

## N–H $\cdots$ O and C–H $\cdots$ F hydrogen bonds in the incommensurately modulated crystal structure of adamantan–1–ammonium 4–fluorobenzoate

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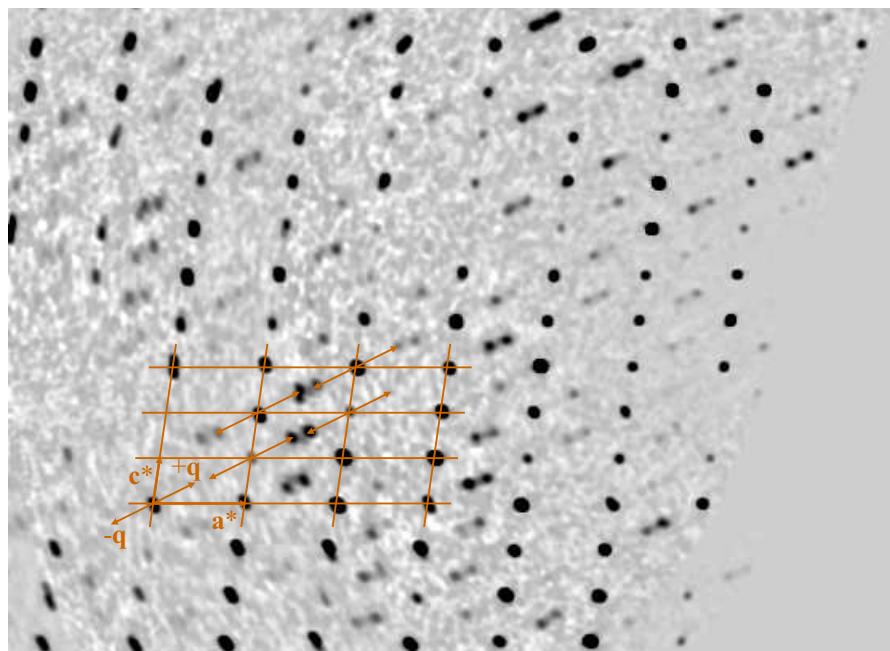
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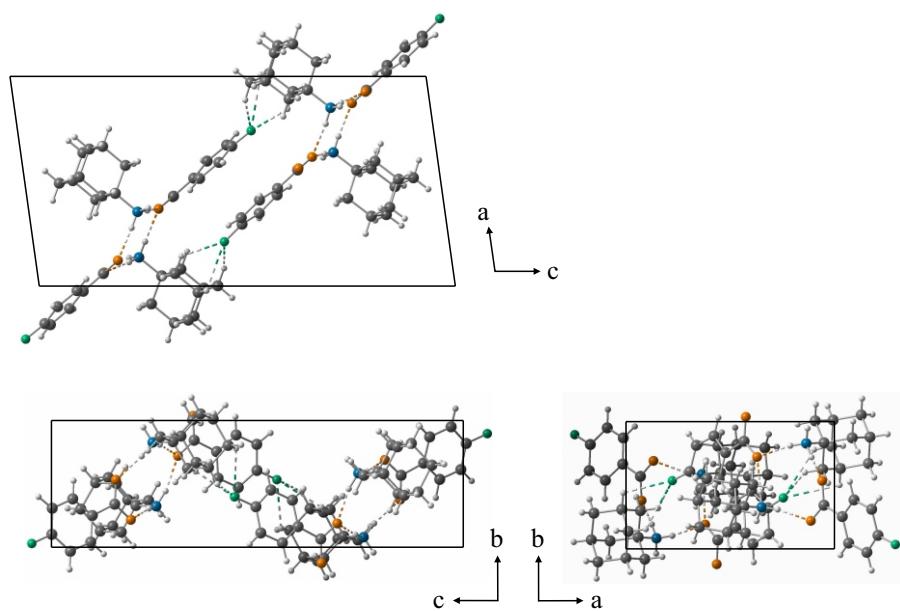
## supplementary material

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**Figure s1:**

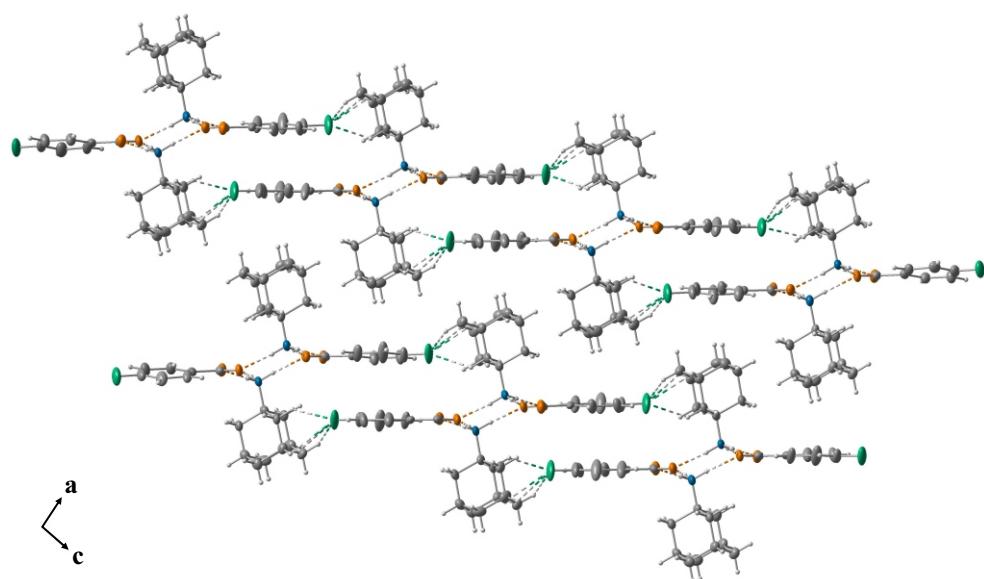
Reconstruction of the diffraction pattern, showing a section of the reciprocal lattice plane  $h1l$ . The net of the reciprocal lattice spanned by  $\mathbf{a}^*$  and  $\mathbf{c}^*$  as well as the modulation wave vector  $\mathbf{q}$  are indicated with which the diffracted intensities can be indexed in a unique way.



