Electronic Supplementary Material (ESI) for ChemComm.

Conserved hydrogen bonding in tetrahydrocarbazolone derivatives: Influence of solution-state assembly on crystal form nucleation

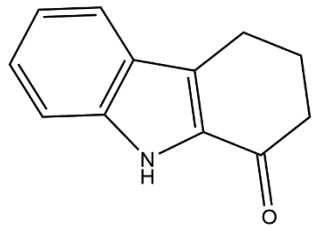
Robert M. Edkins, Elliott Hayden, Jonathan W. Steed, Katharina Fucke*

Supporting information

CSD search

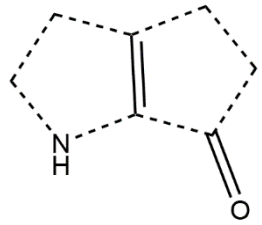
Searches for various fragments of the core tetrahydrocarbazolone and related structures were performed using CSD version 5.35 (February 2014 update). The search inputs and results are detailed below. Where a bond was specified as the 'all' bond-type option, it is drawn as a dashed line.

Searched for fragment:



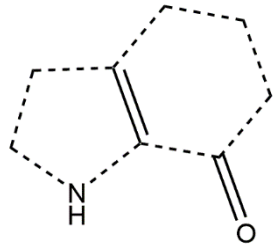
DEXVIM	Dimer	OBUVOY	Dimer
FOVSAL	Dimer	OMABAG	Dimer
FOWXEV	Dimer	QIXMAM	Dimer
GOJWAE	Dimer	QUHZUO	Dimer
HESFOB	Dimer	SACFIN	Dimer
LESBAO	Dimer	SUZGIE	Dimer
LIJPUQ	Dimer	TUJBEF	No 3D coordinates
LOBCIP	No Dimer, additional solvent suspected	UNOLOY	Dimer
MODVAD	Dimer	VIDMOL	Dimer
NEBBUR	No 3D coordinates	WACYAC	Dimer
OBUVEO	Dimer	WADDIQ	Dimer

Searched for fragment:



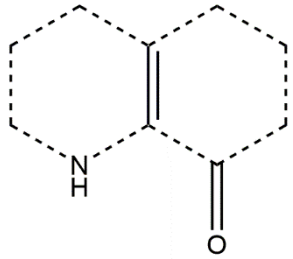
TANHIZ	Dimer
TATZIY	Dimer
VESQEQ	Dimer
VUWSUC	Dimer
YAJJEA	Dimer
YONBUZ	Dimer
YONCAG	Dimer

Searched for fragment:



EBASOP	Dimer	PEMMEZ	Solvate, no dimer
FAVRID	Mixed solvate, no dimer	PEWQUE	No dimer, different synthon
FOSNAC	No dimer	QABXAS	No dimer, different synthon
GEMWUQ	No dimer, different synthon	REMBUH	Dimer
GEXCOB	Dimer	RUGGAB	Solvate, no dimer
LEPRIH	Solvate, no dimer	SEKLOJ	Dimer
NADGOQ	Catemer including additional OH-group	UDOWUG	No dimer, different synthon
		YAKRUZ	No dimer, different synthon

Searched for fragment:



ECANUT	No dimer, different synthon
FOSNAC	No dimer, different synthon
PUYPEE	Solvate, no dimer
QABXAS	No dimer, different synthon
QOHRIP	Dimer
UQEVIW	No dimer, different synthon
UXOCAM	Dimer
WENVEQ	No 3D coordinates

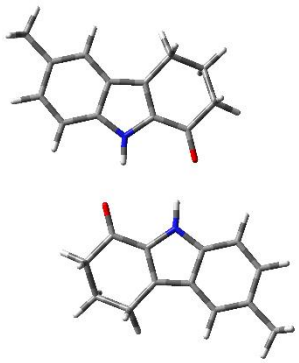


Figure S1 Dimer motif found in the carbazolones with lateral offset of the centro-symmetric dimer. The hydrogen bond acceptor group is shifted towards the indolyl moiety, while the synthon stays overall planar.

Table S1 Crystallisation experiments of OCB and their resulting crystal forms after initial crystallisation and finally after storing for one to two days.

