Structural chemistry of decalins and perfluorodecalins
ESI

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The Coding scheme of some of obtained crystalline phases is presented below.

Code	Meaning
t_pFDec_k200K_100K	Perfluorodecalin (**pFDec**), isomer *trans* (**t**), crystallized at 200K (**k200K**), measured at 100K (**100K**)
t_pFDec_k200K_290K_II	Perfluorodecalin (**pFDec**), isomer *trans* (**t**), crystallized at 200K (**k200K**), measured at 290K (**290K**), attempt 2 (**II**)
t_pFDec_Br2_k200K_200K	Perfluorodecalin (**pFDec**), isomer *trans* (**t**), Br_2 solution (**Br2**), crystallized at 200K (**k200K**), measured at 200K (**200K**)
ct_pFDec_k230K_100K	Perfluorodecalin (**pFDec**), mixture of *cis*, *trans* isomers (**ct**), crystallized at 230K (**k230K**), measured at 100K (**100K**)
c_pFDec_k200K_260K	Perfluorodecalin (**pFDec**), isomer *cis* (**c**), crystallized at 200K (**k200K**), measured at 260K (**260K**)
t_Dec_k200K_100K	Decalin (**Dec**), isomer *trans* (**t**), crystallized at 200K (**k200K**), measured at 100K (**100K**)
c_Dec_k180K_100K_cd_aP	Decalin (**Dec**), isomer *cis* (**c**), crystallized at 180K (**k180K**), measured at 100K (**100K**), after cooling (**cd**), solved in triclinic crystal system (**aP**)
c_Dec_k180K_220K_hu_mI	Decalin (**Dec**), isomer *cis* (**c**), crystallized at 180K (**k180K**), measured at 220K (**220K**), after heating (**hu**), solved in monoclinic crystal system, centered cell *I* (**mI**)

Table S1. Crystal data and refinement parameters for obtained phases.

Name	**t_pFDec_k200K_100K**	**t_pFDec_k200K_200K**	**t_pFDec_k200K_290K_II**	**t_pFDec_Br2_k200K_100K**	**t_pFDec_Br2_k200K_200K**
Compound used for crystallization	Isomer *trans* at 200K	Isomer *trans* at 200K	Isomer *trans* at 200K	*trans*-Perfluorodecalin, saturated Br_2 solution at 200K	*trans*-Perfluorodecalin, saturated Br_2 solution at 200K
Obtained crystals	*trans*-Perfluorodecalin at 100K	*trans*-Perfluorodecalin at 200K	*trans*-Perfluorodecalin at 290K	*trans*-Perfluorodecalin at 100K (no Br_2 detected)	*trans*-Perfluorodecalin at 200K (no Br_2 detected by X-rays)
Formula	$C_{10}F_{18}$	$C_{10}F_{18}$	$C_{10}F_{18}$	$C_{10}F_{18}$	$C_{10}F_{18}$
M_x**/ g mol^{-1}**	462.1	462.1	462.1	462.1	462.1
***T*/ K**	100(2)	200(2)	290(2)	100(2)	200(2)
λ/ Å	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal size/ mm	0.400 × 0.400 × 0.600	0.400 × 0.400 × 0.600	0.400 × 0.400 × 0.600	0.400 × 0.400 × 0.600	0.400 × 0.400 × 0.600
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
Unit cell parameters/ Å, °	a = 5.7433(5) Å b = 7.1269(8) Å c = 9.2269(9) Å α = 111.701(3)° β = 89.034(4)° γ = 111.392(3)°	a = 5.7891(5) Å b = 7.1855(8) Å c = 9.3000(9) Å α = 111.813(3)° β = 89.307(4)° γ = 111.525(3)°	a = 5.8708(7) Å b = 7.2213(7) Å c = 9.3736(12) Å α = 111.871(3)° β = 90.014(4)° γ = 111.475(3)°	a = 5.7499(3) Å b = 7.1098(3) Å c = 9.2311(5) Å α = 111.6889(11)° β = 89.1940(14)° γ = 111.4351(13)°	a = 5.7954(3) Å b = 7.1695(3) Å c = 9.3027(5) Å α = 111.8030(13)° β = 89.4664(16)° γ = 111.5718(15)°
***V*/ Å^3**	323.68(6)	330.64(6)	338.87(7)	323.19(3)	330.10(3)
Z	1	1	1	1	1
D_x**/ g cm^{-3}**	2.371	2.321	2.264	2.374	2.325
μ/ mm^{-1}	0.322	0.315	0.307	0.322	0.316
***F*(000)**	222	222	222	222	222
θ_{min}, θ_{max}	2.40°, 25.05°	2.38°, 25.05°	2.37°, 25.02°	2.40°, 25.04°	2.38°, 25.05°
Index range	-6≤h≤6 -8≤k≤7 -10≤l≤10	-6≤h≤6 -8≤k≤8 -11≤l≤11	-6≤h≤6 -8≤k≤8 -11≤l≤11	-6≤h≤6 -8≤k≤8 -10≤l≤10	-6≤h≤6 -8≤k≤8 -11≤l≤11
Reflections collected	3140	3191	3241	3227	3296
Independent reflections	1048 [R_{int} = 0.0124]	1065 [R_{int} = 0.0101]	1075 [R_{int} = 0.0191]	1052 [R_{int} = 0.0287]	1078 [R_{int} = 0.0250]
Completness for θ_{max}	91.5%	91.3%	89.8%	92.2%	92.5%
Absorption correction	semi-empirical	semi-empirical	semi-empirical	semi-empirical	semi-empirical
T_{min}, T_{max}	0.882 ,0.830	0.884 ,0.833	0.887 ,0.837	0.882, 0.830	0.884, 0.833
Refinement method	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ
Reflections/ restraints/ parameters	1048 / 0 / 127	1065 / 0 / 127	1075 / 0 / 127	1052 / 0 / 128	1078 / 0 / 128
GooF on F^2	1.088	1.124	1.147	1.077	1.147
***R* [I>2σ(I)]** ***R* (all data)**	R1 = 0.0259 wR2 = 0.0749 [1017 data; I>2σ(I)] R1 = 0.0266 wR2 = 0.0757	R1 = 0.0280 wR2 = 0.0832 [1015 data; I>2σ(I)] R1 = 0.0290 wR2 = 0.0848	R1 = 0.0500 wR2 = 0.1375 [947 data; I>2σ(I)] R1 = 0.0543 wR2 = 0.1465	R1 = 0.0309 wR2 = 0.0864 [998 data; I>2σ(I)] R1 = 0.0321 wR2 = 0.0885	R1 = 0.0349 wR2 = 0.0974 [991 data; I>2σ(I)] R1 = 0.0370 wR2 = 0.1007
Extinction	-	-	-	0.052(10)	0.076(12)
ρ_{min}, ρ_{max}/ eÅ^{-3}	0.412, -0.264	0.342, -0.187	0.275, -0.236	0.409, -0.333	0.319, -0.276

Table S2. Crystal data and refinement parameters for obtained phases.