**Figure s2:** View against the three crystallographic axes showing the content of the unit cell. The view along the **b**-axis is also the view along the ribbons generated by the hydrogen bonds.

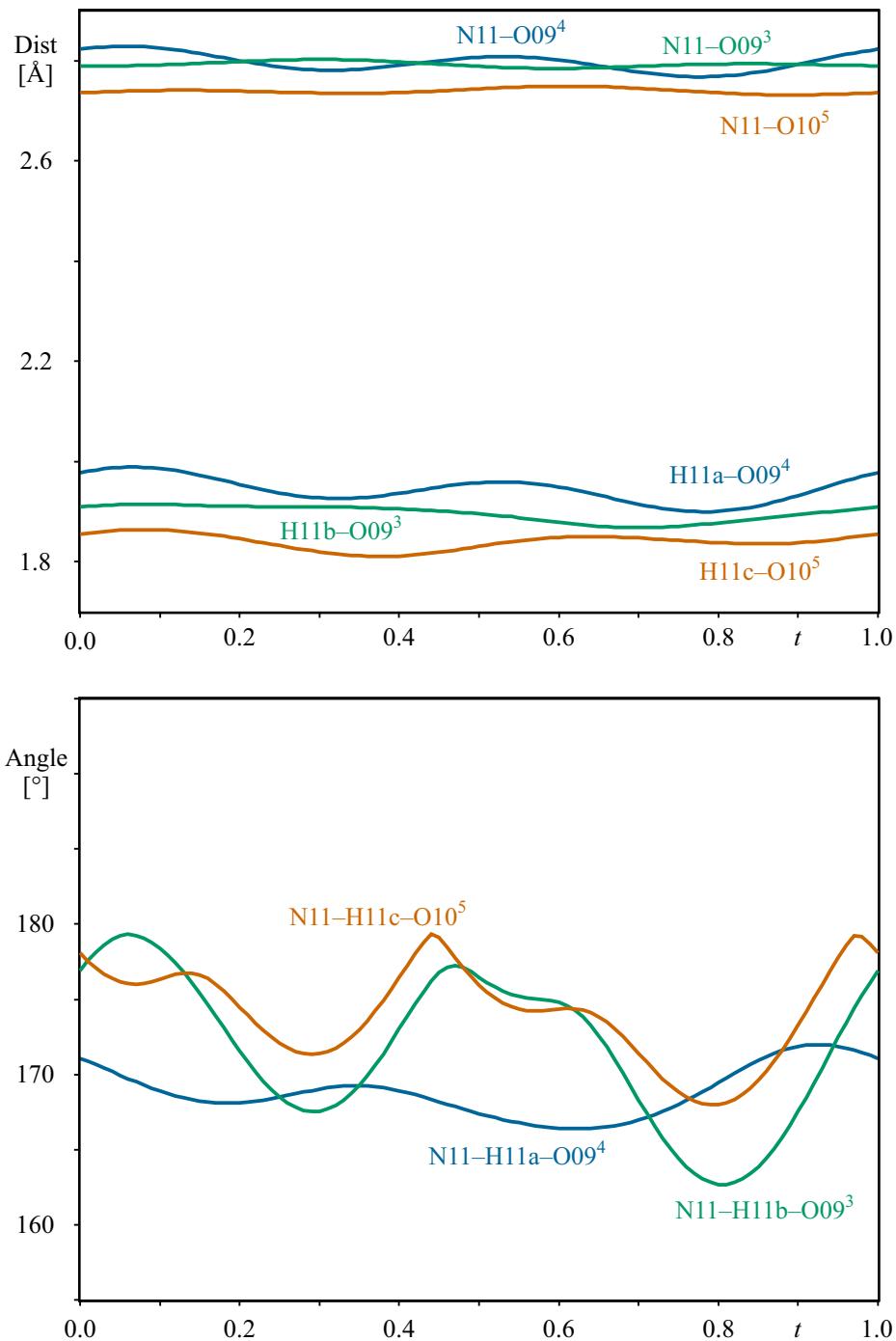
## supplementary material

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**Figure s3:**

View of the structure along **b**. It can be seen that the conformation of the rigid moieties (*e.g.*, the orientation of the phenyl rings in the 4-fluorobenzoate anions) and the ADPs are varying as function of the phase of the modulation *t*.



