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Supporting information for article:

Crystal structures of eight mono-methyl alkanes (C26–C32) *via* single-crystal and powder diffraction and DFT-D optimization

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Supporting Information

Table S1 Bond distances, angles and torsions (Å, º) for 7-methylnanacosane from the single-crystal study.

C1—C2	1.513 (5)	C15—C16	1.524 (4)
C2—C3	1.510 (5)	C16—C17	1.519 (4)
C3—C4	1.536 (5)	C17—C18	1.522 (4)
C4—C5	1.522 (5)	C18—C19	1.518 (4)
C5—C6	1.519 (5)	C19—C20	1.525 (4)
C6—C7	1.523 (5)	C20—C21	1.522 (4)
C7—C8	1.531 (5)	C21—C22	1.528 (4)
C7—C30	1.521 (4)	C22—C23	1.520 (5)
C8—C9	1.526 (5)	C23—C24	1.528 (5)
C9—C10	1.520 (5)	C24—C25	1.522 (4)
C10—C11	1.519 (4)	C25—C26	1.522 (5)
C11—C12	1.516 (4)	C26—C27	1.522 (4)
C12—C13	1.527 (4)	C27—C28	1.527 (5)
C13—C14	1.528 (4)	C28—C29	1.516 (5)
C14—C15	1.525 (4)		

C1—C2—C3	114.1 (3)	C14—C15—C16	113.9 (3)
C2—C3—C4	112.9 (3)	C15—C16—C17	114.2 (3)
C3—C4—C5	115.3 (3)	C16—C17—C18	114.4 (3)
C4—C5—C6	113.0 (3)	C17—C18—C19	114.4 (3)
C5—C6—C7	117.4 (3)	C18—C19—C20	113.9 (3)
C6—C7—C8	110.3 (3)	C19—C20—C21	114.1 (3)
C6—C7—C30	111.9 (3)	C20—C21—C22	114.0 (3)
C8—C7—C30	112.0 (3)	C21—C22—C23	113.9 (3)
C7—C8—C9	115.4 (3)	C22—C23—C24	113.9 (3)
C8—C9—C10	114.6 (3)	C23—C24—C25	114.0 (3)
C9—C10—C11	113.4 (3)	C24—C25—C26	114.4 (3)

C10—C11—C12	114.9 (3)	C25—C26—C27	114.0 (3)
C11—C12—C13	113.3 (3)	C26—C27—C28	113.8 (3)
C12—C13—C14	114.1 (3)	C27—C28—C29	113.5 (3)
C13—C14—C15	113.8 (3)		

C1—C2—C3—C4	178.9 (3)	C15—C16—C17—C18	179.7 (3)
C2—C3—C4—C5	-177.9 (3)	C16—C17—C18—C19	-179.8 (3)
C3—C4—C5—C6	173.8 (3)	C17—C18—C19—C20	-179.9 (3)
C4—C5—C6—C7	-174.0 (3)	C18—C19—C20—C21	179.9 (3)
C5—C6—C7—C8	170.8 (3)	C19—C20—C21—C22	179.4 (3)
C6—C7—C8—C9	-175.4 (3)	C20—C21—C22—C23	-179.8 (3)
C7—C8—C9—C10	177.1 (3)	C21—C22—C23—C24	-179.9 (3)
C8—C9—C10—C11	176.3 (3)	C22—C23—C24—C25	180.0 (3)
C9—C10—C11—C12	-178.4 (3)	C23—C24—C25—C26	-178.6 (3)
C10—C11—C12—C13	178.7 (3)	C24—C25—C26—C27	179.3 (3)
C11—C12—C13—C14	-179.6 (3)	C25—C26—C27—C28	-179.0 (3)
C12—C13—C14—C15	-179.5 (3)	C26—C27—C28—C29	179.1 (3)
C13—C14—C15—C16	-179.8 (3)	C5—C6—C7—C30	-63.8 (5)
C14—C15—C16—C17	180.0 (3)	C30—C7—C8—C9	59.3 (5)

Table S2 Overlay in Mercury of the single-crystal and the DFT-optimised 7-Me-$C_{29}H_{59}$ molecules