Name	**ct_pFDec_k230K_100K**	**ct_pFDec_k230K_230K**	**c_pFDec_k200K_100K**	**c_pFDec_k200K_200K**	**c_pFDec_k200K_260K**
Compound used for crystallization	Mixture of isomers *cis* and *trans* at 230K	Mixture of isomers *cis* and *trans* at 230K	Isomer *cis* at 200K	Isomer *cis* at 200K	Isomer *cis* at 260K HT form
Obtained crystals	Disordered form of *trans*-perfluorodecalin at 100 K (no *cis* isomer detected by X-rays)	Disordered form of *trans*-perfluorodecalin at 230 K (no *cis* isomer detected by X-rays)	*cis*-Perfluorodecalin at 100 K	*cis*-Perfluorodecalin at 200 K	*cis*-Perfluorodecalin at 260 K
Formula	$C_{10}F_{18}$	$C_{10}F_{18}$	$C_{10}F_{18}$	$C_{10}F_{18}$	$C_{10}F_{18}$
M_x**/ g mol^{-1}**	462.1	462.1	462.1	462.1	462.1
***T*/ K**	100(2)	230(2)	100(2)	200(2)	260(2)
λ/ Å	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal size/ mm	0.400 × 0.400 × 0.600	0.400 × 0.400 × 0.600	0.400 × 0.400 × 0.600	0.400 × 0.400 × 0.600	0.400 × 0.400 × 0.600
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	*C*2/*c*	*C*2/*c*	*I*2/*m* (probably)
Unit cell parameters/ Å, °	*a* = 5.940(2) Å *b* = 7.257(2) Å *c* = 9.190(2) Å α = 111.733(10)° β = 89.911(10)° γ = 113.546(9)°	*a* = 6.0143(18) Å *b* = 7.3233(19) Å *c* = 9.274(2) Å α = 111.955(9)° β = 90.006(9)° γ = 113.796(8)°	*a* = 17.0062(11) Å *b* = 6.2091(3) Å *c* = 13.0007(8) Å β = 105.5020(18)°	a = 17.1772(10) Å b = 6.2586(2) Å c = 13.1557(7) Å β = 106.4297(15)°	*a* = 9.2499(7) Å *b* = 6.3171(4) Å *c* = 12.3565(12) Å β = 105.570(2)º
***V*/ Å^3**	332.33(17)	341.11(16)	1322.85(13)	1356.56(12)	695.53(10)
Z	1	1	4	4	2
D_x**/ g cm^{-3}**	2.309	2.249	2.32	2.263	2.206
μ/ mm^{-1}	0.314	0.305	0.315	0.307	
***F*(000)**	222	222	888	888	
θ_{min}, θ_{max}	2.42°, 25.05°	2.41°, 25.04°	2.49°, 25.03°	2.47°, 25.05°	
Index range	-7≤h≤7 -8≤k≤8 -10≤l≤10	-7≤h≤7 -8≤k≤8 -10≤l≤10	-20≤h≤20 -6≤k≤6 -15≤l≤15	-20≤h≤20 -6≤k≤6 -15≤l≤15	
Reflections collected	3560	3698	5996	6356	
Independent reflections	1048 [R_{int} = 0.0351]	1079 [R_{int} = 0.0343]	1121 [R_{int} = 0.0293]	1154 [R_{int} = 0.0275]	
Completness for θ_{max}	90.9%	91.2%	95.6%	95.8%	
Absorption correction	semi-empirical	semi-empirical	semi-empirical	semi-empirical	
Max. and min. transmission	0.885, 0.834	0.888, 0.838	0.884 ,0.833	0.887 ,0.837	
Refinement method	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	
Reflections/ restraints/ parameters	1048 / 133 / 255	1079 / 121 / 255	1121 / 95 / 344	1154 / 155 / 344	
GooF on F^2	1.047	1.071	1.144	1.13	
***R* [*I*>2σ(*I*)]** ***R* (all data)**	R1 = 0.0872 wR2 = 0.2249 [923 data; I>2σ(I)] R1 = 0.0977 wR2 = 0.2401	R1 = 0.0744 wR2 = 0.1951 [835 data; I>2σ(I)] R1 = 0.0966 wR2 = 0.2282	R1 = 0.0444 wR2 = 0.1091 [922 data; I>2σ(I)] R1 = 0.0530 wR2 = 0.1217	R1 = 0.0501 wR2 = 0.1412 [848 data; I>2σ(I)] R1 = 0.0640 wR2 = 0.1741	
Extinction	-	-	-	0.014(3)	
ρ_{min}, ρ_{max}/ eÅ^{-3}	0.373,-0.324	0.243,-0.212	0.138,-0.166	0.135,-0.165	

Table S3. Crystal data and refinement parameters for obtained phases.

Name	**t_Dec_k200K_100K**	**t_Dec_k200K_200K**	**c_Dec_k180K_100K_cd_aP**	**c_Dec_k180K_220K_hu_mI**
Compound used for crystallization	Isomer *trans* at 200K	Isomer *trans* at 200K	Isomer *cis* at 180K	Isomer *cis* at 180K
Obtained crystals	*trans*-Decalin at 100K	*trans*-Decalin at 200K	*cis*-Decalin at 100K LT phase - triclinic	*cis*-Decalin at 220K HT phase – monoclinic
Formula	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$
M_x**/ g mol^{-1}**	138.24	138.24	138.24	138.24
***T*/ K**	100(2)	200(2)	100(2)	220(2)
λ/ Å	0.71073	0.71073	0.71073	0.71073
Crystal size/ mm	0.400 × 0.400 × 0.600	0.400 × 0.400 × 0.600	0.400 × 0.400 x 0.600	0.400 × 0.400 × 0.600
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P\bar{1}$	$I2/a$
Unit cell parameters/ Å, °	a = 5.2670(2) Å b = 10.4832(4) Å c = 7.8148(2) Å β = 90.8405(13)°	a = 5.3191(2) Å b = 10.5640(4) Å c = 7.8580(2) Å β = 90.7843(14)°	a = 8.2602(9) Å b = 10.5243(9) Å c = 11.9532(12) Å α = 113.547(3)° β = 90.225(3)° γ = 112.687(3)°	a = 11.9659(5) Å b = 8.2828(4) Å c = 18.4270(9) Å β = 102.0193(12)°
***V*/ Å^3**	431.45(3)	441.51(3)	863.42(15)	1786.28(14)
Z	2	2	4	8
D_x**/ g cm^{-3}**	1.064	1.04	1.063	1.028
μ/ mm^{-1}	0.059	0.057 [1]	0.058	0.057
***F*(000)**	156	156	312	624
θ_{min}, θ_{max}	3.25°, 25.03°	3.23°, 25.02°	2.27°, 25.05°	2.26°, 25.05°
Index range	-6≤*h*≤6 -12≤*k*≤12 -9≤*l*≤9	-6≤*h*≤6 -12≤*k*≤12 -9≤*l*≤9	-9≤*h*≤9 -11≤*k*≤11 -14≤*l*≤14	-14≤*h*≤14 -9≤*k*≤9 -21≤*l*≤21
Reflections collected	5041	5127	9821	10524
Independent reflections	717 [R_{int} = 0.0127]	727 [R_{int} = 0.0169]	2761 [R_{int} = 0.0264]	1563 [R_{int} = 0.0255]
Completness for θ_{max}	93.1%	93.0%	95.9%	98.7%
Absorption correction	semi-empirical	semi-empirical	semi-empirical	semi-empirical
T_{min}, T_{max}	0.977 ,0.966	0.977 ,0.966	0.977 , 0.966	0.978 , 0.967
Refinement method	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ
Reflections/ restraints/ parameters	717 / 0 / 47	727 / 0 / 47	2761 / 0 / 182	1563 / 25 / 133
GooF on F^2	1.1	1.146	1.053	1.024
***R* [*I*>2σ(*I*)]** ***R* (all data)**	*R*1 = 0.0341 *wR*2 = 0.0815 [681 data; *I*>2σ(*I*)] *R*1 = 0.0356 *wR*2 = 0.0828	*R*1 = 0.0390 *wR*2 = 0.0940 [671 data; *I*>2σ(*I*)] *R*1 = 0.0413 *wR*2 = 0.0963	*R*1 = 0.0423 *wR*2 = 0.0922 [2463 data; *I*>2σ(*I*)] *R*1 = 0.0503 *wR*2 = 0.0990	*R*1 = 0.0477 *wR*2 = 0.1119 [1211 data; *I*>2σ(*I*)] *R*1 = 0.0628 *wR*2 = 0.1258
Extinction	0.036(11)	0.21(2)	-	0.0027(9)
ρ_{min}, ρ_{max}/ eÅ^{-3}	0.224,-0.137	0.196,-0.127	0.186, -0.169	0.106, -0.105

Table S4. Crystal data and refinement parameters for cis-dekalin single crystal refined in two space groups at various temperatures.