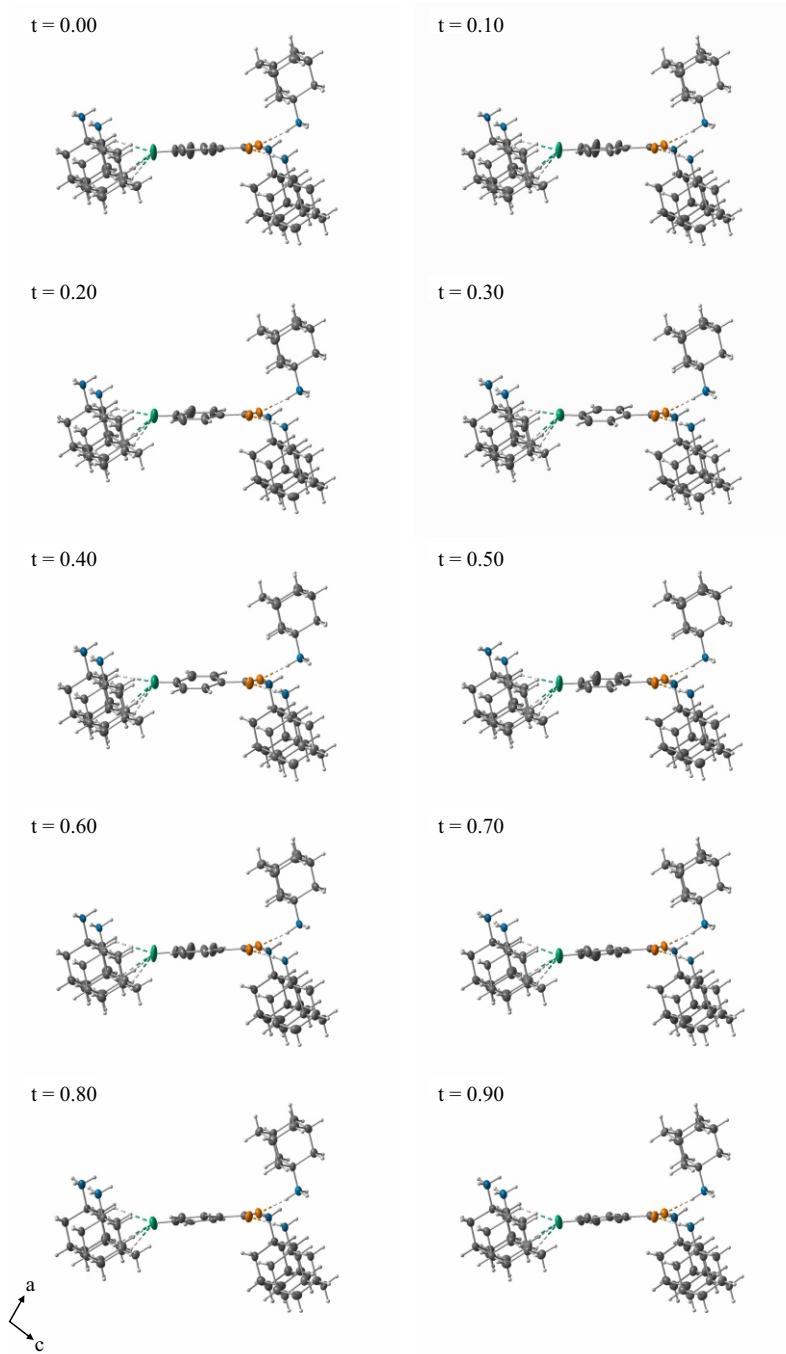
**Figure s4:**

Distances and angles in the intermolecular hydrogen bond motif as function of the phase of the modulation  $t$ . The symmetry operations are (3)  $-x_1, -x_2, -x_3, -x_4$ ; (4)  $x_1 + 1/2, -x_2 + 1/2, x_3 + 1/2, x_4$ ; (5)  $-x_1, -x_2 + 1, -x_3, -x_4$ .

## supplementary material

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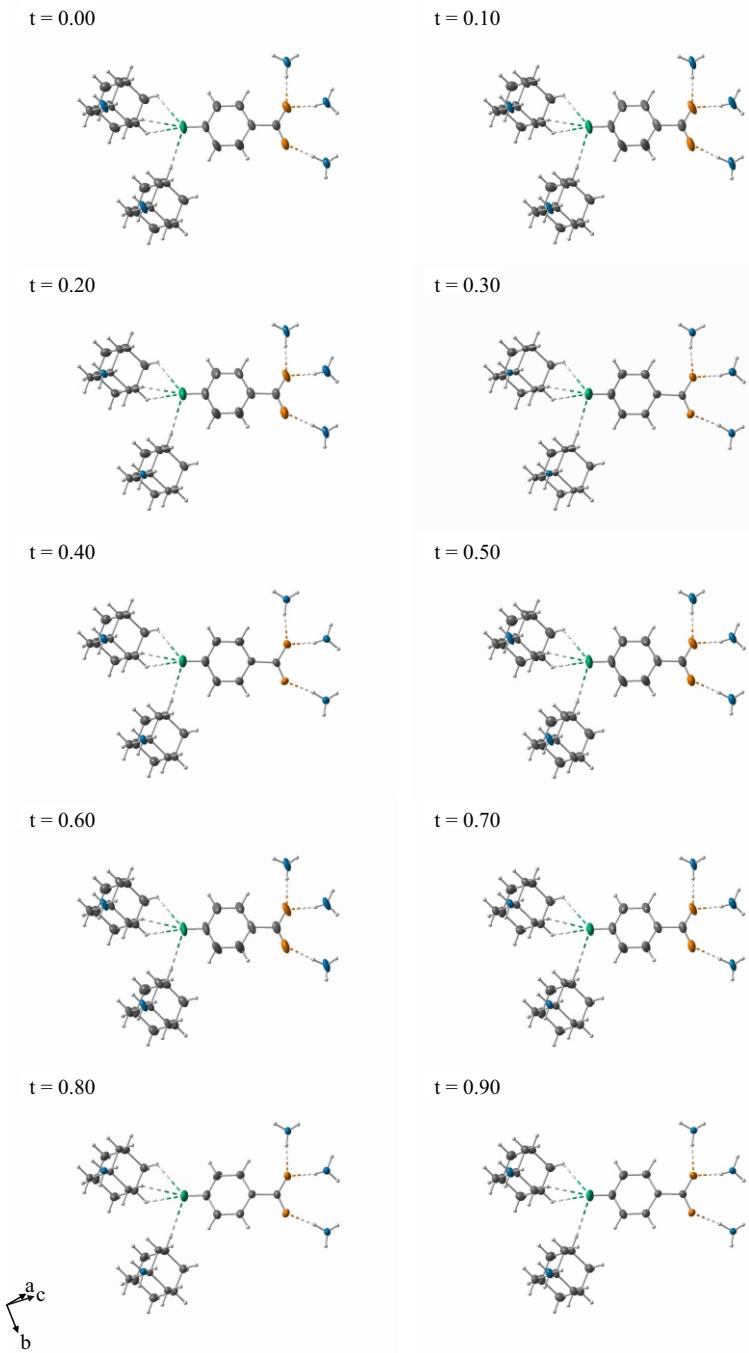
For an animated scheme see Fig. s7 .



