.384(2)
C(3)-C(4)	1.379(2)	C(4)-C(5)	1.393(2)
C(5)-C(6)	1.3948(18)	C(5)-C(26)	1.5238(18)
C(7)-C(8)	1.495(2)	C(9)-C(10)	1.500(2)
C(11)-C(12)	1.370(2)	C(11)-C(20)	1.427(2)
C(12)-C(13)	1.4088(19)	C(13)-C(14)	1.361(2)
C(14)-C(15)	1.4186(19)	C(15)-C(20)	1.4204(17)
C(15)-C(16)	1.4333(19)	C(16)-C(17)	1.3833(19)
C(16)-C(21)	1.4277(18)	C(17)-C(18)	1.4013(19)
C(18)-C(19)	1.370(2)	C(19)-C(20)	1.4158(19)
C(21)-C(22)	1.2036(18)	C(22)-C(22)#1	1.369(3)
C(23)-C(25)	1.516(2)	C(23)-C(24)	1.527(2)
C(26)-C(28)	1.521(3)	C(26)-C(27)	1.521(2)

C(6)-O(1)-C(7)	112.42(11)	C(9)-O(2)-C(8)	113.08(10)
C(11)-O(3)-C(10)	118.13(11)	C(2)-C(1)-C(6)	117.06(12)
C(2)-C(1)-C(23)	122.69(12)	C(6)-C(1)-C(23)	120.20(12)
C(3)-C(2)-C(1)	120.98(13)	C(4)-C(3)-C(2)	120.37(15)
C(3)-C(4)-C(5)	121.25(14)	C(4)-C(5)-C(6)	117.25(12)
C(4)-C(5)-C(26)	120.72(12)	C(6)-C(5)-C(26)	122.00(12)
C(5)-C(6)-O(1)	118.54(11)	C(5)-C(6)-C(1)	123.05(12)
O(1)-C(6)-C(1)	118.39(11)	O(1)-C(7)-C(8)	109.30(12)
O(2)-C(8)-C(7)	108.18(11)	O(2)-C(9)-C(10)	108.45(11)
O(3)-C(10)-C(9)	106.95(12)	O(3)-C(11)-C(12)	125.29(13)
O(3)-C(11)-C(20)	113.67(12)	C(12)-C(11)-C(20)	121.04(12)
C(11)-C(12)-C(13)	119.34(13)	C(14)-C(13)-C(12)	121.71(13)
C(13)-C(14)-C(15)	120.10(12)	C(14)-C(15)-C(20)	119.27(13)
C(14)-C(15)-C(16)	122.91(11)	C(20)-C(15)-C(16)	117.82(12)
C(17)-C(16)-C(21)	119.65(13)	C(17)-C(16)-C(15)	120.95(12)
C(21)-C(16)-C(15)	119.40(12)	C(16)-C(17)-C(18)	120.23(13)
C(19)-C(18)-C(17)	120.29(13)	C(18)-C(19)-C(20)	121.12(12)

C(19)-C(20)-C(15) 119.58(13)	C(19)-C(20)-C(11) 121.90(12)
C(15)-C(20)-C(11) 118.51(12)	C(22)-C(21)-C(16) 179.29(15)
C(21)-C(22)-C(22)#1 179.5(2)	C(25)-C(23)-C(1) 110.77(12)
C(25)-C(23)-C(24) 109.88(12)	C(1)-C(23)-C(24) 114.06(13)
C(28)-C(26)-C(27) 110.17(13)	C(28)-C(26)-C(5) 109.78(13)
C(27)-C(26)-C(5) 112.55(13)	