Name	**c_Dec_k180K_ 100K_cd_aP**	**c_Dec_k180K_ 100K_cd_mI**	**c_Dec_k180K_ 110K_cd_aP**	**c_Dec_k180K_ 110K_cd_mI**	**c_Dec_k180K_ 110K_hu_aP**	**c_Dec_k180K_ 110K_hu_mI**	**c_Dec_k180K_ 120K_cd_aP**	**c_Dec_k180K_ 120K_cd_mI**	**c_Dec_k180K_ 120K_hu_aP**	**c_Dec_K180_ 120K_hu_mI**	**c_Dec_k180K_ 130K_cd_aP**
Compound used for crystallization	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K
Formula	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$
M_x**/ g mol**$^{-1}$	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24
T**/ K**	100(2)	100(2)	110(2)	110(2)	110(2)	110(2)	120(2)	120(2)	120(2)	120(2)	130(2)
λ/ Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal size/ mm	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600
Crystal system	Triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic
Space group	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$
Unit cell parameters/ Å, °	a = 8.2602(9) Å b = 10.5243(9) Å c = 11.9532(12) Å α = 113.547(3)° β = 90.225(3)° γ = 112.687(3)°	a = 11.9250(15) Å b = 8.2439(11) Å c = 17.812(3) Å β = 101.364(4)°	a = 8.2634(9) Å b = 10.5357(9) Å c = 11.9616(12) Å α = 113.547(3)° β = 90.218(3)° γ = 112.694(3)°	a = 11.9376(14) Å b = 8.2488(10) Å c = 17.833(2) Å β = 101.352(3)°	a = 8.2635(9) Å b = 10.5367(9) Å c = 11.9622(12) Å α = 113.553(3)° β = 90.215(3)° γ = 112.692(3)°	a = 11.9334(14) Å b = 8.2466(10) Å c = 17.828(2) Å β = 101.350(3)°	a = 8.2665(7) Å b = 10.5488(7) Å c = 11.9705(10) Å α = 113.550(2)° β = 90.196(3)° γ = 112.709(2)°	a = 11.9467(12) Å b = 8.2518(9) Å c = 17.853(2) Å β = 101.341(3)°	a = 8.2665(7) Å b = 10.5475(7) Å c = 11.9704(9) Å α = 113.554(2)° β = 90.201(3)° γ = 112.704(2)°	a = 11.9439(13) Å b = 8.2503(9) Å c = 17.847(2) Å β = 101.343(3)°	a = 8.2712(6) Å b = 10.5654(5) Å c = 11.9798(8) Å α = 113.5395(18)° β = 90.160(2)° γ = 112.7466(18)°
V**/ Å**^{3}	863.42(15)	1716.7(4)	865.27(15)	1721.7(4)	865.38(15)	1720.1(4)	867.25(12)	1725.6(3)	867.12(12)	1724.3(3)	869.69(10)
Z	4	8	4	8	4	8	4	8	4	8	4
D_x**/ g cm**$^{-3}$	1.063	1.070	1.061	1.067	1.061	1.068	1.059	1.064	1.059	1.065	1.056
μ/ mm^{-1}	0.058	0.059	0.058	0.059	0.058	0.059	0.058	0.059	0.058	0.059	0.058
F**(000)**	312	624	312	624	312	624	312	624	312	624	312
θ_{min}, θ_{max}	2.27°, 25.05°	2.33°, 25.04°	2.27°, 25.05°	2.33°, 25.05°	2.27°, 25.05°	2.33°, 25.04°	2.27°, 25.05°	2.33°, 25.04°	2.27°, 25.04°	2.33°, 25.05°	2.32°, 25.05°
Index range	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$
Reflections collected	9821	9651	10205	9764	10046	9786	10299	9835	10269	9877	10485
Independent reflections	2761 [R_{int} = 0.0264]	1490 [R_{int} = 0.0578]	2818 [R_{int} = 0.0248]	1500 [R_{int} = 0.0533]	2787 [R_{int} = 0.0255]	1499 [R_{int} = 0.0553]	2831 [R_{int} = 0.0222]	1499 [R_{int} = 0.0474]	2823 [R_{int} = 0.0225]	1506 [R_{int} = 0.0497]	2849 [R_{int} = 0.0204]
Completness for θ_{max}	95.9%	97.7%	96.8%	98.0%	96.2%	98.1%	97.2%	97.8%	97.0%	98.3%	97.5%
Absorption correction	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
T_{min}, T_{max}	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966
Refinement method	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ
Reflections/ restraints/ parameters	2761 / 0 / 182	1490 / 0 / 91	2818 / 0 / 182	1500 / 0 / 91	2787 / 0 / 182	1499 / 0 / 91	2831 / 0 / 182	1499 / 0 / 91	2823 / 0 / 182	1506 / 0 / 91	2849 / 0 / 182
GooF on F^2	1.053	1.205	1.056	1.194	1.061	1.198	1.072	1.190	1.079	1.185	1.059
R **[**I**>2σ(**I**)]**	$R1$ = 0.0423 $wR2$ = 0.0922 [2463 data; $I>2\sigma(I)$]	$R1$ = 0.0886 $wR2$ = 0.1674 [1368 data; $I>2\sigma(I)$]	$R1$ = 0.0411 $wR2$ = 0.0953 [2514 data; $I>2\sigma(I)$]	$R1$ = 0.0806 $wR2$ = 0.1539 [1384 data; $I>2\sigma(I)$]	$R1$ = 0.0423 $wR2$ = 0.0965 [2486 data; $I>2\sigma(I)$]	$R1$ = 0.0816 $wR2$ = 0.1590 [1381 data; $I>2\sigma(I)$]	$R1$ = 0.0427 $wR2$ = 0.0950 [2546 data; $I>2\sigma(I)$]	$R1$ = 0.0738 $wR2$ = 0.1425 [1380 data; $I>2\sigma(I)$]	$R1$ = 0.0422 $wR2$ = 0.0946 [2514 data; $I>2\sigma(I)$]	$R1$ = 0.0739 $wR2$ = 0.1461 [1388 data; $I>2\sigma(I)$]	$R1$ = 0.0406 $wR2$ = 0.0938 [2524 data; $I>2\sigma(I)$]
R **(all data)**	$R1$ = 0.0503 $wR2$ = 0.0990	$R1$ = 0.0937 $wR2$ = 0.1698	$R1$ = 0.0486 $wR2$ = 0.1028	$R1$ = 0.0850 $wR2$ = 0.1561	$R1$ = 0.0496 $wR2$ = 0.1025	$R1$ = 0.0856 $wR2$ = 0.1609	$R1$ = 0.0496 $wR2$ = 0.1009	$R1$ = 0.0782 $wR2$ = 0.1448	$R1$ = 0.0500 $wR2$ = 0.1021	$R1$ = 0.0784 $wR2$ = 0.1488	$R1$ = 0.0480 $wR2$ = 0.1003
Extinction	-	-	-	-	-	-	-	-	-	-	-
ρ_{min}, ρ_{max}/ eÅ^{-3}	0.186, -0.169	0.282, -0.241	0.203, -0.155	0.239, -0.192 eÅ^{-3}	0.182, -0.175	0.227, -0.203	0.178, -0.195	0.211, -0.171	0.176, -0.150	0.224, -0.176	0.187, -0.151

cd = cooling down, hu = heating up. Columns coloured in orange stand for data present in the **Table S3** in ESI.