Solvent	**Fast cooling**	**Slow cooling**	
		initial	**final**
Water	No crystallisation	IV	
Methanol	III	I	
Ethanol	III	II	III
1-Propanol	III	IV	I
2-Propanol	III	II	III
1-Butanol	III	III	
2-Butanol	III	IV	
Acetone	No crystallisation	III	I
Acetonitrile	No crystallisation	III	
Nitromethane	III	III	
Ethyl acetate	III	I	
Diethyl ether	III	IV	III
Tetrahydrofuran	No crystallisation	I	
Dioxane	III	I	
Dichloromethane	No crystallisation	No crystallisation	
Chloroform	No crystallisation	No crystallisation	
Dimethylsulfoxide	No crystallisation	No crystallisation	
N,*N*-Dimethylformamide	No crystallisation	No crystallisation	
Toluene	III	IV	
Hexane	II	IV	

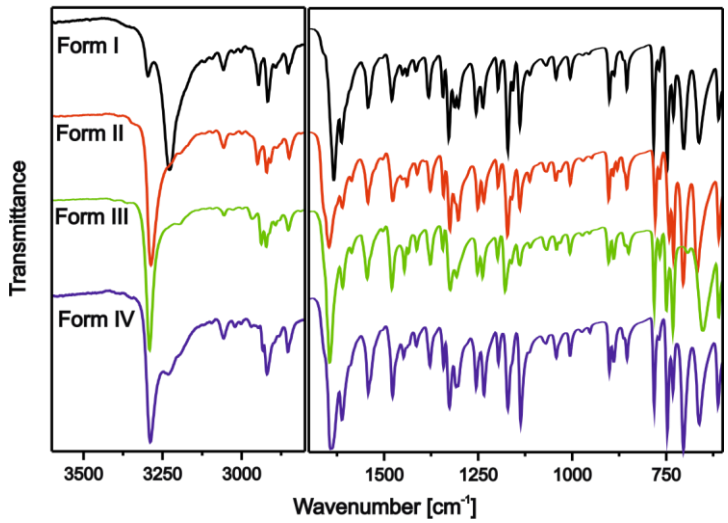


Figure S2 FTIR spectra of the four crystal forms of OCB.

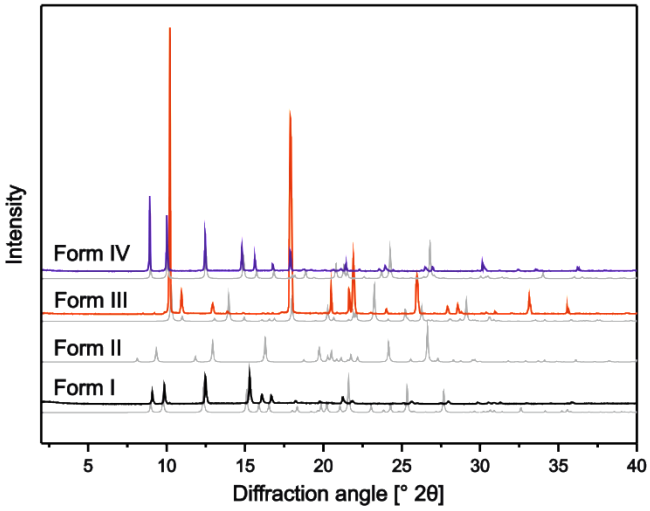


Figure S3 Experimental PXRD patterns of three crystal forms of OCB and the calculated patterns from the crystal structures of all four crystal forms (grey scale).

Table S2 Crystallographic data for the four polymorphs of OCB.

	Form I	**Form II**	**Form III**	**Form IV**
CCDC No.	1 041 114	1 041 115	1 041 116	1 041 117
Formula	$C_{13}H_{13}NO$	$C_{13}H_{13}NO$	$C_{13}H_{13}NO$	$C_{13}H_{13}NO$
M_r	199.25	199.25	199.25	199.25
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_12_12_1$	$P2_1/c$	$P2_1/n$	$P2_1/c$
T [K]	120	120	120	120
a [Å]	4.885(2)	9.4905(5)	10.5236(3)	4.9180(5)
b [Å]	11.442(5)	4.9370(2)	7.1700(2)	17.588(2)
c [Å]	17.634(8)	21.836(1)	13.5856(4)	11.975(1)
α [°]	90	90	90	90
β [°]	90	95.103(5)	93.912(3)	97.432(3)
γ [°]	90	90	90	90
V [Å^3]	985.6(7)	1019.05(9)	1022.70(5)	1027.1(2)
Z	4	4	4	4
ρ_{calcd} [g cm^{-3}]	1.343	1.299	1.294	1.288
λ [Å]	0.68889	0.7107	0.7107	0.7107
μ [mm^{-1}]	0.085	0.082	0.082	0.082
F(000)	424	424	424	424
θ range for data collection	2.06 – 24.10	2.73 – 32.71	2.84 – 32.63	2.07 – 30.07
Index ranges	$-5 < h < 5$	$-13 < h < 12$	$-15 < h < 15$	$-6 < h < 6$
	$-13 < k < 13$	$-5 < k < 7$	$-10 < k < 10$	$-24 < k < 24$
	$-20 < l < 20$	$-32 < l < 32$	$-20 < l < 20$	$-16 < l < 16$
Reflections collected	7409	6965	17019	8627
Independent reflections	1699	3335	3510	2999
Refinement method	Full-matrix least-squares on F^2			
Data/restraints/ parameters	1699/0/138	3335/0/137	3510/0/143	2999/0/138
GOF on F^2	0.902	1.018	1.043	0.999
Final R indices ($I>2\sigma(I)$)	$R_1 = 0.0425$	$R_1 = 0.0860$	$R_1 = 0.0477$	$R_1 = 0.0504$
	$wR_2 = 0.0983$	$wR_2 = 0.1785$	$wR_2 = 0.1162$	$wR_2 = 0.1169$
R indices (all data)	$R_1 = 0.0609$	$R_1 = 0.1384$	$R_1 = 0.0627$	$R_1 = 0.0988$
	$wR_2 = 0.1082$	$wR_2 = 0.2088$	$wR_2 = 0.1274$	$wR_2 = 0.1405$
Largest difference peak/hole [e Å^{-3}]	0.153/-0.157	0.39/-0.39	0.42/-0.28	0.26/-0.28