**Figure s5:**

Molecular conformation, ADPs and intermolecular interactions as function of the phase of the modulation  $t$ .

For an animated scheme see Fig. s7 .



**Figure s6:**

Molecular conformation, ADPs and intermolecular interactions as function of the phase of the modulation  $t$ .

## supplementary material

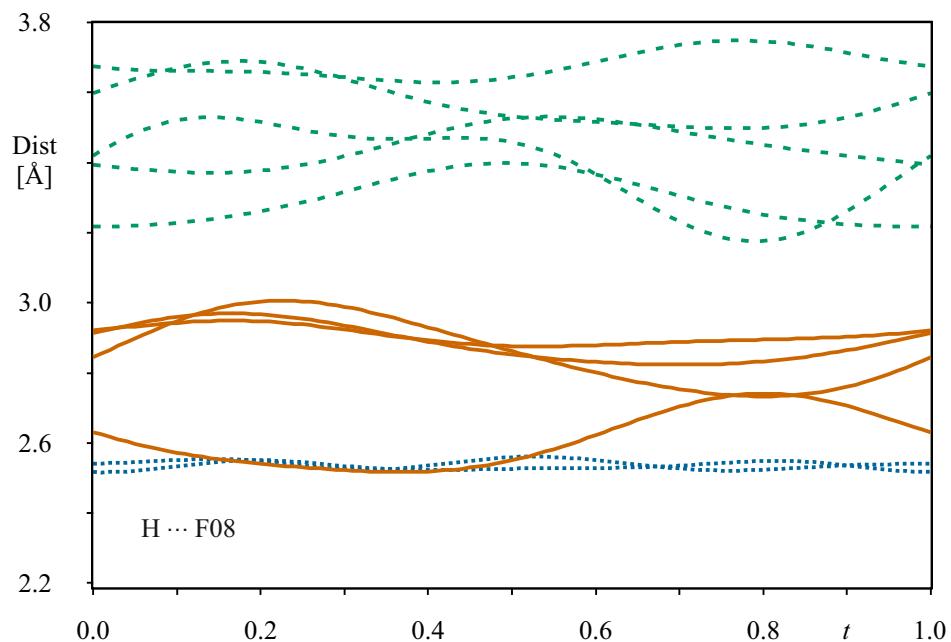
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**Figure s7:**

Molecular conformation, ADPs and intermolecular interactions as function of the phase of the modulation  $t$ .



**Figure s8:**

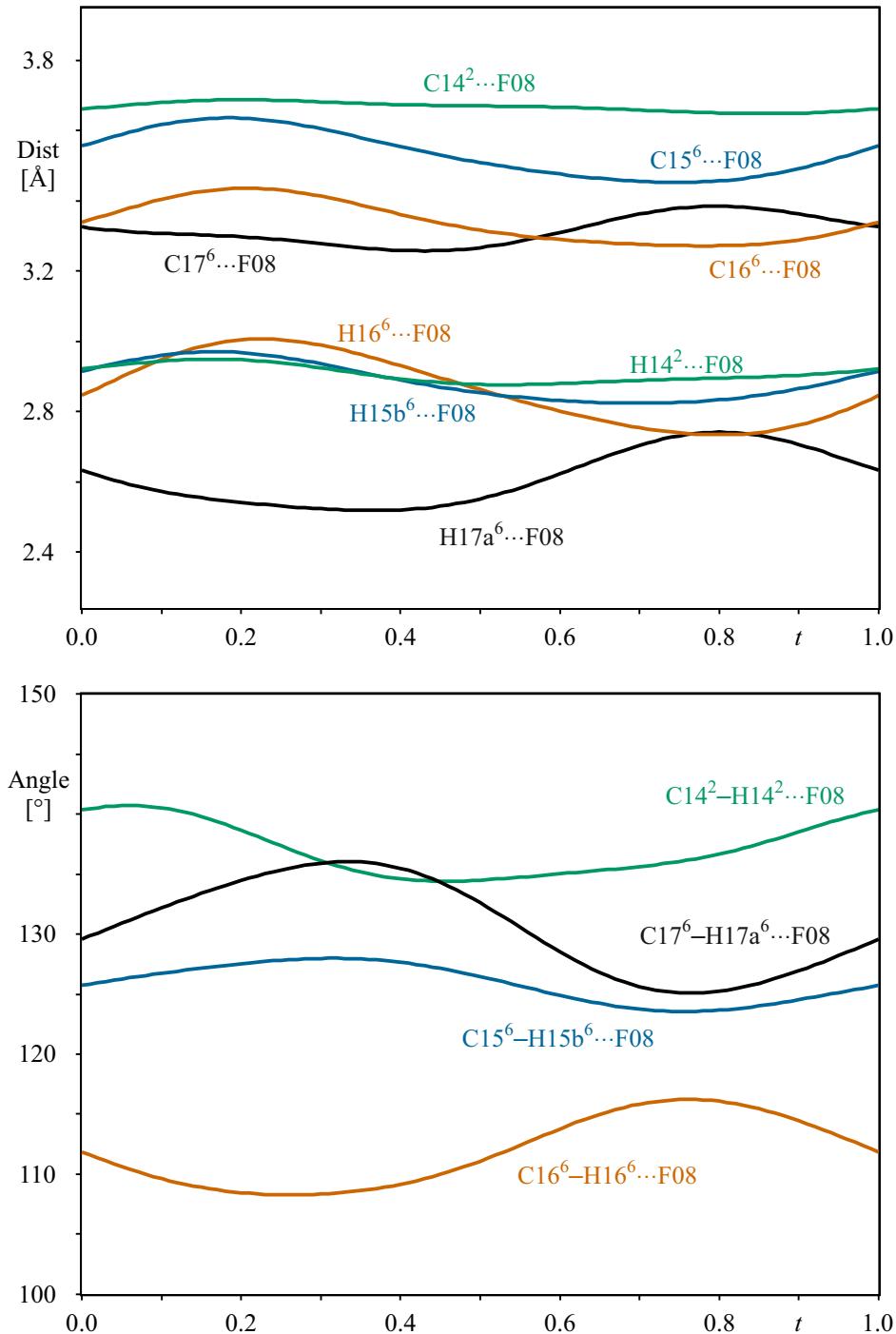
$\text{H}\cdots\text{F}$  distances as function of the phase of the modulation  $t$ .