Table S4. Crystal data and refinement parameters for cis-dekalin single crystal refined in two space groups at various temperatures. Continuation.

Name	c_Dec_k180K_ 130K_cd_mI	c_Dec_k180K_ 130K_hu_aP	c_Dec_k180K_ 130K_hu_mI	c_Dec_k180K_ 140K_cd_aP	c_Dec_k180K_ 140K_cd_mI	c_Dec_k180K_ 140K_hu_aP	c_Dec_k180K_ 140K_hu_mI	c_Dec_k180K_ 150K_cd_aP	c_Dec_k180K_ 150K_cd_mI	c_Dec_k180K_ 150K_hu_aP	c_Dec_k180K_ 150K_hu_mI
Compound used for crystallization	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K
Formula	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$
M_x/ g mol^{-1}	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24
T/ K	132(2)	130(2)	130(2)	140(2)	140(2)	140(2)	140(2)	150(2)	150(2)	150(2)	150(2)
λ/ Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal size/ mm	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600
Crystal system	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic
Space group	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$
Unit cell parameters/ Å, °	a = 11.9609(10) Å b = 8.2593(7) Å c = 17.8832(17) Å β = 101.342(2)°	a = 8.2699(7) Å b = 10.5607(7) Å c = 11.9762(10) Å α = 113.534(2)° β = 90.179(3)° γ = 112.733(3)°	a = 11.9553(11) Å b = 8.2563(8) Å c = 17.8738(18) Å β = 101.343(3)°	a = 8.2775(4) Å b = 10.5829(4) Å c = 11.9879(5) Å α = 113.5061(11)° β = 90.1124(13)° γ = 112.8047(12)°	a = 11.9735(7) Å b = 8.2678(5) Å c = 17.9172(12) Å β = 101.3605(17)°	a = 8.2770(4) Å b = 10.5807(4) Å c = 11.9867(5) Å α = 113.5057(12)° β = 90.1279(14)° γ = 112.7902(12)°	a = 11.9706(8) Å b = 8.2662(6) Å c = 17.9123(13) Å β = 101.3588(18)°	a = 8.2823(5) Å b = 10.6037(5) Å c = 11.9909(7) Å α = 113.4279(16)° β = 90.0435(19)° γ = 112.8878(17)°	a = 11.9833(5) Å b = 8.2770(3) Å c = 17.9669(8) Å β = 101.4018(10)°	a = 8.2827(3) Å b = 10.6032(3) Å c = 11.9913(4) Å α = 113.4349(8)° β = 90.0430(9)° γ = 112.8814(8)°	a = 11.9840(5) Å b = 8.2774(3) Å c = 17.9659(8) Å β = 101.3997(10)°
V/ Å^3	1732.2(3)	869.00(12)	1729.8(3)	872.36(7)	1738.95(19)	872.11(7)	1737.7(2)	875.02(9)	1746.89(12)	875.04(5)	1746.99(12)
Z	8	4	8	4	8	4	8	4	8	4	8
D_x/ g cm^{-3}	1.060	1.057	1.062	1.053	1.056	1.053	1.057 g/cm^3	1.049 g/cm^3	1.051 g/cm^3	1.049 g/cm^3	1.051 g/cm^3
μ/ mm^{-1}	0.058	0.058	0.058	0.058	0.058	0.058	0.058 mm^{-1}	0.058 mm^{-1}	0.058 mm^{-1}	0.058 mm^{-1}	0.058 mm^{-1}
F(000)	624	312	624	312	624	312	624	312	624	312	624
θ_{min}, θ_{max}	2.32°, 25.05°	2.32°, 25.05°	2.32°, 25.05°	2.32°, 25.05°	2.32°, 25.04°	2.32°, 25.05°	2.32°, 25.05°	2.31°, 25.05°	2.31°, 25.04°	2.31°, 25.05°	2.31°, 25.04°
Index range	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-11\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-12\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$
Reflections collected	10072	10418	10030	10556	9991	10639	10181	10713	10310	10768	10367
Independent reflections	1514 [R_{int} = 0.0413]	2849 [R_{int} = 0.0214]	1511 [R_{int} = 0.0441]	2863 [R_{int} = 0.0157]	1522 [R_{int} = 0.0282]	2871 [R_{int} = 0.0189]	1522 [R_{int} = 0.0336]	2893 [R_{int} = 0.0166]	1531 [R_{int} = 0.0190]	2894 [R_{int} = 0.0192]	1530 [R_{int} = 0.0228]
Completness for θ_{max}	98.4%	97.4%	98.3%	97.8%	98.4%	97.9%	98.4%	93.2%	98.6%	93.2%	98.6%
Absorption correction	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
T_{min}, T_{max}	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966
Refinement method	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ
Reflections/ restraints/ parameters	1514 / 0 / 91	2849 / 0 / 182	1511 / 0 / 91	2863 / 0 / 182	1522 / 0 / 91	2871 / 0 / 182	1522 / 0 / 91	2893 / 92 / 264	1531 / 55 / 133	2894 / 110 / 264	1530 / 31 / 133
GooF on F^2	1.170	1.044	1.168	1.066	1.065	1.046	1.089	1.027	1.056	1.023	1.037
R [I>2σ(I)]	$R1$ = 0.0627 $wR2$ = 0.1283 [1390 data; I>2σ(I)]	$R1$ = 0.0409 $wR2$ = 0.0937 [2522 data; I>2σ(I)]	$R1$ = 0.0643 $wR2$ = 0.1311 [1393 data; I>2σ(I)]	$R1$ = 0.0424 $wR2$ = 0.1036 [2473 data; I>2σ(I)]	$R1$ = 0.0494 $wR2$ = 0.1150 [1360 data; I>2σ(I)]	$R1$ = 0.0417 $wR2$ = 0.1011 [2486 data; I>2σ(I)]	$R1$ = 0.0511 $wR2$ = 0.1157 [1371 data; I>2σ(I)]	$R1$ = 0.0414 $wR2$ = 0.0978 [2399 data; I>2σ(I)]	$R1$ = 0.0399 $wR2$ = 0.1014 1341 data; I>2σ(I)	$R1$ = 0.0422 $wR2$ = 0.0967 [2438 data; I>2σ(I)]	$R1$ = 0.0410 $wR2$ = 0.0959 [1364 data; I>2σ(I)]
R (all data)	$R1$ = 0.0675 $wR2$ = 0.1317	$R1$ = 0.0480 $wR2$ = 0.1004	$R1$ = 0.0688 $wR2$ = 0.1339	$R1$ = 0.0505 $wR2$ = 0.1124	$R1$ = 0.0549 $wR2$ = 0.1198	$R1$ = 0.0495 $wR2$ = 0.1084	$R1$ = 0.0561 $wR2$ = 0.1199	$R1$ = 0.0500 $wR2$ = 0.1061	$R1$ = 0.0459 $wR2$ = 0.1074	$R1$ = 0.0504 $wR2$ = 0.1043	$R1$ = 0.0462 $wR2$ = 0.1004
Extinction	-	-	-	-	-	-	-	0.008(2)	0.0018(7)	0.007(3)	0.0013(7)
ρ_{min}, ρ_{max}/ eÅ^{-3}	0.203, -0.175	0.168, -0.160	0.216, -0.166	0.191, -0.152	0.194, -0.151	0.201, -0.148	0.208, -0.156	0.154, -0.138	0.186, -0.146	0.158, -0.131	0.170, -0.137

cd = cooling down, hu = heating up. Columns coloured in orange stand for data present in the **Table S3** in ESI.