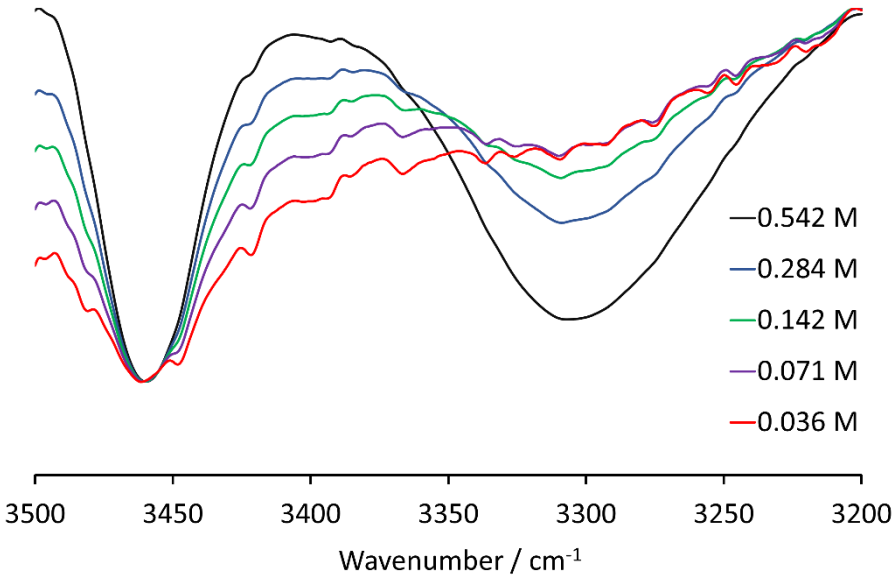


Figure S4 FTIR spectra of the titration of OCB in chloroform solution. The spectra have been normalised at the maximum intensity band at *ca*. 3460 cm^{-1}, which is assigned as the monomer band. The broader peak at *ca*. 3300 cm^{-1} is assigned to the dimer.

Table S3 Crystallisation experiments of PCB and their resulting crystal forms.

Solvent	Fast cooling	Slow cooling
Water	No crystallisation	No crystallisation
Methanol	I[a]	I[a]
Ethanol	IV	IV
1-Propanol	I[a]	I[a]
2-Propanol	I[a]	I[a]
1-Butanol	I[a]	IV
2-Butanol	I[a]	I[a]
Acetone	IV	I[a]
Acetonitrile	I[a]	I[a]
Nitromethane	I[a]	IV
Ethyl acetate	IV	I[a]
Diethyl ether	IV	IV
Tetrahydrofuran	I[a]	IV
Dioxane	IV	No crystallisation
Dichloromethane	I[a]	IV
Chloroform	I[a]	I[a]
Dimethylsulfoxide	I + IV	IV
N,*N*-Dimethylformamide	I[a]	I[a]
Toluene	IV	IV
Hexane	IV	IV

[a] The crystallisation results in a mixture of which form I is the predominant part.

PCB crystal forms II and III were obtained only from the melt; form V was obtained only once as a large single crystal by slow cooling of a solution in DMSO. Unlike OCB, no transformation to a more stable form was observed for any one initially produced form upon storage in contact with any solvent for a period of a few days.

Table S4 Crystallographic data for the three polymorphs of PCB.