The two (blue) dotted lines in the lower part of the figure, between 2.5 and 2.6 Å, are the intramolecular distances  $\text{H}04\cdots\text{F}$  and  $\text{H}06\cdots\text{F}$ , while the four (orange) continuous ones, between 2.6 and 3 Å, are further analysed in Fig. s9.

The five (green) dashed lines in the upper part, above 3.2 Å, represent interatomic distances not suitable for  $\text{C}-\text{H}\cdots\text{F}$  interactions anymore.

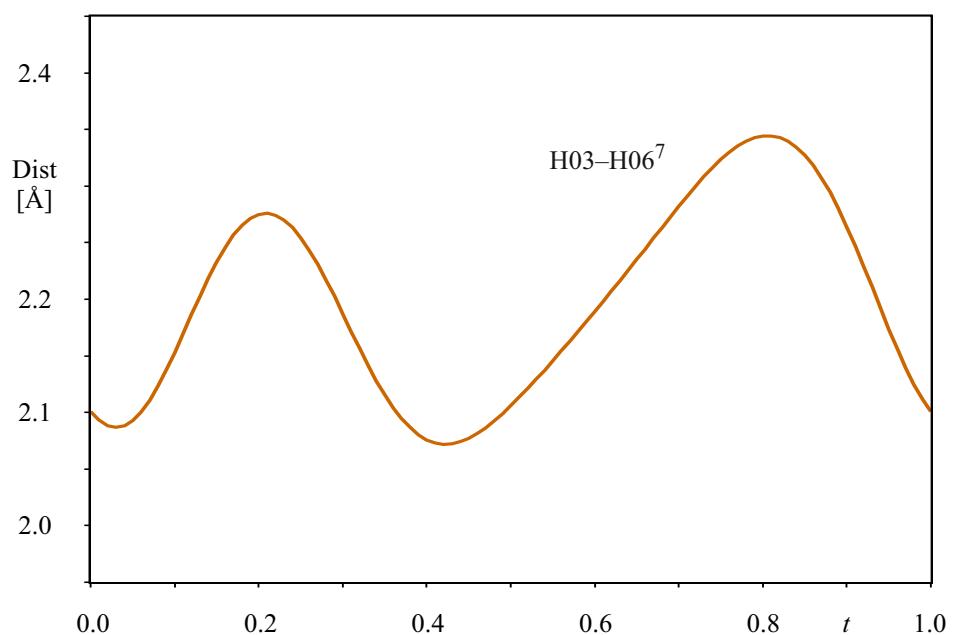
## supplementary material

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**Figure s9:**

Distances and angles in the possible intermolecular C–H $\cdots$ F interactions as function of the phase of the modulation  $t$ . The symmetry operations are (2)  $-x_1 + 1/2$ ,  $x_2 + 1/2$ ,  $-x_3 + 1/2$ ,  $-x_4$ ; (6)  $-x_1 + 1/2$ ,  $x_2 - 1/2$ ,  $-x_3 + 1/2$ ,  $-x_4$ .