Table S4. Crystal data and refinement parameters for cis-dekalin single crystal refined in two space groups at various temperatures. Continuation.

Name	**c_Dec_k180K_ 160K_cd_aP**	**c_Dec_k180K_ 160K_cd_mI**	**c_Dec_k180K_ 160K_hu_aP**	**c_Dec_k180K_ 160K_hu_mI**	**c_Dec_k180K_ 170K_cd_aP**	**c_Dec_k180K_ 170K_cd_mI**	**c_Dec_k180K_ 170K_hu_aP**	**c_Dec_k180K_ 170K_hu_mI**	**c_Dec_k180K_ 180K_cd_aP**	**c_Dec_k180K_ 180K_cd_mI**	**c_Dec_k180K_ 180K_hu_aP**
Compound used for crystallization	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K
Formula	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$
M_x/ g mol^{-1}	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24
T/ K	160(2)	160(2)	160(2)	160(2)	170(2)	170(2)	170(2)	170(2)	180(2)	180(2)	180(2)
λ/ Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal size/ mm	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600
Crystal system	triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic
Space group	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$
Unit cell parameters/ Å, °	a = 8.2845(3) Å b = 10.6177(3) Å c = 11.9890(4) Å α = 113.3017(8)° β = 90.0282(9)° γ = 112.8787(9)°	a = 11.9832(4) Å b = 8.2803(3) Å c = 18.0209(6) Å β = 101.4727(10)°	a = 8.2838(3) Å b = 10.6169(3) Å c = 11.9887(4) Å α = 113.3097(8)° β = 90.0250(10)° γ = 112.8789(9)°	a = 11.9843(4) Å b = 8.2804(3) Å c = 18.0191(6) Å β = 101.4692(10)°	a = 8.2847(3) Å b = 10.6319(3) Å c = 11.9834(4) Å α = 113.1322(9)° β = 90.0204(10)° γ = 112.8539(9)°	a = 11.9781(4) Å b = 8.2808(3) Å c = 18.0841(7) Å β = 101.5685(10)°	a = 8.2852(3) Å b = 10.6314(3) Å c = 11.9844(4) Å α = 113.1411(9)° β = 90.0216(10)° γ = 112.8556(9)°	a = 11.9791(4) Å b = 8.2813(3) Å c = 18.0809(7) Å β = 101.5642(10)°	a = 8.2855(3) Å b = 10.6479(3) Å c = 11.9802(4) Å α = 112.9570(10)° β = 90.0180(10)° γ = 112.8180(10)°	a = 11.9739(4) Å b = 8.2807(3) Å c = 18.1504(7) Å β = 101.6659(10)°	a = 8.2862(3) Å b = 10.6476(3) Å c = 11.9806(4) Å α = 112.9610(9)° β = 90.0220(10)° γ = 112.8190(10)°
V/ Å^3	877.41(5)	1752.39(11)	877.19(5)	1752.42(11)	879.77(5)	1757.29(11)	879.77(5)	1757.26(11)	882.64(5)	1762.48(11)	882.66(5)
Z	4	8	4	8	4	8	4	8	4	8	4
D_x/ g cm^{-3}	1.047 g/cm^3	1.048 g/cm^3	1.047 g/cm^3	1.048 g/cm^3	1.044 g/cm^3	1.045 g/cm^3	1.044 g/cm^3	1.045 g/cm^3	1.040 g/cm^3	1.042 g/cm^3	1.040 g/cm^3
μ/ mm^{-1}	0.058 mm^{-1}	0.058 mm^{-1}	0.058 mm^{-1}	0.058 mm^{-1}	0.057 mm^{-1}	0.057 mm^{-1}	0.057 mm^{-1}	0.057 mm^{-1}	0.057 mm^{-1}	0.057 mm^{-1}	0.057 mm^{-1}
F(000)	312	624	312	624	312	624	312	624	312	624	312
θ_{min}, θ_{max}	2.71°, 25.05°	2.31°, 25.05°	2.71°, 25.05°	2.31°, 25.05°	2.71°, 25.05°	2.71°, 25.05°	2.71°, 25.05°	2.71°, 25.05°	2.71°, 25.05°	2.71°, 25.05°	2.71°, 25.04°
Index range	$-9\le h\le 9$ $-12\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-12\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-12\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-12\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-12\le k\le 11$ $-14\le l\le 14$	$-14\le h\le 14$ $-9\le k\le 9$ $-21\le l\le 21$	$-9\le h\le 9$ $-12\le k\le 11$ $-14\le l\le 14$
Reflections collected	10773	10355	10811	10395	10783	10346	10842	10437	10811	10405	10850
Independent reflections	2905 [R_{int} = 0.0163]	1536 [R_{int} = 0.0177]	2907 [R_{int} = 0.0191]	1537 [R_{int} = 0.0216]	2914 [R_{int} = 0.0170]	1538 [R_{int} = 0.0191]	2916 [R_{int} = 0.0214]	1536 [R_{int} = 0.0265]	2921 [R_{int} = 0.0174]	1540 [R_{int} = 0.0195]	2922 [R_{int} = 0.0244]
Completness for θ_{max}	93.2%	98.7%	93.4%	98.7%	93.5%	98.7%	93.6%	98.6%	93.6%	98.7%	93.7%
Absorption correction	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	none	multi-scan	multi-scan	multi-scan
T_{min}, T_{max}	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966	0.977, 0.966
Refinement method	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ
Reflections/ restraints/ parameters	2905 / 0 / 264	1536 / 25 / 133	2907 / 0 / 264	1537 / 25 / 133	2914 / 50 / 264	1538 / 25 / 133	2916 / 0 / 263	1536 / 25 / 133	2921 / 50 / 264	1540 / 25 / 133	2922 / 0 / 263
GooF on F^2	1.053	1.045	1.071	1.043	1.023	1.048	1.055	1.044	1.038	1.051	1.051
R [I>2σ(I)]	$R1$ = 0.0408 $wR2$ = 0.1014 [2377 data; $I>2\sigma(I)$]	$R1$ = 0.0398 $wR2$ = 0.0993 [1334 data; $I>2\sigma(I)$]	$R1$ = 0.0420 $wR2$ = 0.1038 [2405 data; $I>2\sigma(I)$]	$R1$ = 0.0412 $wR2$ = 0.0992 [1354 data; $I>2\sigma(I)$]	$R1$ = 0.0450 $wR2$ = 0.1057 [2345 data; $I>2\sigma(I)$]	$R1$ = 0.0409 $wR2$ = 0.1037 [1319 data; $I>2\sigma(I)$]	$R1$ = 0.0442 $wR2$ = 0.1074 [2360 data; $I>2\sigma(I)$]	$R1$ = 0.0412 $wR2$ = 0.1007 [1328 data; $I>2\sigma(I)$]	$R1$ = 0.0469 $wR2$ = 0.1125 [2303 data; $I>2\sigma(I)$]	$R1$ = 0.0419 $wR2$ = 0.1046 [1297 data; $I>2\sigma(I)$]	$R1$ = 0.0473 $wR2$ = 0.1143 [2315 data; $I>2\sigma(I)$]
R (all data)	$R1$ = 0.0506 $wR2$ = 0.1112	$R1$ = 0.0461 $wR2$ = 0.1061	$R1$ = 0.0510 $wR2$ = 0.1137	$R1$ = 0.0469 $wR2$ = 0.1052	$R1$ = 0.0565 $wR2$ = 0.1164	$R1$ = 0.0484 $wR2$ = 0.1111	$R1$ = 0.0551 $wR2$ = 0.1194	$R1$ = 0.0477 $wR2$ = 0.1083	$R1$ = 0.0604 $wR2$ = 0.1257	$R1$ = 0.0504 $wR2$ = 0.1135	$R1$ = 0.0605 $wR2$ = 0.1286
Extinction	0.009(3)	0.0027(7)	0.007(3)	0.0021(7)	0.011(3)	0.0024(8)	-	0.0028(9)	0.013(3)	0.0035(8)	-
ρ_{min}, ρ_{max}/ eÅ^{-3}	0.127, -0.138	0.156, -0.135	0.128, -0.149	0.150, -0.141	0.169, -0.127	0.129, -0.122	0.133, -0.138	0.127, -0.134	0.180, -0.124	0.115, -0.109	0.150, -0.134

cd = cooling down, hu = heating up. Columns coloured in orange stand for data present in the **Table S3** in ESI.