	Form I	**Form IV**	**Form V[a]**
CCDC No.	1 041 118	1 041 119	1 041 120
Formula	$C_{13}H_{13}NO$	$C_{13}H_{13}NO$	$C_{13}H_{13}NO$
M_r	199.25	199.25	199.25
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	$P2_1/n$	$P2_1/n$	$Pbca$
T [K]	120	120	120
a [Å]	9.3763(6)	12.726(1)	14.682(2)
b [Å]	6.5586(4)	5.4479(5)	6.6231(8)
c [Å]	16.793(1)	14.793(1)	20.970(3)
α [°]	90	90	90
β [°]	102.558(2)	103.039(3)	90
γ [°]	90	90	90
V [Å^3]	1008.0(1)	999.1(2)	2039.1(5)(2)
Z	4	4	8
ρ_{calcd} [g cm^{-3}]	1.3129	1.3245	1.2980
λ [Å]	0.7107	0.7107	0.7107
μ [mm^{-1}]	0.083	0.084	0.082
F(000)	424	424	848
θ range for data collection	2.30 – 26.00	2.40 – 26.00	2.77 – 28.94
Index ranges	$-12 < h < 10$ $-8 < k < 8$ $-20 < l < 21$	$-17 < h < 14$ $-6 < k < 7$ $-19 < l < 20$	$-19 < h < 18$ $-8 < k < 8$ $-26 < l < 27$
Reflections collected	12395	15697	12113
Independent reflections	1974	1967	2458
Refinement method			
Data/restraints/parameters	1974/0/136	1967/0/136	2458/0/136
GOF on F^2	1.0606	1.0528	1.3261
Final R indices ($I>2\sigma(I)$)	$R_1 = 0.0703$ $wR_2 = 0.1707$	$R_1 = 0.0666$ $wR_2 = 0.1655$	$R_1 = 0.1958$ $wR_2 = 0.4158$
R indices (all data)	$R_1 = 0.0766$ $wR_2 = 0.1793$	$R_1 = 0.0831$ $wR_2 = 0.1807$	$R_1 = 0.2986$ $wR_2 = 0.0.4813$
Largest difference peak/hole [e Å^{-3}]	0.6048/-0.3161	0.5582/-0.3439	2.4296/-1.1369

[a] Structure refined stably, but the crystal showed a streaking diffraction pattern, most likely due to twinning or strain, resulting in rather high R-values.

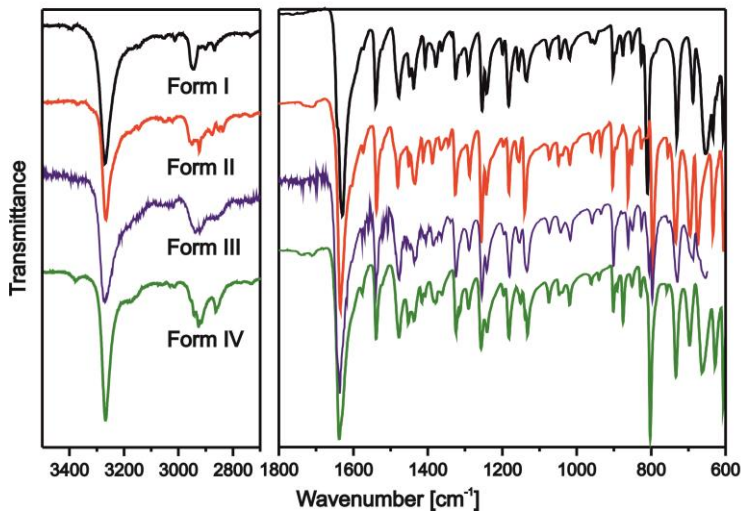


Figure S5 FTIR spectra of the four crystal forms of PCB.

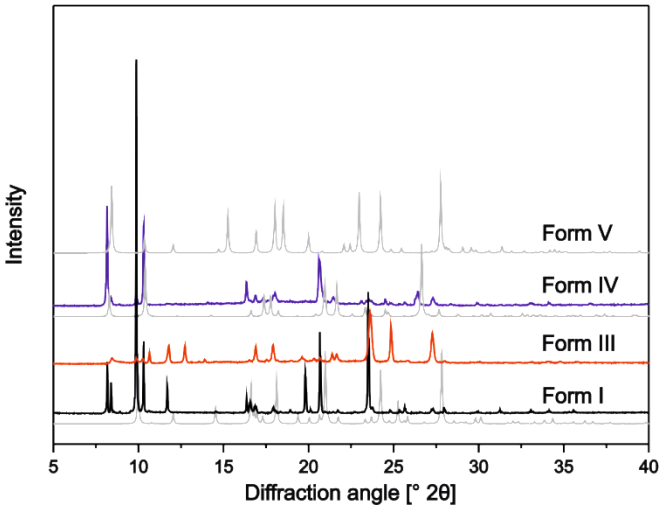


Figure S6 Experimental PXRD patterns of three crystal forms of PCB and the calculated patterns from the crystal structures (grey scale).