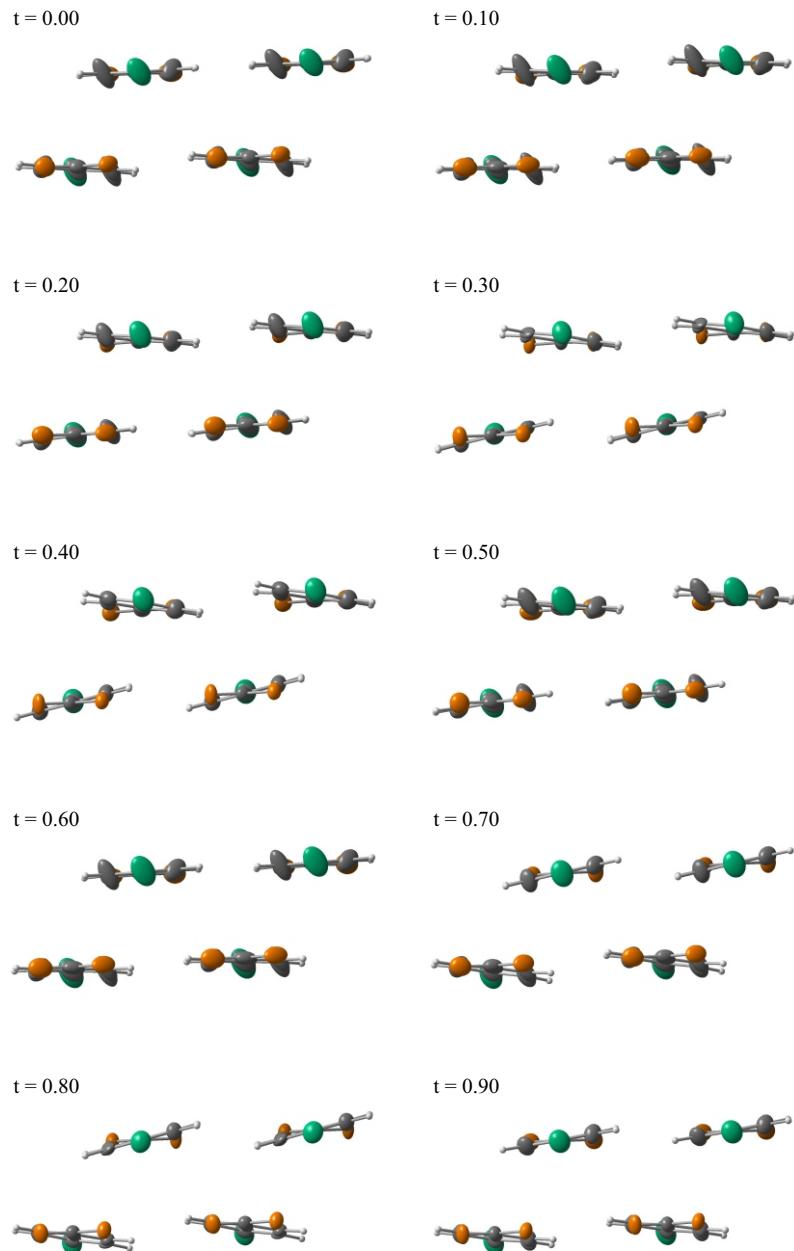
**Figure s10:**

Intermolecular distance  $H03 - H06^7$  as function of the phase of the modulation  $t$ .  
The symmetry operation is (7)  $x_1, x_2 + 1, x_3, x_4$ .

## supplementary material

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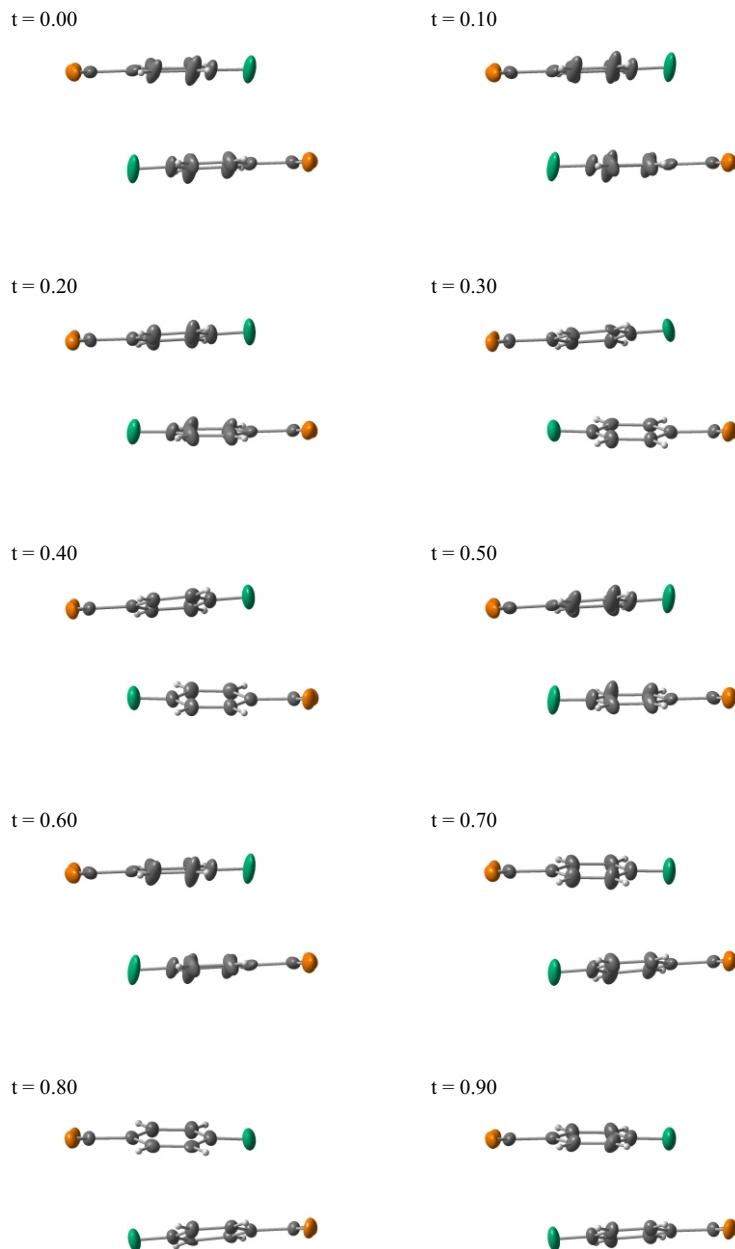
For an animated scheme see Fig. s13 .



**Figure s11:**

Relative orientations of the *p*-fluorobenzoate anions as function of the phase of the modulation  $t$ .

For an animated scheme see Fig. s13 .