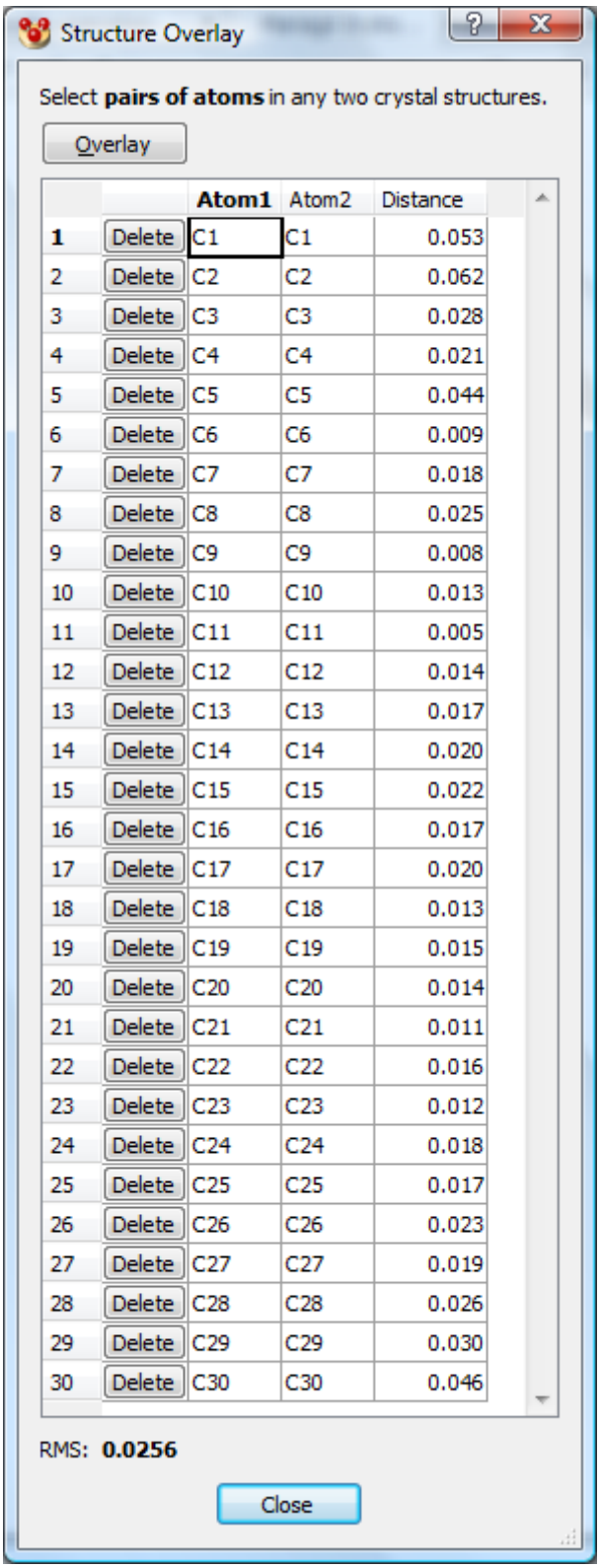
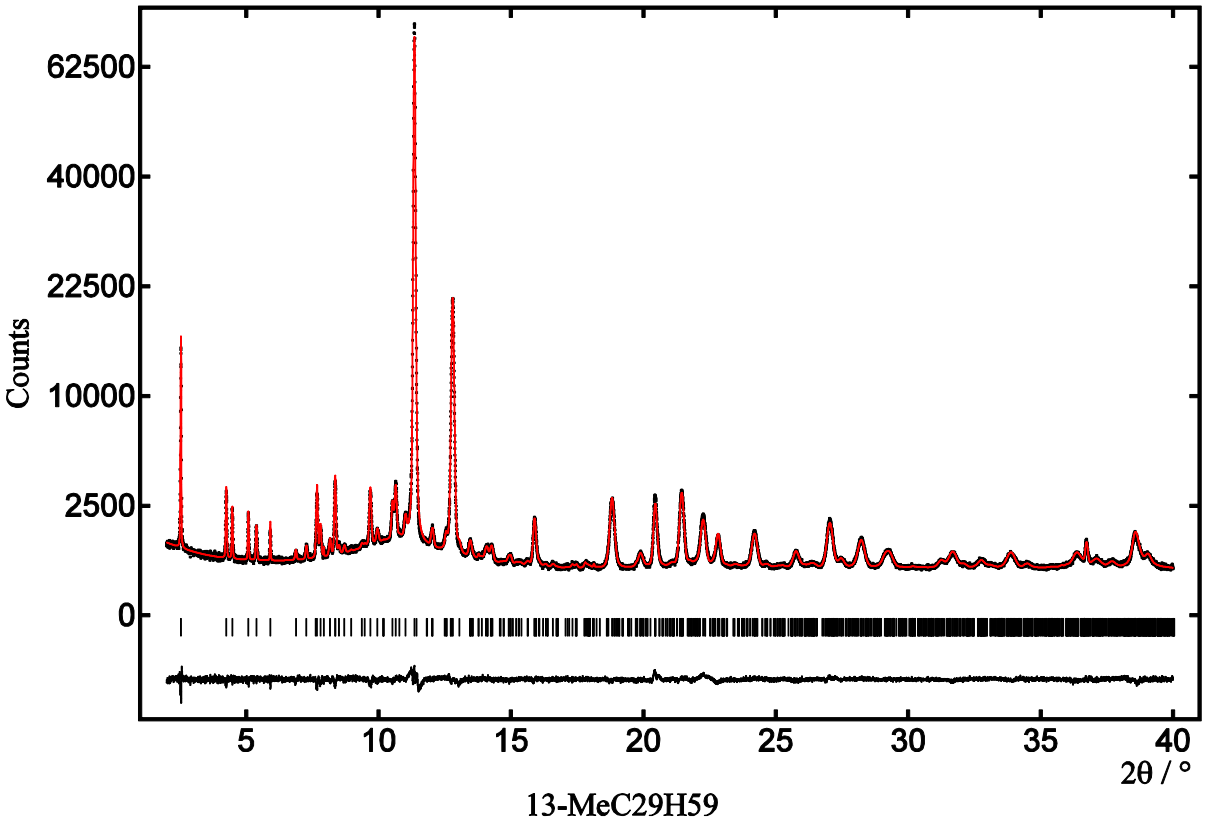
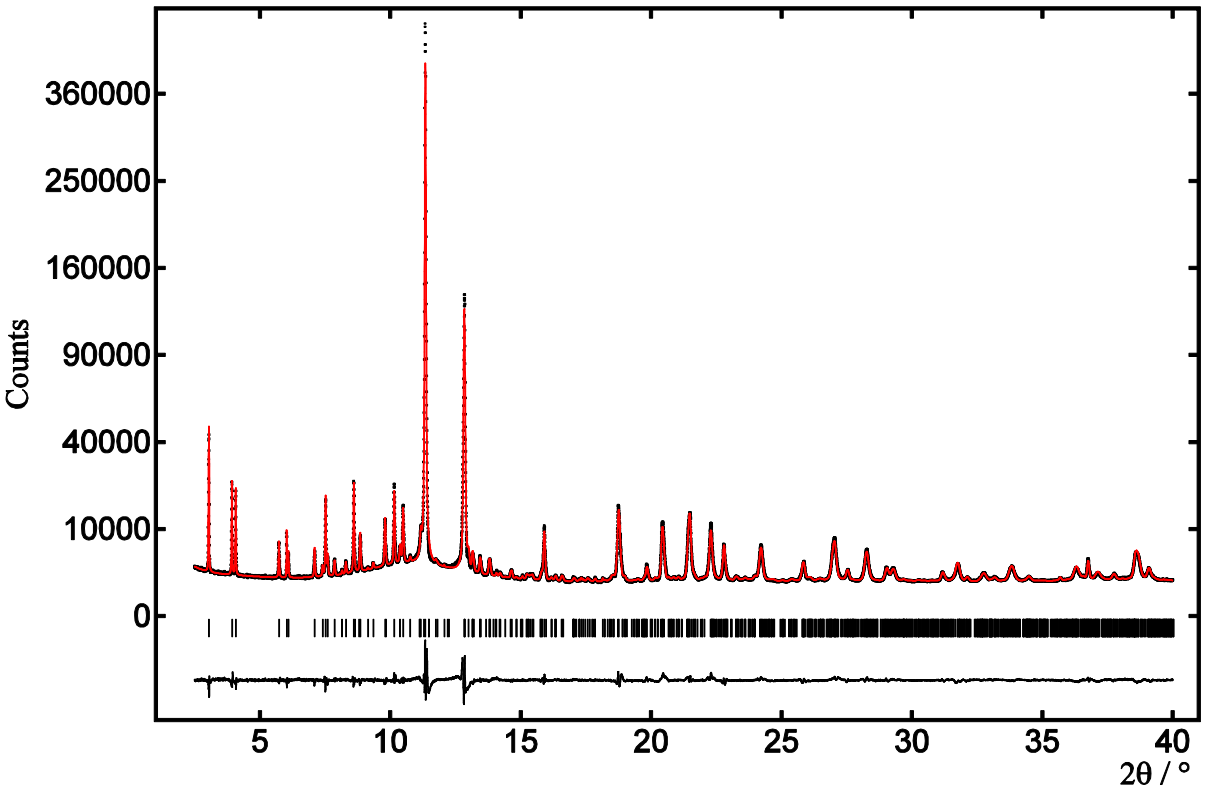
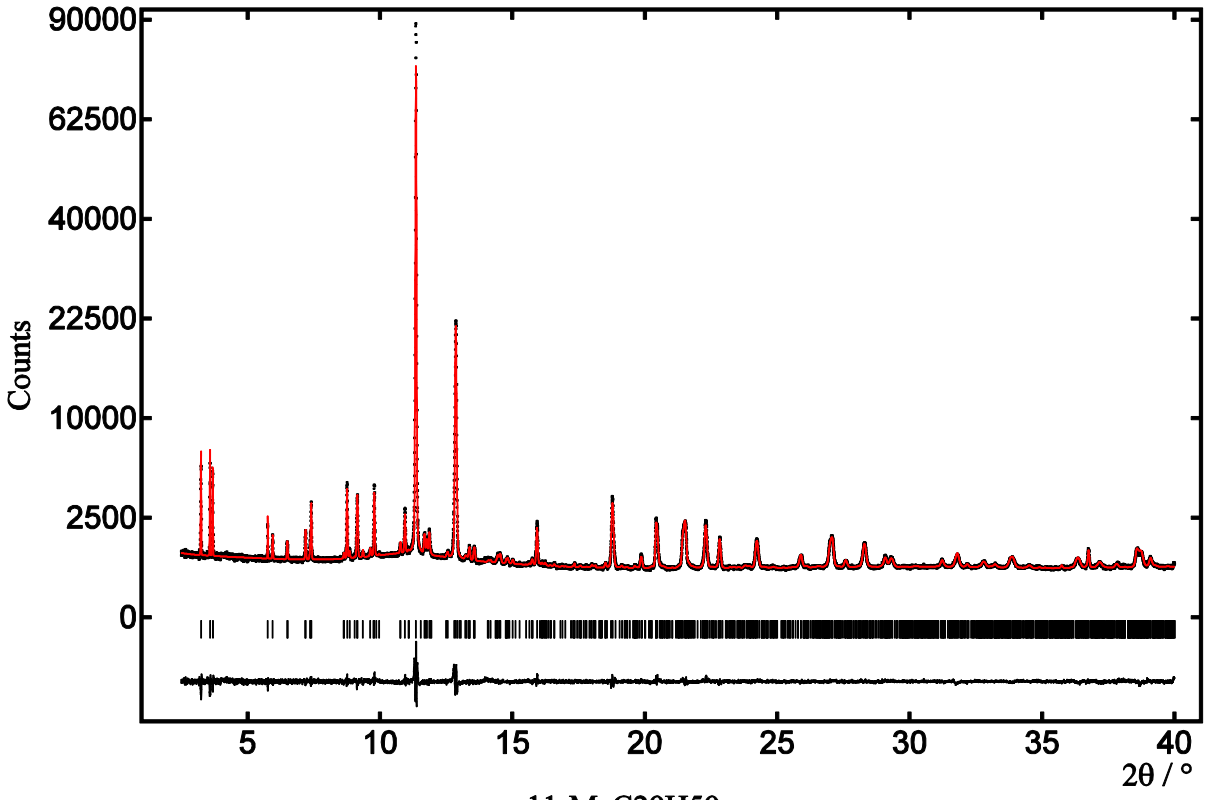


Figure S1 Observed (points), calculated (red line) and difference profiles for the powder diffraction patterns for the eight samples after a final rigid body fit of the molecules obtained from the DFT-D optimisation. Note the square-root counts scale.