DFT Calculations

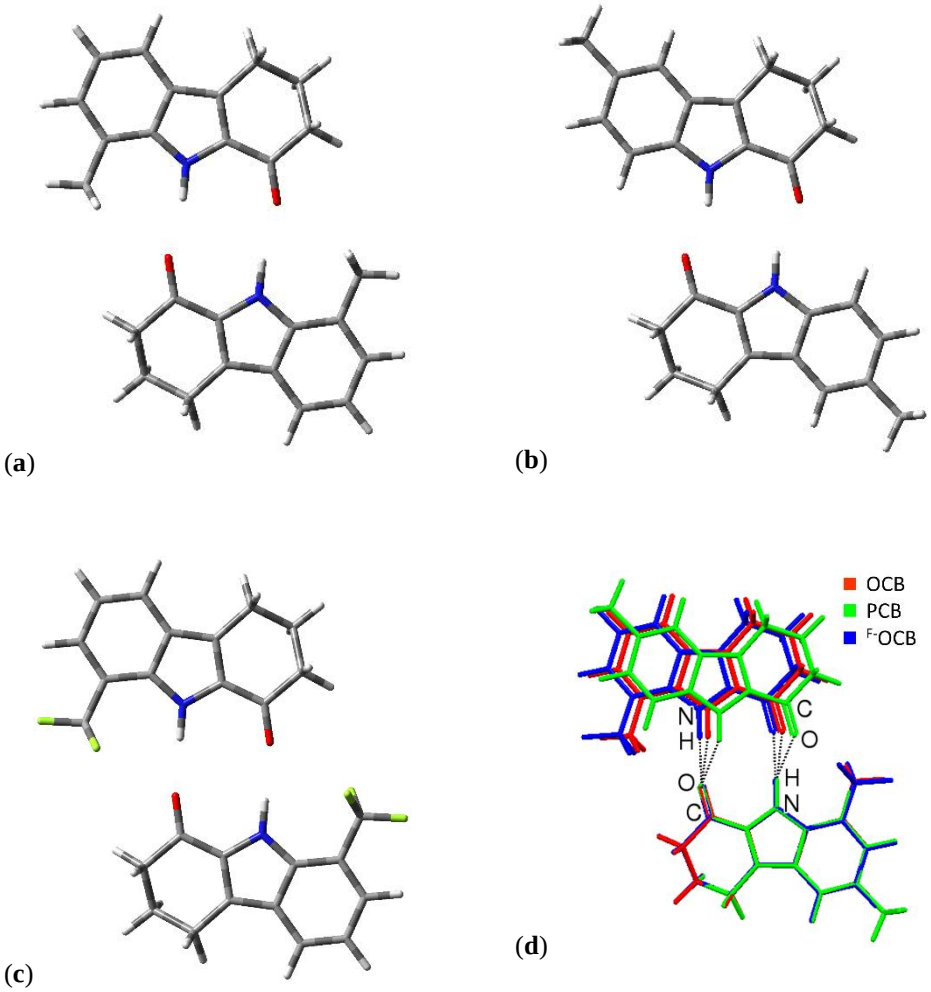


Figure S7 DFT optimised structures of the dimers of (**a**) OCB, (**b**) PCB and (**c**) $^{F-}$OCB at the B3LYP/6-311+G(d) level of theory with GD3BJ dispersion correction. (**d**) Overlap of the lower molecules of the dimers to illustrate the difference in offset.

Experimental

The compounds OCB and PCB were prepared according to the literature.[1] Solvents and all reagents were obtained from Sigma Aldrich or Fisher Scientific and were used as received.

Crystallisation

For the slow cooling, a vial containing a saturated solution at boiling point in the appropriate solvent was placed into a wooden block and allowed to cool slowly to room temperature. The fast cooling was performed by placing a vial containing a hot saturated solution into an ice-water bath to quench the solution, and the precipitate was characterised immediately after formation.

FTIR spectroscopy

Fourier-transform infrared spectra were recorded with a Perkin Elmer Spectrum 100 ATR instrument (Perkin-Elmer, Norwalk, CT, USA). For each spectrum, 64 scans were conducted over a spectral range of 4000 to 600 cm^{-1} with a resolution of 1 cm^{-1}. The analysis was carried out with the Spectrum Express 1.01 software. Normalisation of spectra was performed in Microsoft Excel.