Table S4. Crystal data and refinement parameters for cis-dekalin single crystal refined in two space groups at various temperatures. Continuation.

Name	**c_Dec_k180K_ 180K_hu_mI**	**c_Dec_k180K_ 190K_hu_aP**	**c_Dec_k180K_ 190K_hu_mI**	**c_Dec_k180K_ 200K_hu_aP**	**c_Dec_k180K_ 200K_hu_mI**	**c_Dec_k180K_ 210K_hu_aP**	**c_Dec_k180K_ 210K_hu_mI**	**c_Dec_k180K_ 220K_hu_aP**	**c_Dec_k180K_ 220K_hu_mI**
Compound used for crystallization	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K	Isomer *cis* at 180K
Formula	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$	$C_{10}H_{18}$
M_x/ **g mol^{-1}**	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24	138.24
T/ **K**	180(2)	190(2)	190(2)	200(2)	200(2)	210(2)	210(2)	220(2)	220(2)
λ/ Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal size/ mm	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600	0.400×0.400×0.600
Crystal system	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	Monoclinic
Space group	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$	$P\bar{1}$	$I2/a$
Unit cell parameters/ Å, °	a = 11.9744(4) Å b = 8.2815(3) Å c = 18.1491(7) Å β = 101.6636(10)°	a = 8.2860(7) Å b = 10.6634(7) Å c = 11.9779(9) Å α = 112.795(2)° β = 90.023(2)° γ = 112.784(2)°	a = 11.9719(5) Å b = 8.2815(3) Å c = 18.2151(8) Å β = 101.7554(11)°	a = 8.2858(4) Å b = 10.6794(3) Å c = 11.9757(5) Å α = 112.6404(11)° β = 90.0236(12)° γ = 112.7497(12)°	a = 11.9701(5) Å b = 8.2817(4) Å c = 18.2789(9) Å β = 101.8375(12)°	a = 8.2864(7) Å b = 10.6979(7) Å c = 11.9743(10) Å α = 112.477(2)° β = 90.024(3)° γ = 112.708(3)°	a = 11.9678(5) Å b = 8.2815(4) Å c = 18.3482(9) Å β = 101.9207(12)°	a = 8.2873(4) Å b = 10.7178(3) Å c = 11.9719(5) Å α = 112.2899(11)° β = 90.0213(12)° γ = 112.6630(12)°	a = 11.9659(5) Å b = 8.2828(4) Å c = 18.4270(9) Å β = 102.0193(12)°
V/ **Å^3**	1762.61(11)	885.34(12)	1768.06(12)	887.97(6)	1773.50(14)	891.07(12)	1779.30(14)	894.47(6)	1786.28(14)
Z	8	4	8	4	8	4	8	4	8
D_x/ **g cm^{-3}**	1.042 g/cm^3	1.037 g/cm^3	1.039	1.034	1.036	1.030	1.032	1.027	1.028
μ/ mm^{-1}	0.057 mm^{-1}	0.057 mm^{-1}	0.057	0.057	0.057	0.057	0.057	0.056	0.057
F**(000)**	624	312	624	312	624	312	624	312	624
θ_{min}, θ_{max}	2.71°, 25.05°	2.71°, 25.04°	2.71°, 25.05°	2.26°, 25.05°	2.28°, 25.05°	2.27°, 25.05°	2.71°, 25.05°	2.26°, 25.05°	2.26°, 25.05°
Index range	$-14 \le h \le 14$ $-9 \le k \le 9$ $-21 \le l \le 21$	$-9 \le h \le 9$ $-12 \le k \le 11$ $-14 \le l \le 14$	$-14 \le h \le 14$ $-9 \le k \le 9$ $-21 \le l \le 21$	$-9 \le h \le 9$ $-12 \le k \le 11$ $-14 \le l \le 14$	$-14 \le h \le 14$ $-9 \le k \le 9$ $-21 \le l \le 21$	$-9 \le h \le 9$ $-12 \le k \le 11$ $-14 \le l \le 14$	$-14 \le h \le 14$ $-9 \le k \le 9$ $-21 \le l \le 21$	$-9 \le h \le 9$ $-12 \le k \le 11$ $-14 \le l \le 14$	$-14 \le h \le 14$ $-9 \le k \le 9$ $-21 \le l \le 21$
Reflections collected	10445	10885	10451	10904	10486	10958	10543	10934	10524
Independent reflections	1539 [R_{int} = 0.0297]	2930 [R_{int} = 0.0191]	1544 [R_{int} = 0.0209]	2944 [R_{int} = 0.0177]	1554 [R_{int} = 0.0199]	2954 [R_{int} = 0.0193]	1558 [R_{int} = 0.0217]	2959 [R_{int} = 0.0222]	1563 [R_{int} = 0.0255]
Completness for θ_{max}	98.6%	93.5%	98.5%	93.4%	98.6%	93.5%	98.6%	93.5%	98.7%
Absorption correction	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
T_{min}, T_{max}	0.977, 0.966	0.978, 0.967	0.978, 0.967	0.978, 0.967	0.978, 0.967	0.978, 0.967	0.978, 0.967	0.978, 0.967	0.978, 0.967
Refinement method	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ	Full matrix LSQ
Reflections/ restraints/ parameters	1539 / 25 / 133	2930 / 0 / 263	1544 / 25 / 133	2944 / 0 / 263	1554 / 25 / 133	2954 / 0 / 263	1558 / 25 / 133	2959 / 0 / 263	1563 / 25 / 133
GooF on F^2	1.056	1.055	1.051	1.076	1.087	1.075	1.079	1.046	1.024
R **[I>2σ(I)]**	$R1$ = 0.0429 $wR2$ = 0.1061 [1303 data; $I>2\sigma(I)$]	$R1$ = 0.0493 $wR2$ = 0.1195 [2292 data; $I>2\sigma(I)$]	$R1$ = 0.0433 $wR2$ = 0.1051 [1284 data; $I>2\sigma(I)$]	$R1$ = 0.0519 $wR2$ = 0.1233 [2249 data; $I>2\sigma(I)$]	$R1$ = 0.0457 $wR2$ = 0.1100 [1290 data; $I>2\sigma(I)$]	$R1$ = 0.0536 $wR2$ = 0.1342 [2216 data; $I>2\sigma(I)$]	$R1$ = 0.0460 $wR2$ = 0.1144 [1247 data; $I>2\sigma(I)$]	$R1$ = 0.0555 $wR2$ = 0.1333 [2158 data; $I>2\sigma(I)$]	$R1$ = 0.0477 $wR2$ = 0.1119 [1211 data; $I>2\sigma(I)$]
R **(all data)**	$R1$ = 0.0507 $wR2$ = 0.1144	$R1$ = 0.0635 $wR2$ = 0.1341	$R1$ = 0.0519 $wR2$ = 0.1134	$R1$ = 0.0680 $wR2$ = 0.1393	$R1$ = 0.0557 $wR2$ = 0.1195	$R1$ = 0.0716 $wR2$ = 0.1557	$R1$ = 0.0583 $wR2$ = 0.1281	$R1$ = 0.0778 $wR2$ = 0.1576	$R1$ = 0.0628 $wR2$ = 0.1258
Extinction	0.0027(10)	-	0.0032(9)	-	0.0029(9)	-	0.0023(10)	-	0.0027(9)
ρ_{min}, ρ_{max}/ eÅ^{-3}	0.110, -0.128	0.150, -0.130	0.105, -0.106	0.145, -0.139	0.115, -0.103	0.129, -0.129	0.105, -0.105	0.150, -0.132	0.106, -0.105

cd = cooling down, hu = heating up. Columns coloured in orange stand for data present in the **Table S3** in ESI.