11-MeC27H55



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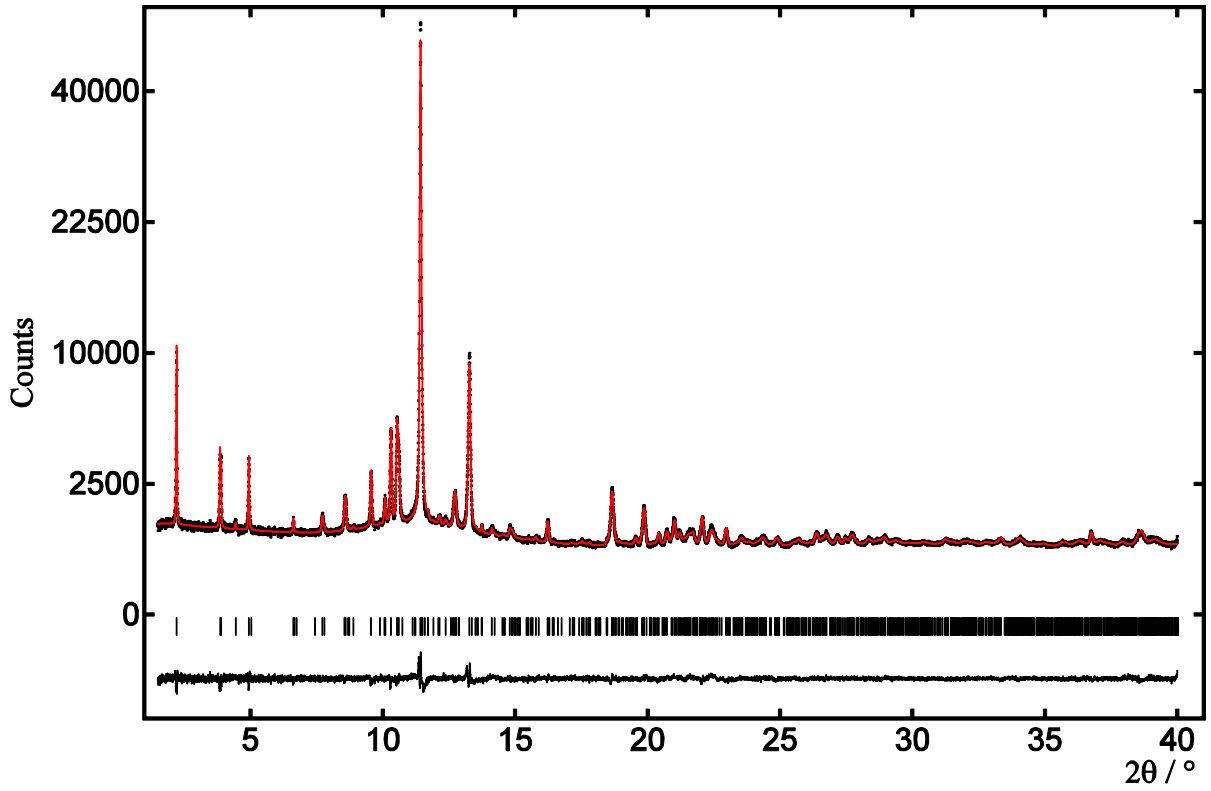
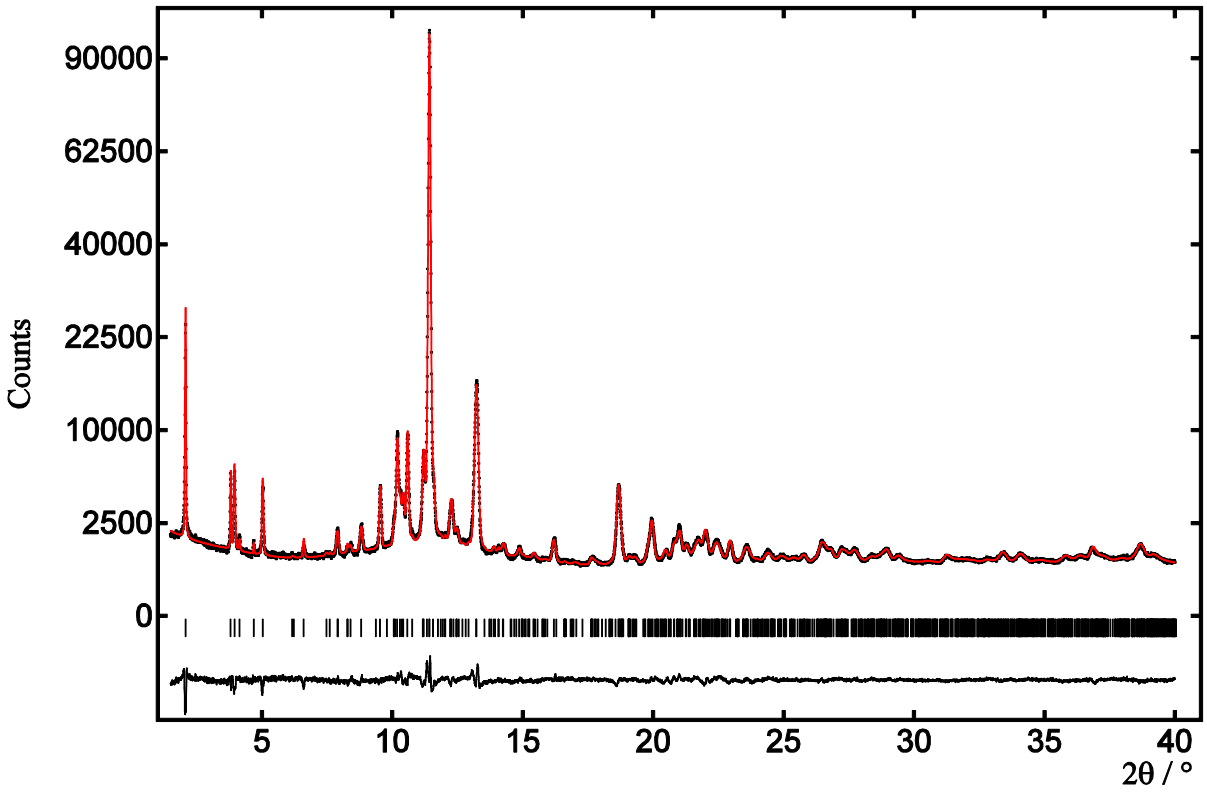