Thermal microscopy

Hot-stage microscopic investigations were performed on an Olympus BX51 microscope (Olympus, Southend-on-Sea, UK) equipped with a Linkam THMS600 hot stage, operated with a TMS94 controller (Linkam Scientific Instruments Ltd., Tadworth, UK).

PXRD

Powder X-ray diffraction patterns were recorded using a D8 diffractometer (Bruker, Coventry, UK) in Bragg-Brentano geometry with Cu Kα (λ = 1.5418 Å) radiation, graphite monochromator, 20 mm variable Soller slits and scintillation counter detector. The X-ray tube was operated at 40 kV and 40 mA. Each sample was prepared on a low-background silicone-slide sample holder as a dry powder.

Single-crystal X-ray crystallography

Single crystals of OCB forms II, III and IV as well as PCB form V were measured on an Agilent Excalibur Gemini diffractometer using Mo Kα radiation (λ = 0.71073 Å). Crystals of PCB forms I and IV were measured on a Bruker D8 Quest diffractometer using Mo Kα radiation (λ = 0.71073 Å). Crystals of OCB form I were too small for laboratory-based diffractometry and were thus measured on the I19 small-organic single-crystal beamline at the Diamond Light Source, Oxfordshire, UK (λ = 0.68890 Å). All crystals were cooled to 120 K by an open-flow liquid-nitrogen Cryoflex device, except for OCB form I, which was cooled to 150 K, Data reduction was performed for OCB forms II, III and IV and PCB form V using Agilent Crysalis software and for OCB form I and PCB forms I and IV using Bruker ApexII software. Structure solution and refinement were performed for all crystal structures using the Olex2 software suite.[2]

DFT calculations

All calculations were performed using the Gaussian 09 (revision D.01) package.[3] The output files were viewed and analysed in GaussView 5 and molecular overlays were generated in Mercury CSD version 3.3. The monomer structures of OCB and PCB were optimised using the exchange-correlation functional B3LYP,[4] the basis set 6-311+G(d) and the third atom-pairwise dispersion correction from Grimme and coworkers with Becke-Johnson damping (GD3BJ).[5] Frequency calculations were

performed at the same level of theory and have been scaled by the typical value of 0.965.[6] From the optimised monomer structures, initial starting geometries for the dimers were constructed, namely a coplanar geometry with a realistic hydrogen-bonding distance of 2 Å. The structures of the dimers of OCB and PCB were then optimised at the same level of theory as the monomers. The structure of the ^{F}-OCB Dimer was optimised starting from that of the OCB dimer by replacement of the methyl hydrogen atoms with fluorine atoms. Two laterally offset but coplanar geometries were used as starting points for optimisation of each of the dimers: one offset to the phenyl side (similar to that observed in the crystal structures), the other to the cyclohenxenyl side, in order to see if there was another stable minimum with the latter relationship; however, the same geometry was obtained in each case. The counterpoise method,[7] as implemented in Gaussian 09, was used to correct the dimerisation energies for the basis-set superposition error, which accounts for *ca*. +3.5-4 kJ mol^{-1}.

DFT Cartesian coordinates of optimised structures

OCB Monomer (B3LYP/6-311+G(d) with GD3BJ dispersion correction)

Symbol	X	Y	Z
C	-2.961317	-1.720937	-0.035234
C	-3.439198	-0.392653	0.012876
C	-2.59076	0.706308	0.03299
C	-1.214569	0.419702	0.001183
C	-0.703836	-0.911443	-0.047296
C	-1.606191	-1.991741	-0.06492
H	-3.676606	-2.536705	-0.049005
H	-4.512118	-0.223959	0.035321
H	-1.246009	-3.014818	-0.103147
C	1.023146	0.539827	-0.027643
C	0.723127	-0.808881	-0.060773
N	-0.143363	1.279887	0.012201
H	-0.162193	2.286885	0.036881
C	3.472814	0.079427	-0.185799
H	4.377639	0.502064	0.257476
H	3.678791	-0.037404	-1.25932
C	3.119202	-1.284059	0.432932
H	3.036572	-1.170337	1.519823
H	3.934751	-1.991484	0.254235
C	1.795081	-1.855604	-0.107014
H	1.502923	-2.738313	0.471379
H	1.933002	-2.205086	-1.140267
C	2.358243	1.112798	-0.062187
O	2.563222	2.318712	-0.031673
C	-3.091464	2.125197	0.085332
H	-2.731391	2.649778	0.97771
H	-2.761072	2.704472	-0.784438
H	-4.182184	2.158347	0.104638

OCB Dimer (B3LYP/6-311+G(d) with GD3BJ dispersion correction)