Symmetry transformations used to generate equivalent atoms:
#1 -x-1,-y+1,-z

Table S6 Anisotropic displacement parameters ($Å^2 \times 10^3$) for dimer **3**. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
O(1)	34(1)	28(1)	27(1)	-2(1)	-4(1)	1(1)
O(2)	48(1)	31(1)	34(1)	-6(1)	-18(1)	6(1)
O(3)	32(1)	44(1)	31(1)	0(1)	-5(1)	9(1)
C(1)	35(1)	34(1)	29(1)	2(1)	-7(1)	-1(1)
C(2)	48(1)	54(1)	24(1)	-6(1)	-7(1)	5(1)
C(3)	53(1)	66(1)	33(1)	-17(1)	-6(1)	16(1)
C(4)	45(1)	58(1)	36(1)	-11(1)	-7(1)	18(1)
C(5)	37(1)	40(1)	26(1)	-3(1)	-5(1)	6(1)
C(6)	33(1)	31(1)	24(1)	-1(1)	-2(1)	0(1)
C(7)	43(1)	32(1)	35(1)	3(1)	-11(1)	-5(1)
C(8)	50(1)	28(1)	41(1)	-2(1)	-17(1)	4(1)
C(9)	35(1)	40(1)	33(1)	-12(1)	-7(1)	6(1)
C(10)	33(1)	42(1)	28(1)	-9(1)	-4(1)	6(1)
C(11)	32(1)	31(1)	28(1)	-6(1)	-10(1)	4(1)
C(12)	33(1)	36(1)	29(1)	-5(1)	-1(1)	1(1)
C(13)	41(1)	34(1)	25(1)	-1(1)	-4(1)	0(1)
C(14)	35(1)	30(1)	26(1)	-2(1)	-9(1)	3(1)
C(15)	32(1)	26(1)	24(1)	-6(1)	-8(1)	1(1)
C(16)	34(1)	29(1)	25(1)	-6(1)	-7(1)	3(1)
C(17)	35(1)	37(1)	26(1)	-6(1)	-2(1)	2(1)
C(18)	44(1)	37(1)	23(1)	0(1)	-3(1)	2(1)
C(19)	38(1)	33(1)	26(1)	-2(1)	-9(1)	5(1)
C(20)	32(1)	29(1)	24(1)	-6(1)	-7(1)	1(1)

C(21)	34(1)	35(1)	28(1)	-6(1)	-2(1)	2(1)
C(22)	34(1)	37(1)	27(1)	-3(1)	-1(1)	3(1)
C(23)	42(1)	34(1)	31(1)	1(1)	-13(1)	2(1)
C(24)	45(1)	57(1)	44(1)	20(1)	-10(1)	1(1)
C(25)	44(1)	61(1)	51(1)	15(1)	5(1)	10(1)
C(26)	47(1)	42(1)	30(1)	-5(1)	-11(1)	16(1)
C(27)	45(1)	66(1)	49(1)	4(1)	-18(1)	-6(1)
C(28)	57(1)	110(2)	41(1)	25(1)	-8(1)	-14(1)

Table S7 Hydrogen atom coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for dimer **3**.

	x	*y*	*z*	U_{eq}
H(2)	5518	2830	3418	50
H(3)	3872	4636	3279	61
H(4)	2947	4935	2497	55
H(7A)	3634	101	1868	44
H(7B)	4838	-946	2055	44
H(8A)	5641	-886	1219	48
H(8B)	4295	-1819	1273	48
H(9A)	3229	-1375	554	43
H(9B)	4573	-745	333	43
H(10A)	3481	1717	193	41
H(10B)	2920	341	-148	41
H(12)	1874	2525	-413	39
H(13)	161	3993	-762	40
H(14)	-1828	4178	-385	37
H(17)	-3579	2130	1068	39
H(18)	-1892	587	1398	41
H(19)	83	405	1002	39
H(23)	6505	-52	2557	43
H(24A)	7492	-618	3314	73
H(24B)	5982	-259	3406	73
H(24C)	7066	1017	3536	73
H(25A)	7872	1967	2295	78
H(25B)	8653	772	2641	78

H(25C)	8193	2400	2859	78
H(26)	3608	2539	1439	47
H(27A)	1537	2679	1843	80
H(27B)	1531	3511	1315	80
H(27C)	1622	4523	1809	80
H(28A)	3698	5801	1601	104
H(28B)	3564	4998	1070	104
H(28C)	4880	4798	1391	104

Table S8 Torsion angles [°] for **3**.