9-MeC25H51



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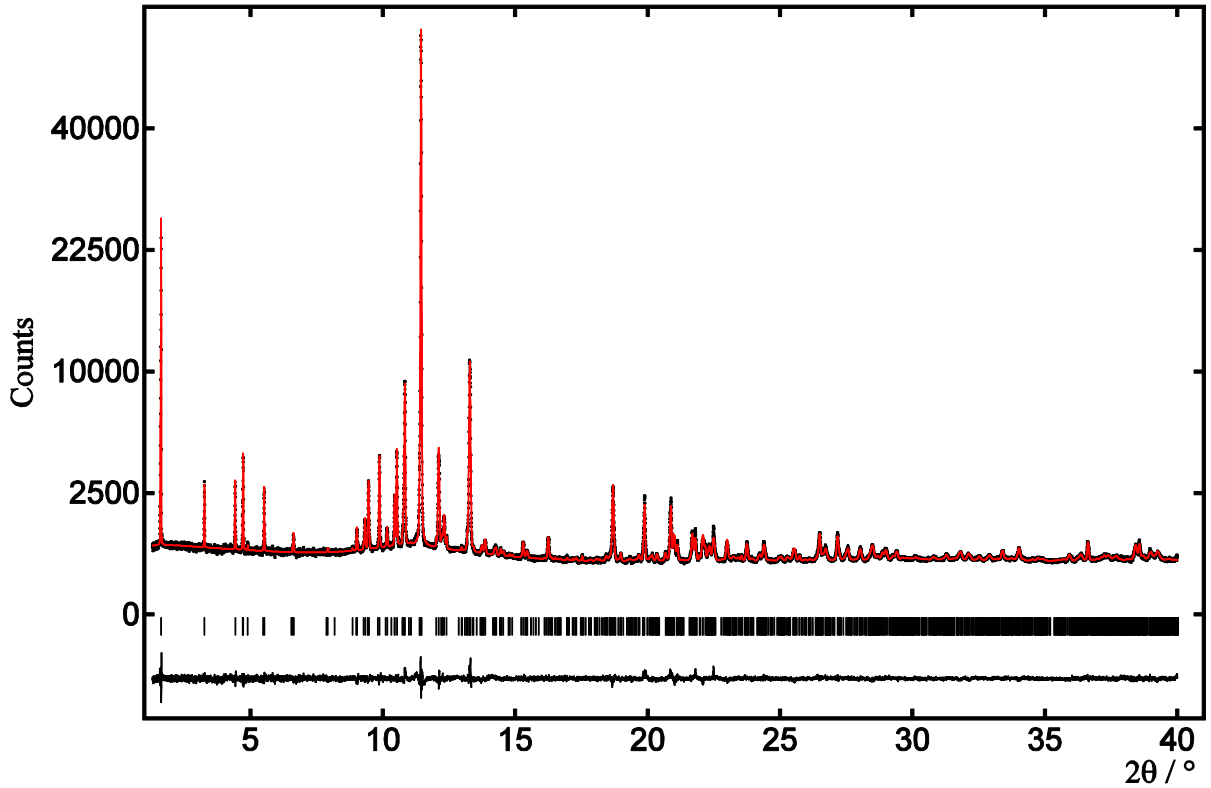
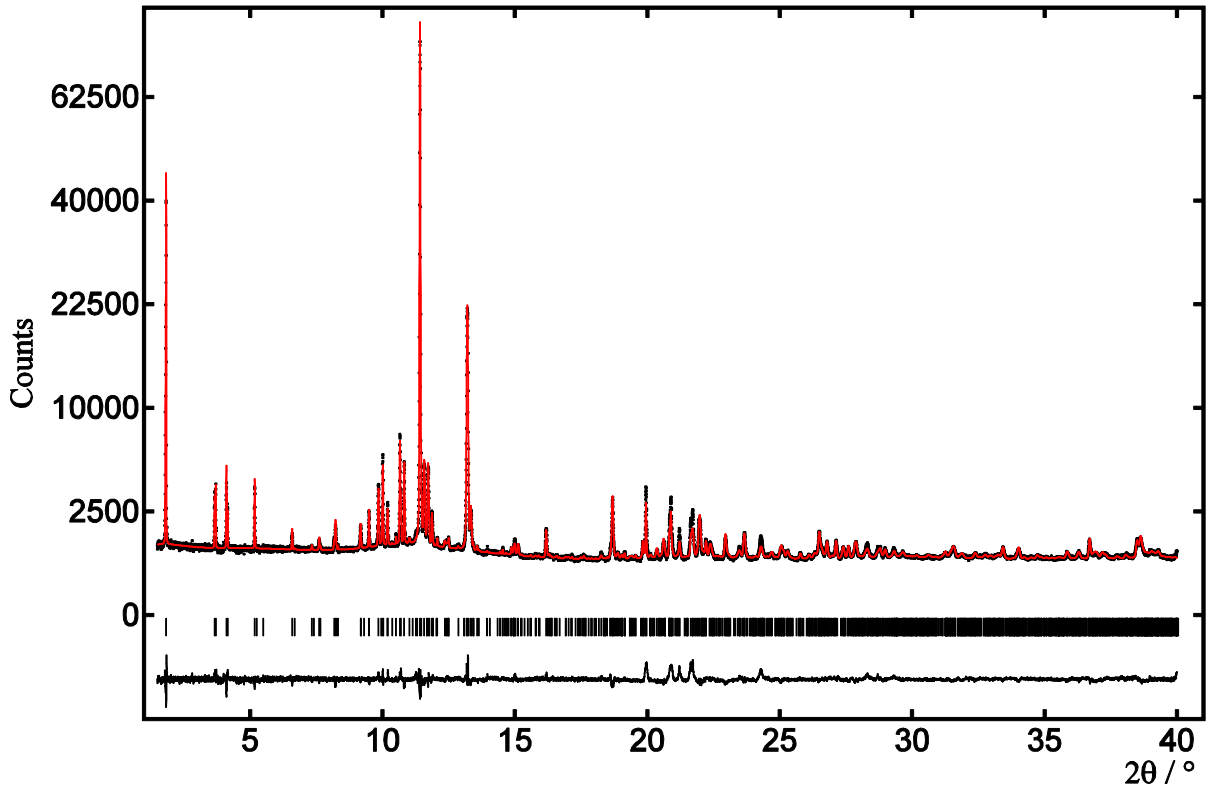