Powder patterns of perfluorodecalins and decalins

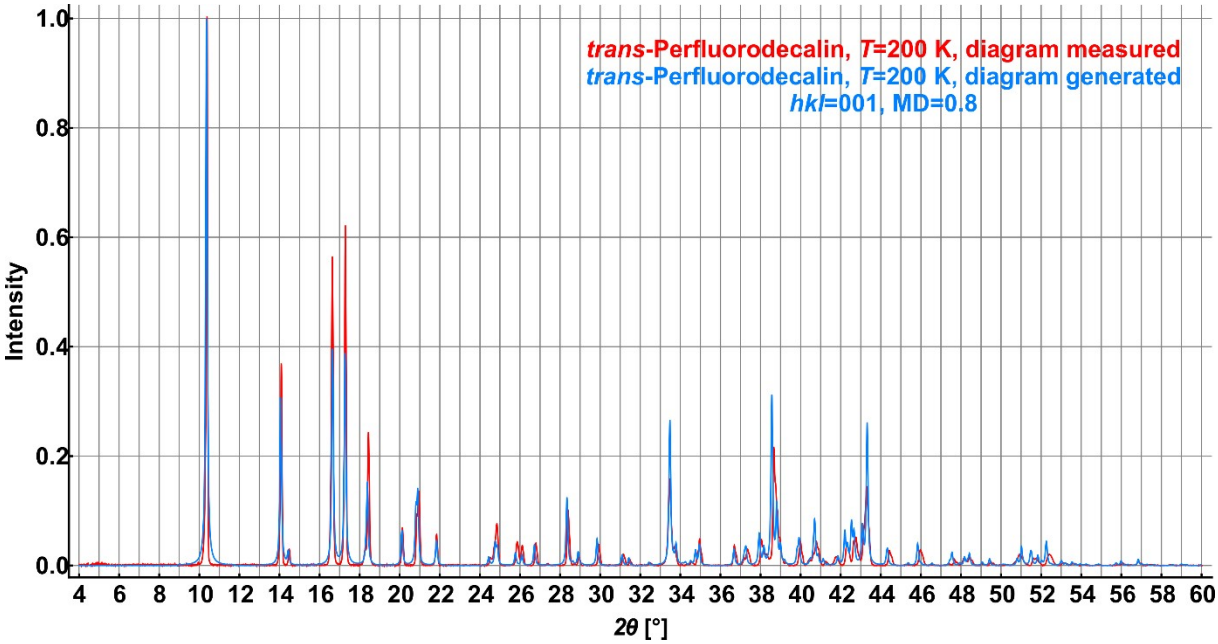

Fig. S1. Overlay of experimental and generated powder diagrams for *trans*-perfluorodecalin. Relatively good fit is observed when texture effect is included in generated diagrams for *MD*=0.8 (March-Dollase parameter) with enhanced intensities of *hkl*=001 group of reflections – crystals form plates with index of the base face equal to (001).

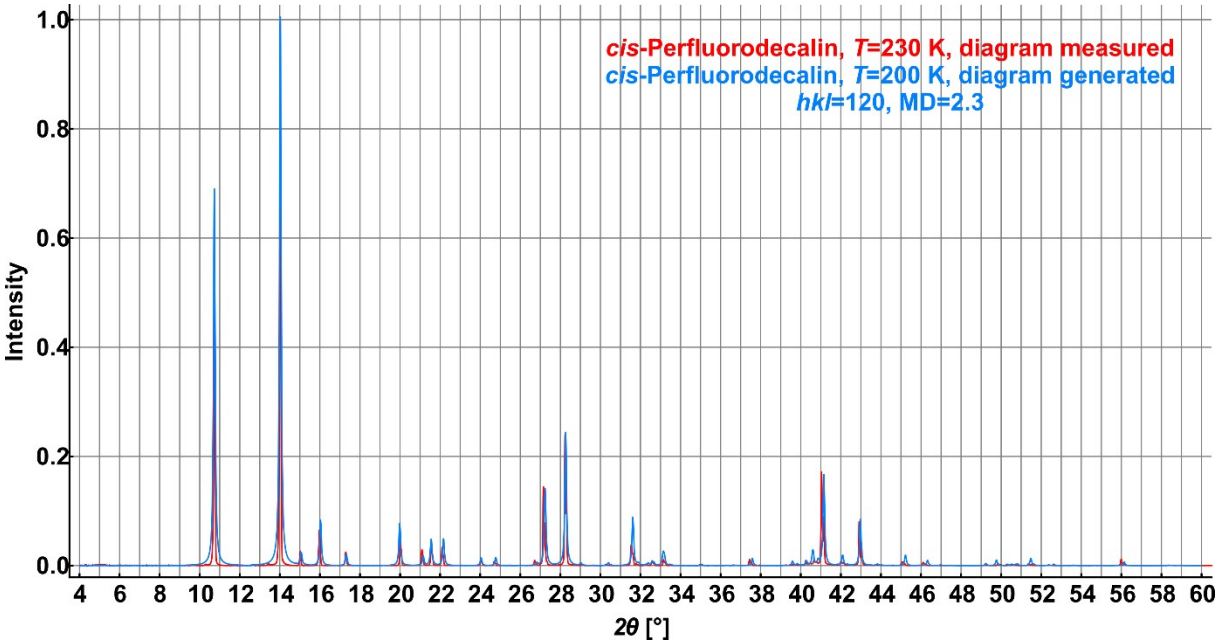

Fig. S2. Overlay of experimental and generated powder diagrams for *cis*-perfluorodecalin. Relatively good fit is observed when texture effect is included in generated diagrams for *MD*=2.3 (March-Dollase parameter) with decreased intensities of *hkl*=120 group of reflections – crystals form needles elongated the [120] direction and parallel to the capillary.