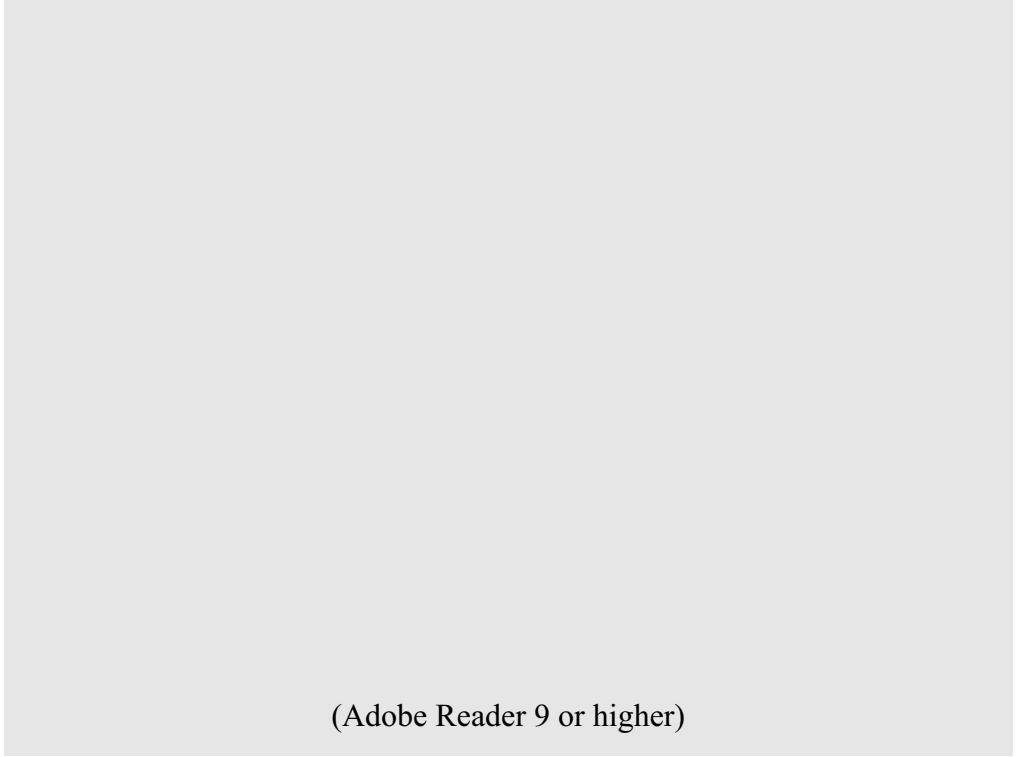
**Figure s12:**

Relative orientations of the *p*-fluorobenzoate anions as function of the phase of the modulation  $t$ .

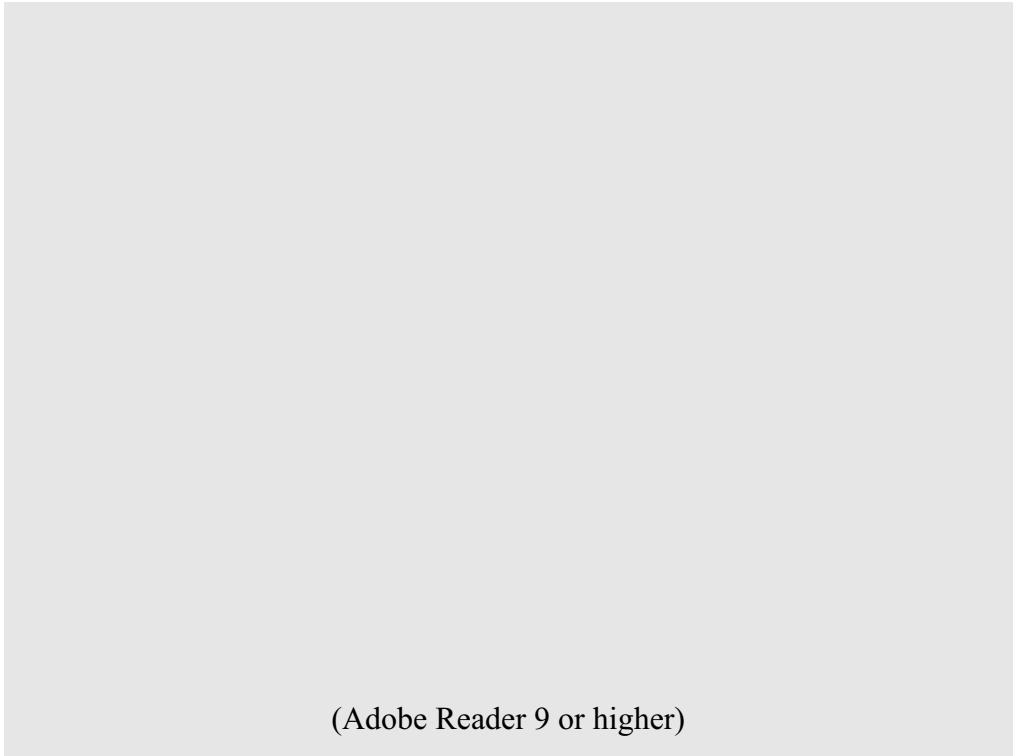
## **supplementary material**

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**Figure s13:**

Relative orientations of the *p*-fluorobenzoate anions as function of the phase of the modulation  $t$ .

**Table s1:**

Covalent bond lengths ( $\text{\AA}$ ) in the adamantan-1-ammonium cation and the 4-fluorobenzoate anion.

bond	average	minimum	maximum	$\Delta$
N11–C12	1.491 (5)	1.479 (5)	1.499 (5)	0.020
C12–C13	1.535 (4)	1.528 (4)	1.540 (4)	0.012
C12–C17	1.533 (4)	1.520 (4)	1.548 (4)	0.028
C12–C18	1.533 (4)	1.526 (4)	1.542 (4)	0.016
C13–C14	1.520 (5)	1.513 (5)	1.527 (5)	0.014
C14–C15	1.538 (4)	1.527 (4)	1.551 (4)	0.024
C14–C21	1.531 (5)	1.524 (5)	1.535 (5)	0.011
C15–C16	1.541 (5)	1.535 (5)	1.547 (4)	0.012
C16–C17	1.525 (5)	1.518 (5)	1.531 (5)	0.013
C16–C20	1.532 (5)	1.521 (5)	1.544 (5)	0.023
C18–C19	1.523 (5)	1.515 (5)	1.532 (5)	0.017
C19–C20	1.537 (4)	1.516 (4)	1.558 (4)	0.042
C19–C21	1.539 (5)	1.530 (5)	1.548 (5)	0.018
C01–C02	1.513 (5)	1.498 (5)	1.528 (5)	0.030
C01–O09	1.261 (4)	1.239 (5)	1.280 (4)	0.041
C01–O10	1.254 (4)	1.236 (4)	1.268 (4)	0.032
C02–C03	1.386 (5)	1.365 (5)	1.405 (5)	0.040
C02–C07	1.388 (5)	1.368 (5)	1.406 (5)	0.038
C03–C04	1.382 (6)	1.371 (6)	1.393 (6)	0.022
C04–C05	1.360 (5)	1.344 (5)	1.380 (5)	0.036
C05–C06	1.377 (6)	1.356 (6)	1.402 (6)	0.046
C05–F08	1.355 (5)	1.346 (5)	1.365 (5)	0.019
C06–C07	1.388 (6)	1.380 (7)	1.397 (6)	0.017