7-MeC29H59



9-MeC31H63

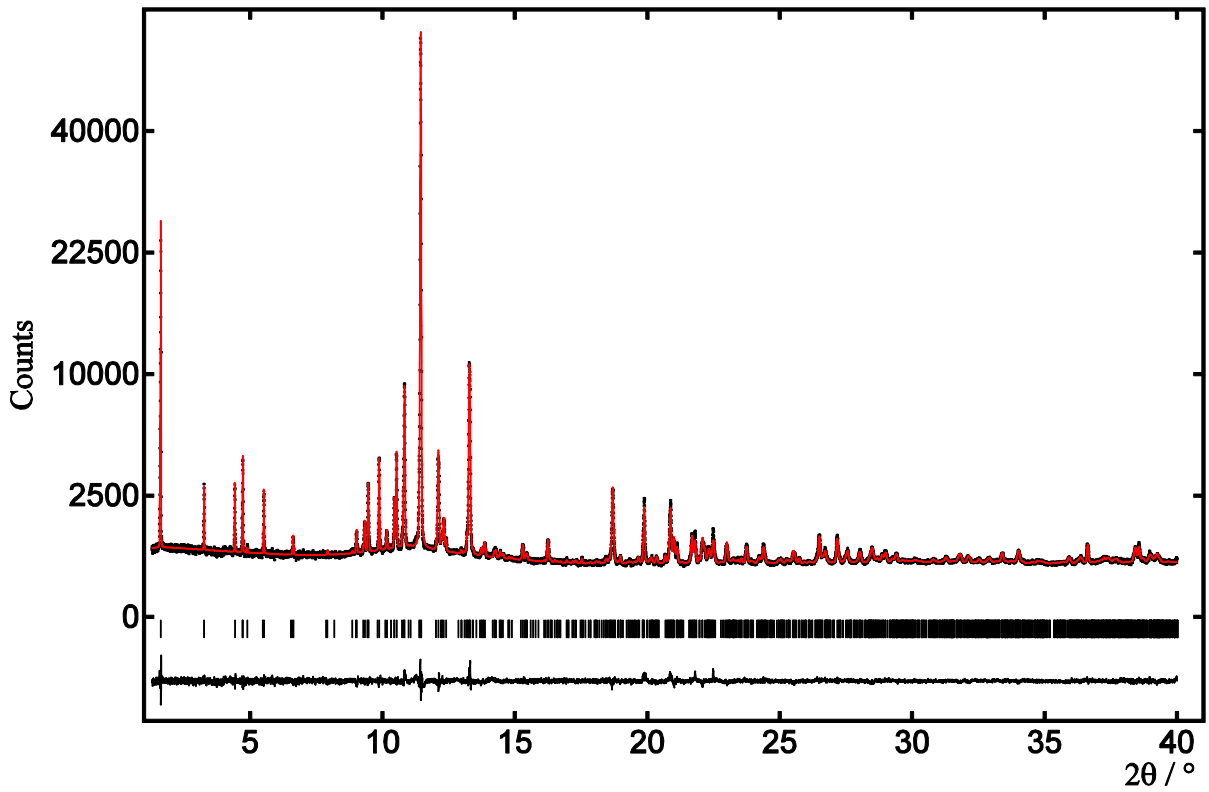
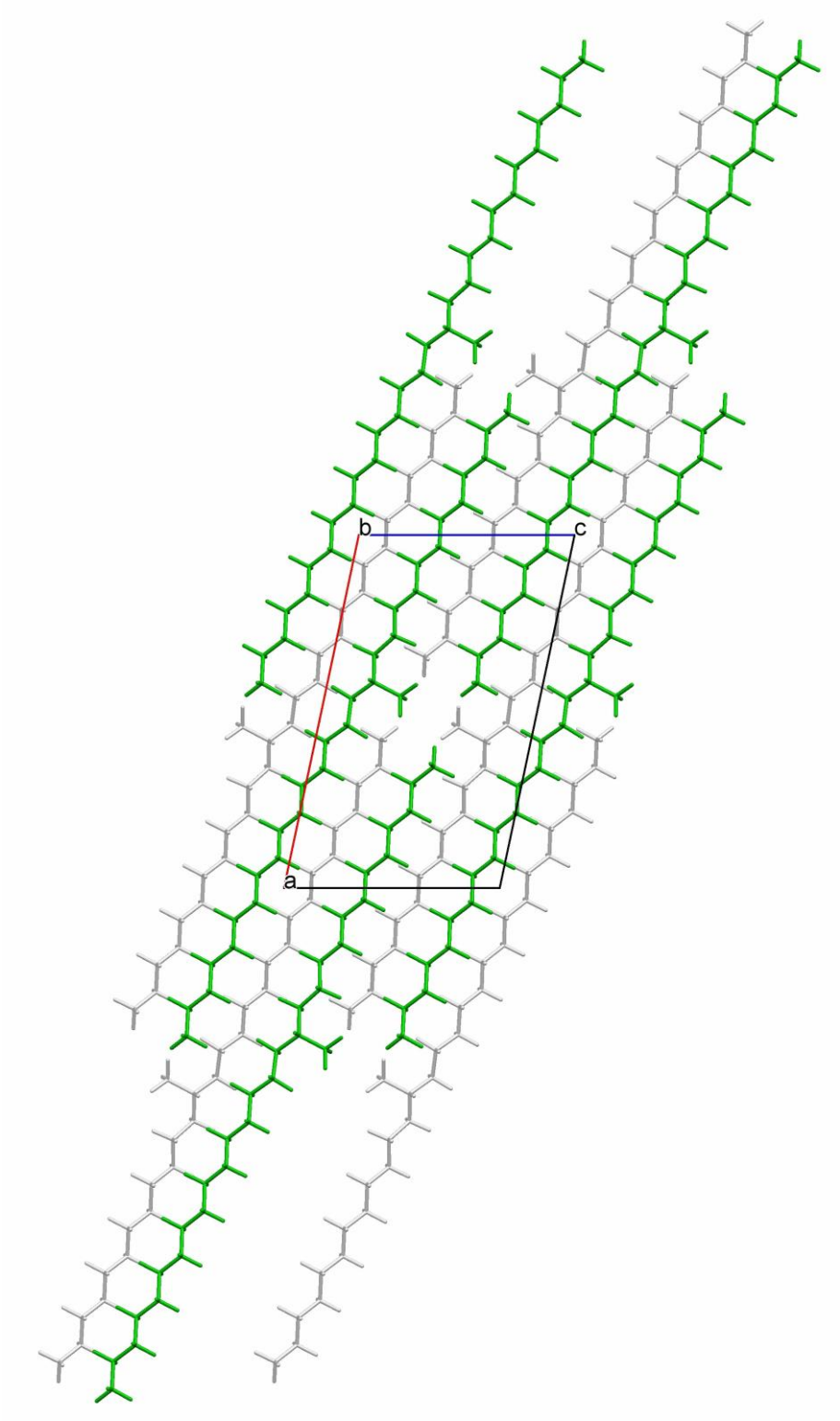
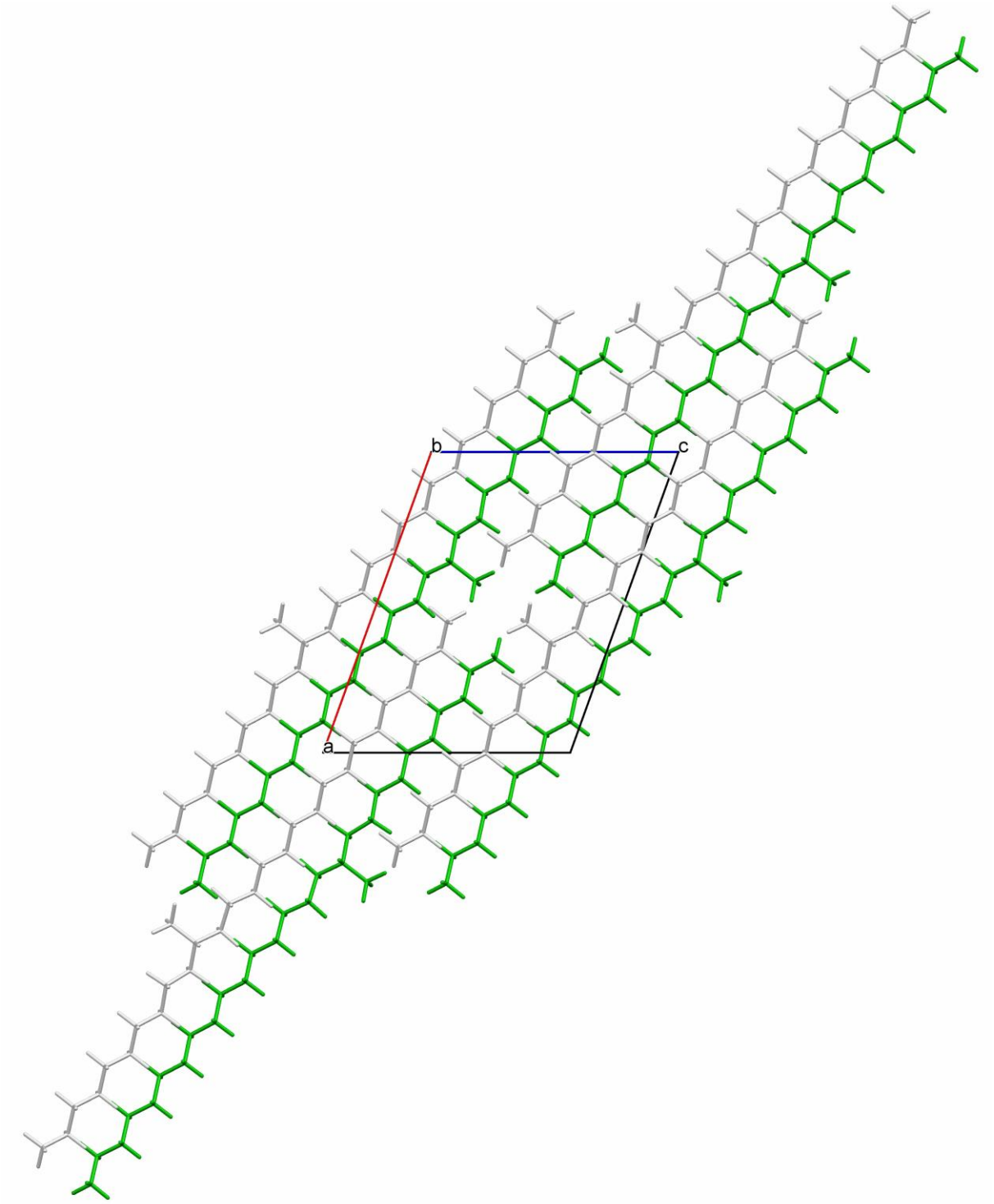