C(6)-C(1)-C(2)-C(3)	-1.2(2)
C(23)-C(1)-C(2)-C(3)	176.51(15)
C(1)-C(2)-C(3)-C(4)	-0.6(3)
C(2)-C(3)-C(4)-C(5)	1.7(3)
C(3)-C(4)-C(5)-C(6)	-1.0(3)
C(3)-C(4)-C(5)-C(26)	-178.70(16)
C(4)-C(5)-C(6)-O(1)	-179.14(13)
C(26)-C(5)-C(6)-O(1)	-1.5(2)
C(4)-C(5)-C(6)-C(1)	-0.9(2)
C(26)-C(5)-C(6)-C(1)	176.81(14)
C(7)-O(1)-C(6)-C(5)	-86.59(14)
C(7)-O(1)-C(6)-C(1)	95.06(14)
C(2)-C(1)-C(6)-C(5)	1.9(2)
C(23)-C(1)-C(6)-C(5)	-175.82(13)
C(2)-C(1)-C(6)-O(1)	-179.80(12)
C(23)-C(1)-C(6)-O(1)	2.46(19)
C(6)-O(1)-C(7)-C(8)	159.17(11)
C(9)-O(2)-C(8)-C(7)	-159.92(12)
O(1)-C(7)-C(8)-O(2)	-69.97(15)
C(8)-O(2)-C(9)-C(10)	175.32(13)
C(11)-O(3)-C(10)-C(9)	-175.05(11)
O(2)-C(9)-C(10)-O(3)	-70.26(14)
C(10)-O(3)-C(11)-C(12)	-0.65(18)
C(10)-O(3)-C(11)-C(20)	179.01(11)
O(3)-C(11)-C(12)-C(13)	179.34(12)
C(20)-C(11)-C(12)-C(13)	-0.30(19)
C(11)-C(12)-C(13)-C(14)	0.8(2)

C(12)-C(13)-C(14)-C(15)	-0.01(19)
C(13)-C(14)-C(15)-C(20)	-1.29(18)
C(13)-C(14)-C(15)-C(16)	179.48(12)
C(14)-C(15)-C(16)-C(17)	178.80(12)
C(20)-C(15)-C(16)-C(17)	-0.44(17)
C(14)-C(15)-C(16)-C(21)	-1.09(18)
C(20)-C(15)-C(16)-C(21)	179.67(11)
C(21)-C(16)-C(17)-C(18)	179.65(12)
C(15)-C(16)-C(17)-C(18)	-0.25(19)
C(16)-C(17)-C(18)-C(19)	0.20(19)
C(17)-C(18)-C(19)-C(20)	0.6(2)
C(18)-C(19)-C(20)-C(15)	-1.26(19)
C(18)-C(19)-C(20)-C(11)	178.88(12)
C(14)-C(15)-C(20)-C(19)	-178.11(11)
C(16)-C(15)-C(20)-C(19)	1.17(17)
C(14)-C(15)-C(20)-C(11)	1.76(17)
C(16)-C(15)-C(20)-C(11)	-178.97(11)
O(3)-C(11)-C(20)-C(19)	-0.80(17)
C(12)-C(11)-C(20)-C(19)	178.88(12)
O(3)-C(11)-C(20)-C(15)	179.34(11)
C(12)-C(11)-C(20)-C(15)	-0.98(18)
C(2)-C(1)-C(23)-C(25)	-93.87(18)
C(6)-C(1)-C(23)-C(25)	83.75(16)
C(2)-C(1)-C(23)-C(24)	30.7(2)
C(6)-C(1)-C(23)-C(24)	-151.66(13)
C(4)-C(5)-C(26)-C(28)	74.7(2)
C(6)-C(5)-C(26)-C(28)	-102.94(17)
C(4)-C(5)-C(26)-C(27)	-48.4(2)
C(6)-C(5)-C(26)-C(27)	133.96(15)

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