Symbol	X	Y	Z
C	8.587797	-2.876446	-0.350995
C	8.23538	-1.696865	0.344804
C	7.11477	-0.942769	0.03027
C	6.329835	-1.422663	-1.036688
C	6.666655	-2.612037	-1.754971
C	7.817025	-3.340982	-1.396738
H	9.47906	-3.417282	-0.051195
H	8.870036	-1.364969	1.161228
H	8.086872	-4.246552	-1.929988
C	4.776596	-1.7277	-2.616152
C	5.669236	-2.784701	-2.75587
N	5.180695	-0.905932	-1.578813
H	4.681657	-0.073385	-1.270153
C	3.352949	-2.653097	-4.444766
H	2.766869	-2.22771	-5.262427
H	2.711848	-3.401467	-3.957828
C	4.639516	-3.318802	-4.951287
H	5.219377	-2.584886	-5.521649
H	4.389157	-4.129918	-5.641207
C	5.504561	-3.845662	-3.796776
H	6.478847	-4.176687	-4.169668
H	5.031994	-4.733647	-3.353363
C	3.594157	-1.55157	-3.421291
O	2.802711	-0.617492	-3.292605
C	6.750453	0.312755	0.771125
H	6.723768	1.178705	0.103514
H	5.753997	0.244884	1.215299
H	7.469367	0.516042	1.567097
C	-1.615869	3.921186	-3.690377
C	-1.269104	2.736158	-4.379734
C	-0.180899	1.951257	-4.028866
C	0.574042	2.402711	-2.928381
C	0.243065	3.597711	-2.21677
C	-0.871878	4.360323	-2.61469
H	-2.481031	4.486823	-4.019442
H	-1.880524	2.426299	-5.22214
H	-1.138405	5.26906	-2.085173
C	2.079591	2.662552	-1.295547
C	1.214386	3.745653	-1.186676
N	1.691221	1.855615	-2.350403
H	2.156236	0.990752	-2.621003
C	3.341201	3.433839	0.714608
H	4.392223	3.450978	1.011369
H	2.780848	3.038702	1.5737
C	2.826802	4.834504	0.356031

H	3.460215	5.255325	-0.432564
H	2.919147	5.495361	1.222817
C	1.37352	4.801439	-0.139698
H	1.080708	5.781086	-0.530097
H	0.69791	4.596556	0.702928
C	3.190464	2.418415	-0.410253
O	3.952413	1.456257	-0.505843
C	0.184076	0.696307	-4.77037
H	1.189141	0.760715	-5.196961
H	0.193068	-0.174799	-4.110127
H	-0.520885	0.506236	-5.581935

PCB Monomer (B3LYP/6-311+G(d) with GD3BJ dispersion correction)

Symbol	X	Y	Z
C	-3.451288	0.976041	-0.003818
C	-3.677692	-0.421035	-0.107133
C	-2.646613	-1.343894	-0.141869
C	-1.336637	-0.856936	-0.069354
C	-1.072615	0.53999	0.035222
C	-2.149634	1.445964	0.066107
H	-4.702483	-0.777786	-0.161493
H	-2.850359	-2.4068	-0.22241
H	-1.957053	2.511985	0.146832
C	0.883425	-0.581583	0.009374
C	0.347292	0.691035	0.079667
N	-0.131518	-1.514509	-0.083056
H	0.027333	-2.507676	-0.140812
C	3.204069	0.304454	0.240182
H	4.181355	0.065016	-0.185098
H	3.353328	0.423892	1.322575
C	2.622468	1.599477	-0.353499
H	2.569816	1.497418	-1.443367
H	3.297598	2.435448	-0.147272
C	1.212502	1.909046	0.182775
H	0.771298	2.746176	-0.368077
H	1.275546	2.234721	1.230817
C	2.297766	-0.907974	0.054979
O	2.716601	-2.055494	-0.012363
C	-4.632605	1.915869	0.028235
H	-4.315482	2.958199	0.106184
H	-5.242391	1.822332	-0.876308
H	-5.288081	1.705067	0.879563

PCB Dimer (B3LYP/6-311+G(d) with GD3BJ dispersion correction)