40000
22500
10000
2500
0
Counts
5
10
15
20
25
30
35
40
2θ / °
7-MeC29H59

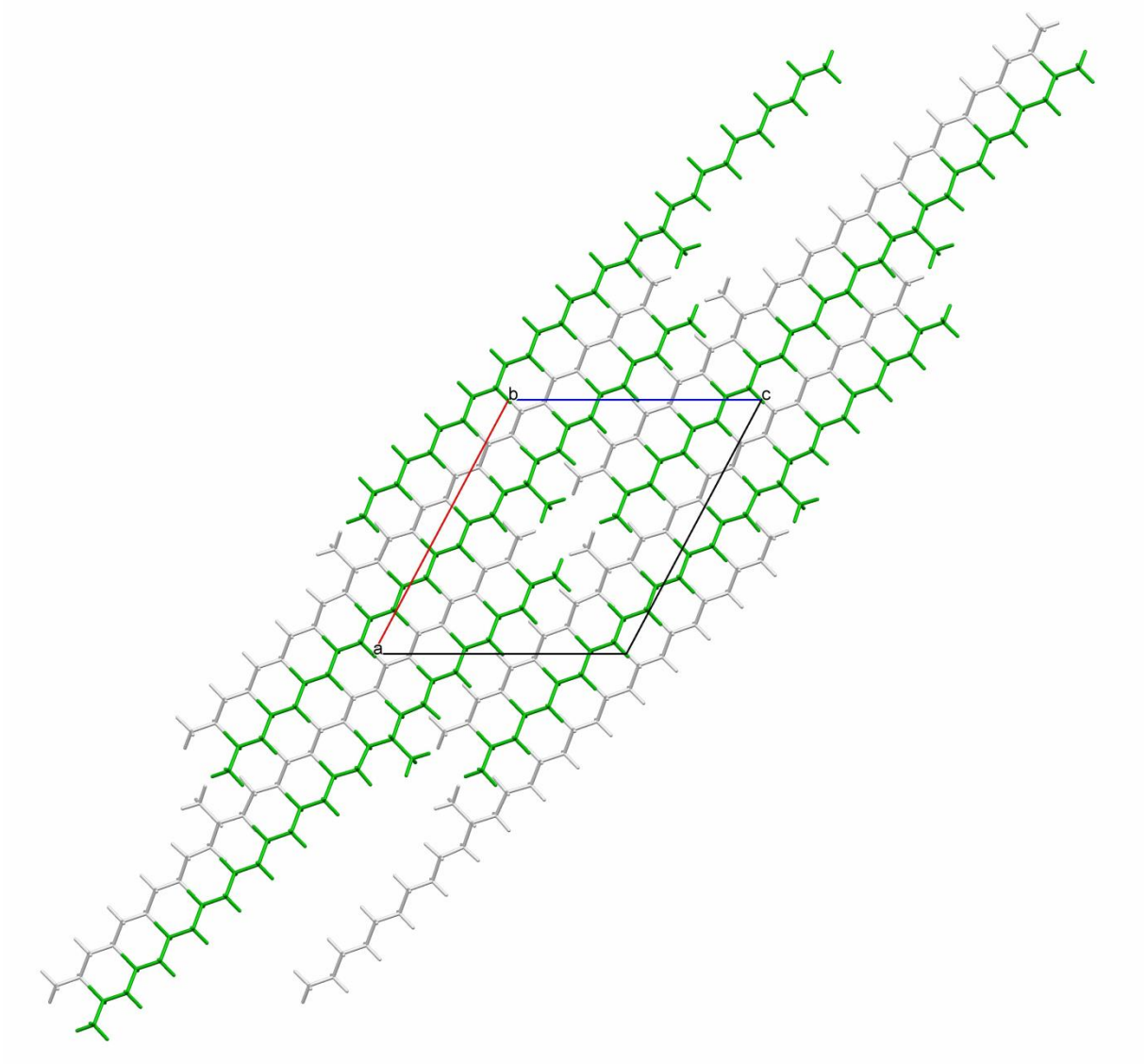
Figure S2 The DFT-minimised structures viewed along the *b* axis. Grey and green molecules are related by a 2_1 screw axis.