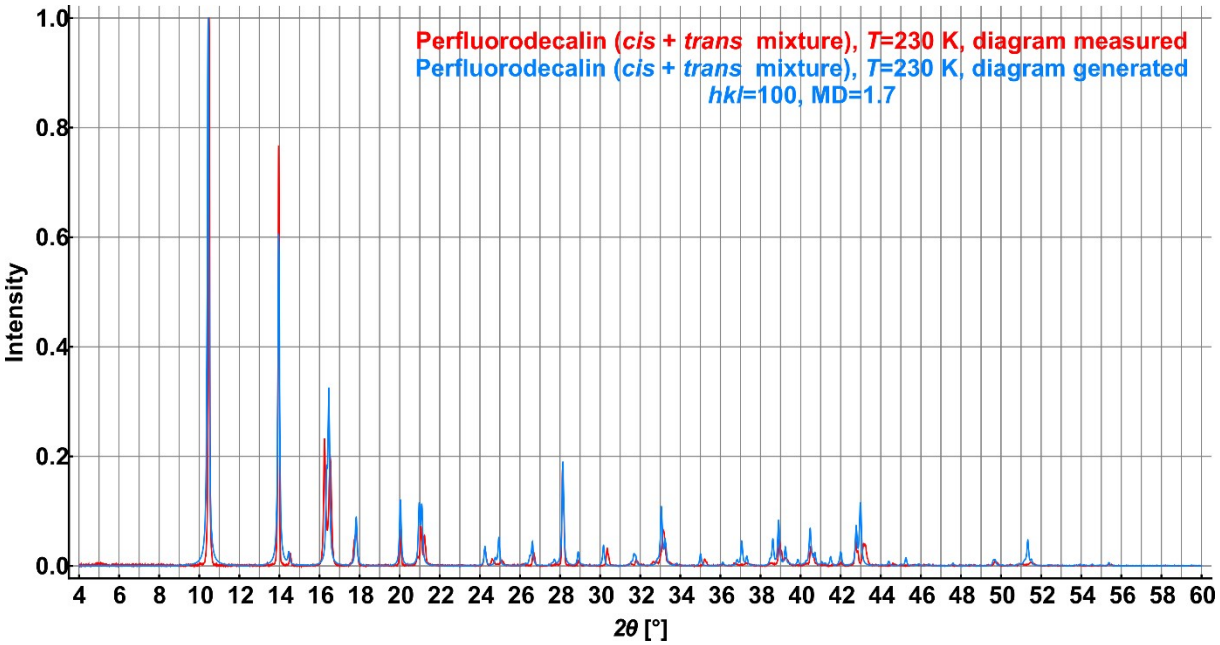

Fig. S3. Overlay of experimental and generated powder diagrams for disordered form of *trans*-perfluorodecalin. Relatively good fit is observed when texture effect is included in generated diagrams for *MD*=1.7 (March-Dollase parameter) with decreased intensities of *hkl*=100 group of reflections – crystals form needles elongated the [100] direction and parallel to the capillary.

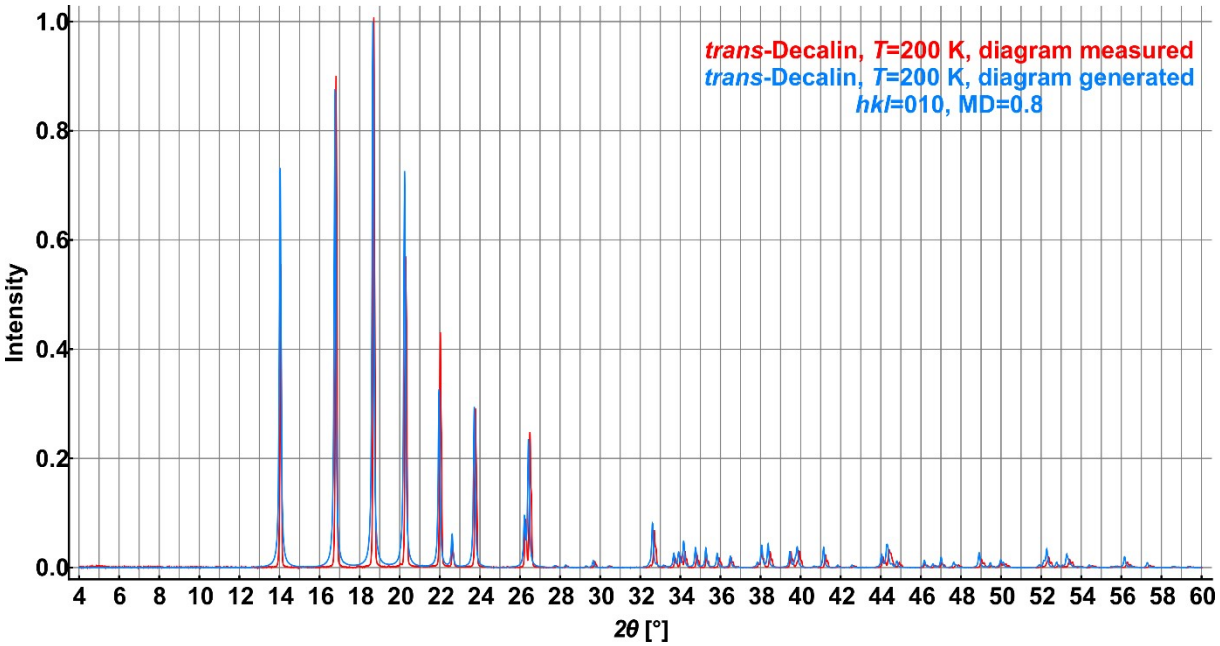

Fig S4. Overlay of experimental and generated powder diagrams for *trans*-decalin. Relatively good fit is observed when texture effect is included in generated diagrams for *MD*=0.8 (March-Dollase parameter) with enhanced intensities of *hkl*=010 group of reflections – crystals form plates with index of the base face equal to (010).

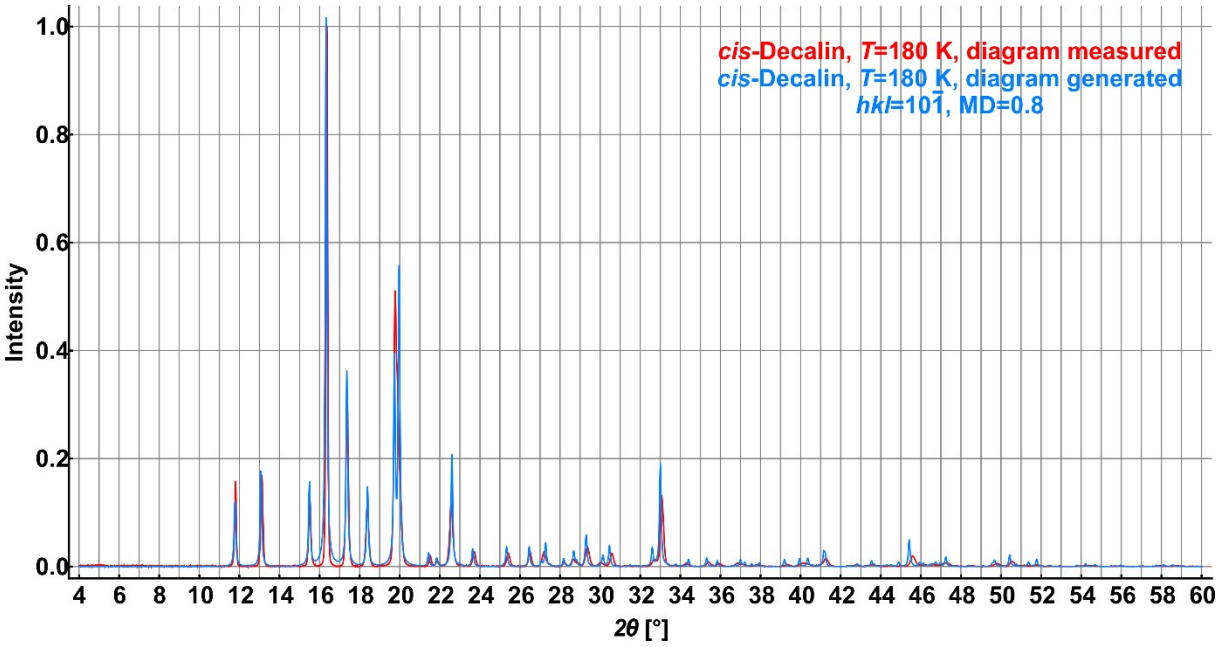

Fig. S5. Overlay of experimental and generated powder diagrams for *cis*-decalin. Relatively good fit is observed when texture effect is included in generated diagrams for *MD*=0.8 (March-Dollase parameter) with enhanced intensities of *hkl*=10-1 group of reflections – crystals form plates with index of the base face equal to (10-1).