Symbol	X	Y	Z
C	-0.870696	1.625902	-0.024746
C	0.369268	0.93319	-0.09008
C	1.585883	1.58298	-0.166287
C	1.570468	2.98425	-0.176757
C	0.344347	3.712337	-0.113006
C	-0.874882	3.008807	-0.036911
H	0.354486	-0.152999	-0.079691
H	2.522151	1.038882	-0.216007
H	-1.814404	3.551272	0.014109
C	2.078587	5.155652	-0.23125
C	0.689135	5.093129	-0.153153
N	2.603646	3.877417	-0.246713
H	3.588751	3.620663	-0.299214
C	2.005745	7.648102	-0.15971
H	2.562906	8.452538	-0.644936
H	1.948778	7.907696	0.906846
C	0.591401	7.504246	-0.738619
H	0.664015	7.351226	-1.820933
H	0.034597	8.4335	-0.586766
C	-0.166205	6.319399	-0.120329
H	-1.107595	6.149465	-0.6522
H	-0.442502	6.555586	0.917205
C	2.838966	6.37846	-0.255551
O	4.070088	6.423709	-0.310977
C	-2.153353	0.83681	0.057196
H	-3.024179	1.494375	0.099427
H	-2.275886	0.179844	-0.809971
H	-2.175872	0.199613	0.947196
C	10.053185	7.363593	-0.475466
C	8.812639	8.056405	-0.423588
C	7.593711	7.406931	-0.399538
C	7.607425	6.005866	-0.426925
C	8.834022	5.277698	-0.479512
C	10.055579	5.980913	-0.503293
H	8.828833	9.142418	-0.402476
H	6.65698	7.951106	-0.360533
H	10.995678	5.438375	-0.541305
C	7.095363	3.834962	-0.460771
C	8.486334	3.897292	-0.504574
N	6.571637	5.113051	-0.415516
H	5.585878	5.370007	-0.378475
C	7.172949	1.341843	-0.424674
H	6.574861	0.542968	-0.868619
H	7.323036	1.069624	0.629629
C	8.53116	1.493065	-1.123703

H	8.364032	1.658445	-2.193662
H	9.098684	0.562421	-1.031919
C	9.340598	2.671118	-0.560661
H	10.231936	2.84751	-1.170892
H	9.706445	2.42328	0.445977
C	6.335224	2.612112	-0.431975
O	5.103987	2.566835	-0.37907
C	11.338477	8.152325	-0.498198
H	12.209297	7.494727	-0.540032
H	11.384487	8.818783	-1.36556
H	11.439633	8.779767	0.393266

$^{F-}$OCB Dimer (B3LYP/6-311+G(d) with GD3BJ dispersion correction)

Symbol	X	Y	Z
C	8.794263	-2.60537	-0.030311
C	8.3712	-1.452985	0.659212
C	7.235623	-0.751397	0.282844
C	6.500124	-1.223725	-0.821978
C	6.927142	-2.396257	-1.525824
C	8.082813	-3.079656	-1.116318
H	9.688807	-3.118897	0.302579
H	8.945974	-1.101956	1.506567
H	8.409472	-3.968721	-1.645554
C	5.053799	-1.592043	-2.48232
C	5.990434	-2.607002	-2.580682
N	5.364477	-0.757346	-1.42149
H	4.806743	0.053865	-1.157309
C	3.759795	-2.55475	-4.39159
H	3.19916	-2.147936	-5.235379
H	3.124112	-3.328889	-3.939324
C	5.098193	-3.165498	-4.830162
H	5.677515	-2.406429	-5.36698
H	4.917754	-3.981938	-5.534939
C	5.924087	-3.666178	-3.634825
H	6.928913	-3.953631	-3.959615
H	5.466676	-4.575519	-3.220565
C	3.90439	-1.451667	-3.354235
O	3.088136	-0.543801	-3.256712
C	6.806391	0.471902	1.034025
C	-1.952333	3.513776	-3.864034
C	-1.551799	2.336395	-4.524167
C	-0.408098	1.644272	-4.155047
C	0.358258	2.15153	-3.087146
C	-0.046153	3.348939	-2.412811
C	-1.20998	4.022845	-2.815076
H	-2.854724	4.018304	-4.189435
H	-2.151218	1.957798	-5.342083

H	-1.521302	4.929233	-2.306391
C	1.855251	2.575525	-1.48563
C	0.926544	3.599218	-1.400028
N	1.510197	1.703414	-2.505292
H	2.059801	0.884302	-2.761914
C	3.09538	3.494146	0.481088
H	4.146451	3.5873	0.761154
H	2.573348	3.092816	1.361047
C	2.484418	4.843666	0.079532
H	3.078379	5.276844	-0.732588
H	2.543534	5.540257	0.920425
C	1.029174	4.699975	-0.392535
H	0.669572	5.644454	-0.812599
H	0.378561	4.481584	0.465798
C	2.996367	2.431178	-0.602831
O	3.803324	1.513329	-0.682015
C	-0.00213	0.395222	-4.876197
F	5.569811	0.331251	1.570306
F	7.64102	0.770274	2.055785
F	6.760594	1.567973	0.23706
F	1.205271	0.525067	-5.479484
F	0.095954	-0.665699	-4.038537
F	-0.882169	0.047224	-5.842629

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