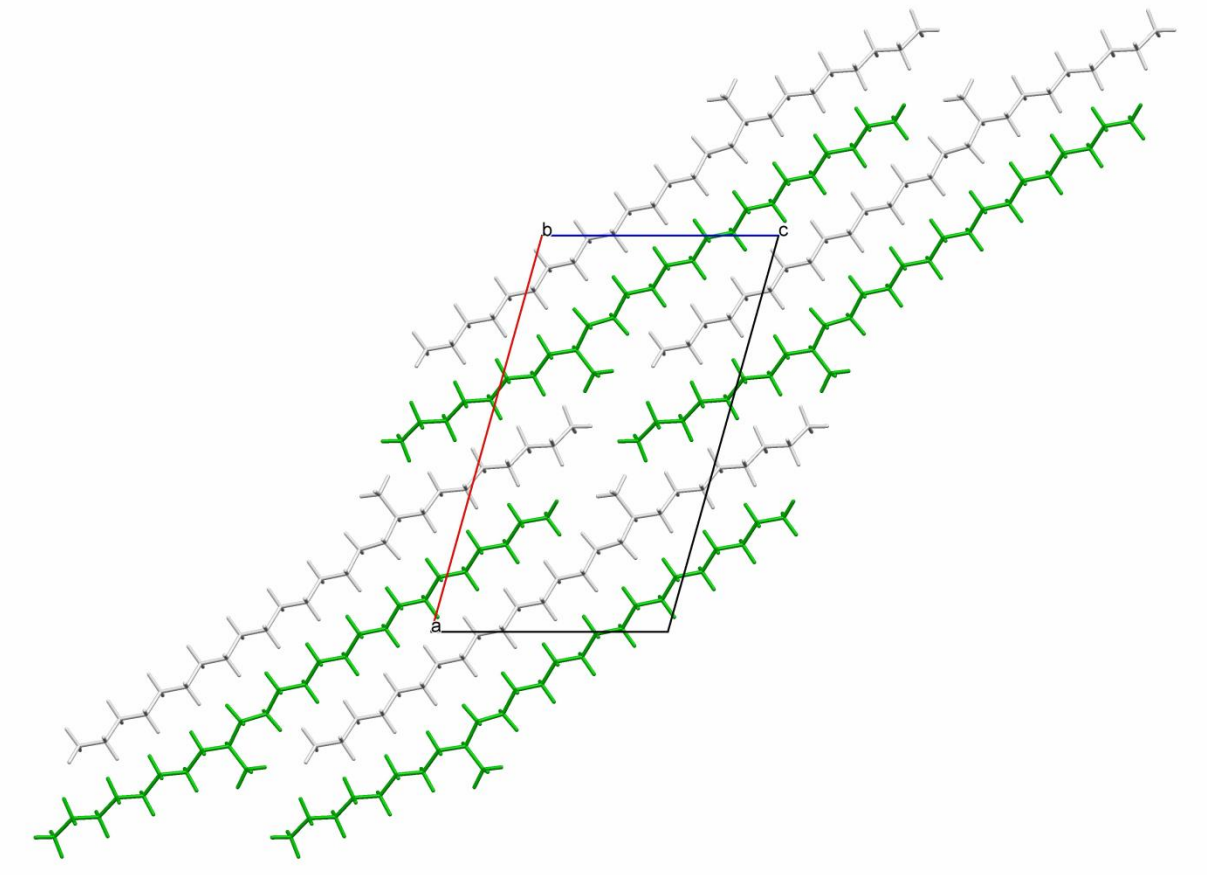
13-Me$C_{29}H_{59}$



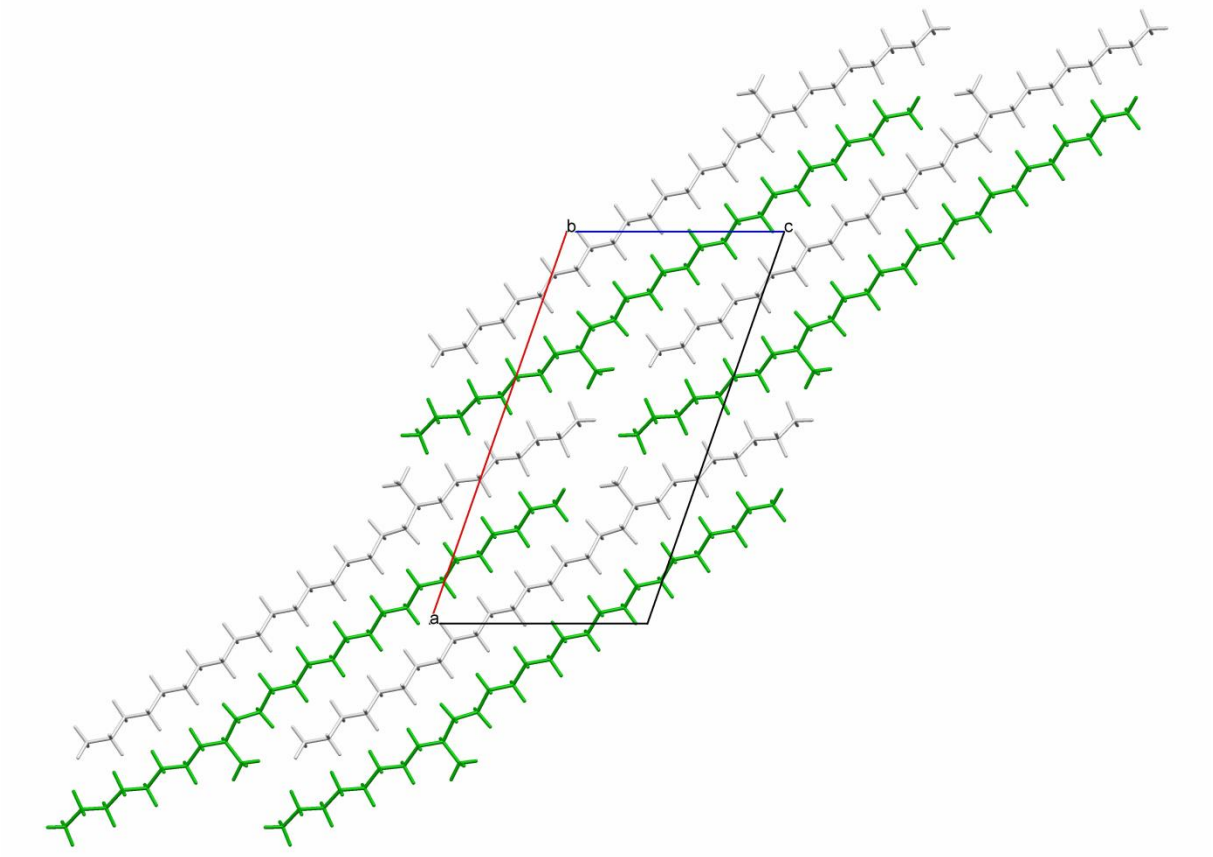
11-Me$C_{27}H_{55}$



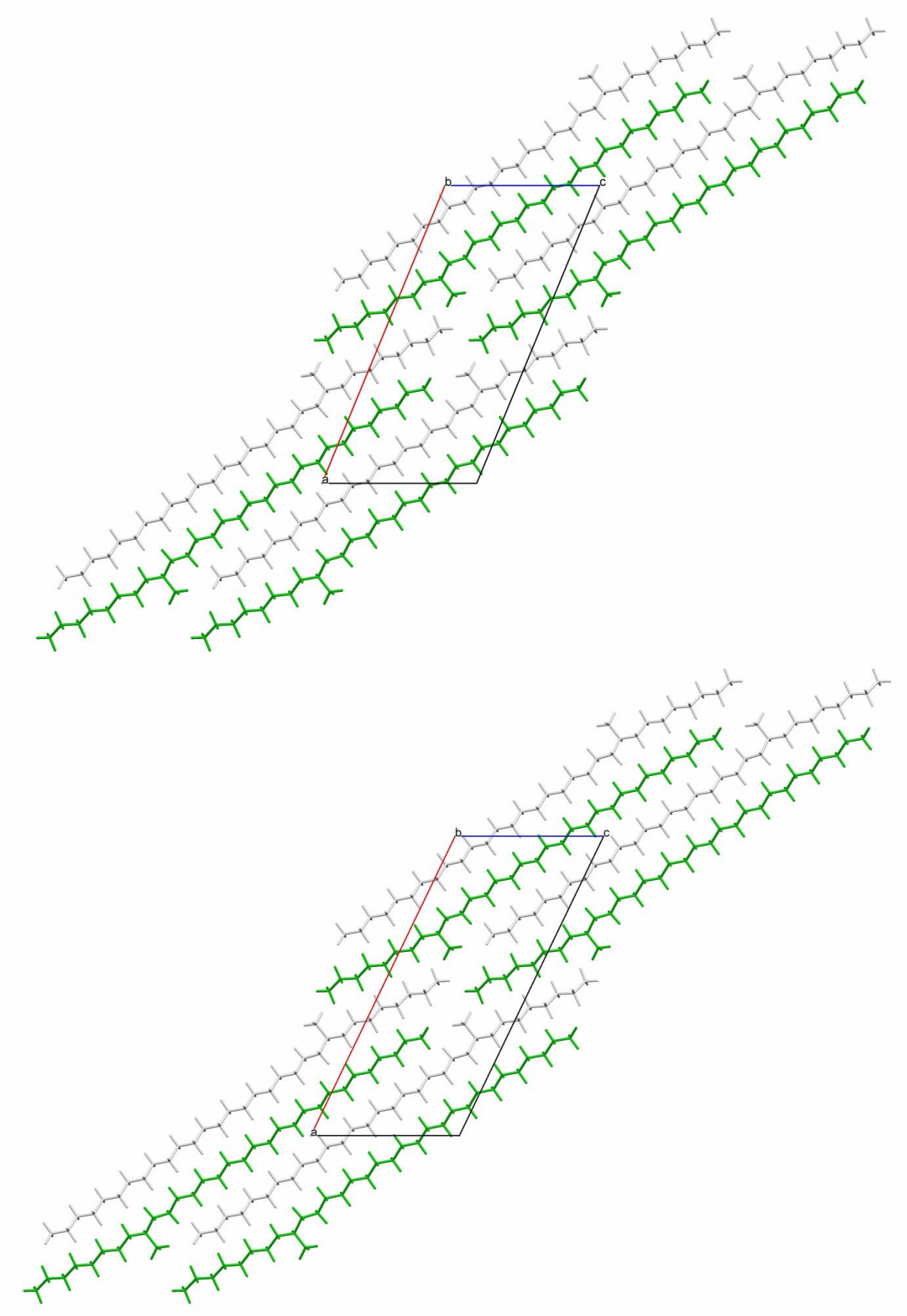
11-$MeC_{29}H_{59}$



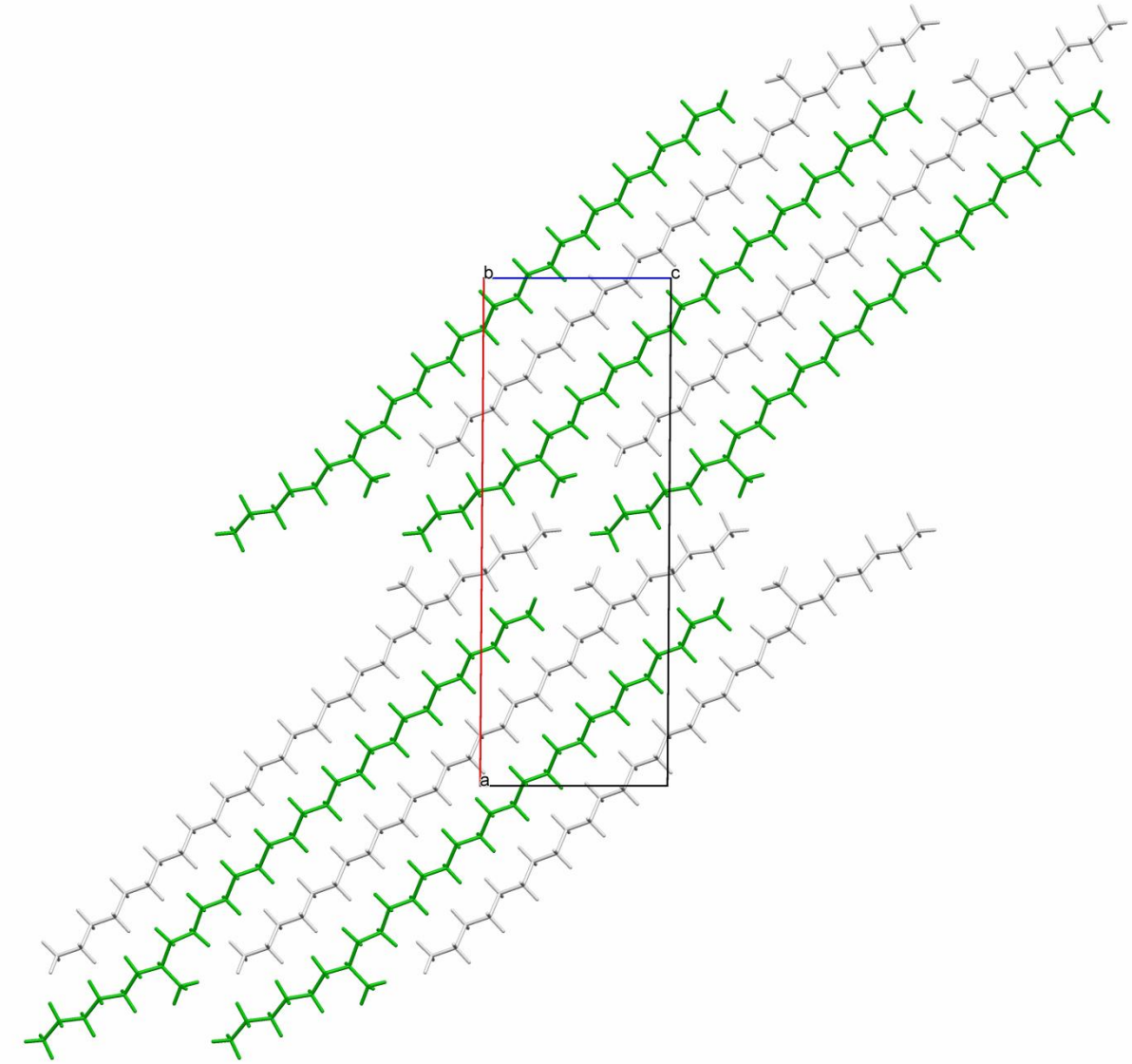
9-$MeC_{25}H_{51}$



9-Me$C_{27}H_{55}$

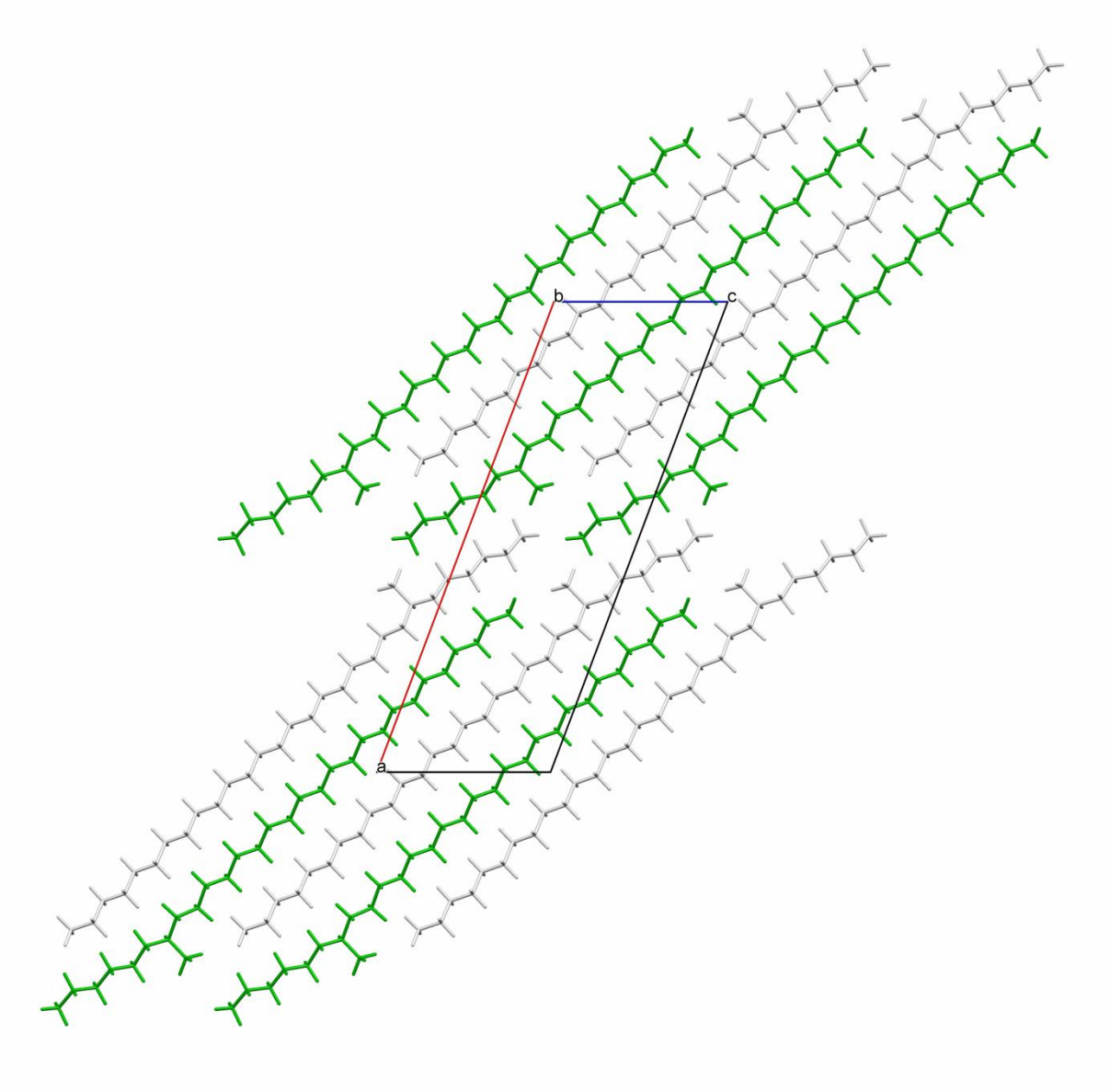


9-Me$C_{29}H_{59}$



9-Me$C_{31}H_{63}$

7-Me$C_{29}H_{59}$



7-Me$C_{29}H_{59}$ with the unit cell transformed via $\vec{a'} = \vec{a} - \vec{c}$, followed by a translation of the molecules by ½$\vec{c}$.