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**Table s2:**

Covalent bond angles ( $^{\circ}$ ) in the adamantan-1-ammonium cation and the 4-fluorobenzoate anion.

bond	average	minimum	maximum	$\Delta$
N11-C12-C13	109.2 (3)	108.8 (3)	109.5 (3)	0.7
N11-C12-C17	109.2 (3)	108.9 (3)	109.5 (3)	0.6
N11-C12-C18	109.4 (3)	108.5 (3)	110.2 (3)	1.7
C13-C12-C17	109.6 (3)	109.1 (3)	110.2 (3)	1.1
C13-C12-C18	109.6 (2)	109.1 (3)	110.0 (2)	0.9
C17-C12-C18	109.8 (2)	109.4 (2)	110.4 (3)	1.0
C12-C13-C14	109.3 (3)	109.1 (3)	109.6 (3)	0.5
C13-C14-C15	109.8 (3)	109.6 (3)	110.0 (3)	0.4
C13-C14-C21	109.8 (3)	109.4 (3)	110.1 (3)	0.7
C15-C14-C21	109.3 (3)	108.6 (3)	109.7 (3)	1.1
C14-C15-C16	109.1 (3)	108.4 (3)	109.9 (3)	1.5
C15-C16-C17	109.6 (3)	109.4 (3)	109.9 (3)	0.5
C15-C16-C20	109.1 (3)	108.8 (3)	109.3 (3)	0.5
C17-C16-C20	109.7 (3)	109.5 (3)	110.0 (3)	0.5
C12-C18-C19	109.3 (3)	108.8 (3)	109.7 (3)	0.9
C18-C19-C20	109.7 (3)	109.5 (3)	110.1 (3)	0.6
C18-C19-C21	109.4 (3)	109.0 (3)	109.6 (3)	0.6
C20-C19-C21	109.1 (3)	108.4 (3)	109.7 (3)	1.3
C16-C20-C19	109.6 (3)	109.0 (3)	110.0 (3)	1.0
C14-C21-C19	109.5 (3)	109.1 (3)	109.9 (3)	0.8
C02-C01-O09	118.6 (3)	117.0 (3)	119.7 (3)	2.7
C02-C01-O10	116.8 (3)	116.0 (3)	117.7 (3)	1.7
O09-C01-O10	124.7 (3)	123.9 (3)	125.5 (4)	1.6
C01-C02-C03	119.1 (3)	118.1 (3)	119.7 (3)	1.6
C01-C02-C07	122.4 (3)	121.7 (3)	123.1 (3)	1.4
C03-C02-C07	118.5 (3)	117.8 (4)	119.4 (3)	1.6
C02-C03-C04	121.6 (3)	120.9 (3)	122.3 (3)	1.4
C03-C04-C05	118.1 (4)	117.4 (4)	118.9 (4)	1.5
C04-C05-C06	122.6 (4)	121.4 (4)	124.1 (4)	2.7
C04-C05-F08	118.9 (4)	118.1 (4)	119.4 (4)	1.3
C06-C05-F08	118.5 (3)	117.6 (4)	119.4 (3)	1.8
C05-C06-C07	118.5 (4)	117.5 (4)	119.7 (3)	2.2
C02-C07-C06	120.5 (4)	120.1 (4)	120.8 (4)	0.7

**Table s3:**

Equation of best plane  $A \cdot x + B \cdot y + C \cdot z - D = 0$  as function of the phase of the modulation  $t$  for the carboxylate group through atoms C02, O09 and O10 and distances ( $\text{\AA}$ ) of other atoms to this plane.

	A	B	C	D
Reference	8.9921 (36)	0.1206 (38)	-14.3767 (93)	-1.6813 (23)
$t = 0.000$	8.9122	0.1015	-14.5836	-1.7063
0.100	9.0106	0.0485	-14.3338	-1.6275
0.200	9.0902	0.0502	-14.1213	-1.5786
0.300	9.0964	0.1159	-14.0994	-1.6004
0.400	9.0485	0.1769	-14.2205	-1.6576
0.500	9.0068	0.1748	-14.3311	-1.6979
0.600	8.9915	0.1340	-14.3767	-1.7117
0.700	8.9666	0.1175	-14.4431	-1.7238
0.800	8.9132	0.1376	-14.5774	-1.7458
0.900	8.8752	0.1433	-14.6721	-1.7504

	C01
Reference	0.004(1)
$t = 0.000$	0.003
0.100	0.009
0.200	0.007
0.300	-0.001
0.400	-0.003
0.500	0.004
0.600	0.011
0.700	0.008
0.800	0.000
0.900	-0.003

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**Table s4:** Equation of best plane  $A \cdot x + B \cdot y + C \cdot z - D = 0$  as function of the phase of the modulation  $t$  for the fluorophenyl group through atoms C01, C04 and C06 and distances ( $\text{\AA}$ ) of other atoms to this plane.

	A	B	C	D
Reference	9.0418 (28)	0.1916 (60)	-14.2359 (78)	-1.6873 (16)
$t = 0.000$	9.0261	0.2117	-14.2739	-1.6979
0.100	8.7228	-0.8443	-14.7484	-1.3451
0.200	8.4905	-1.2811	-14.9026	-1.1639
0.300	8.6868	-0.9025	-14.7916	-1.3019
0.400	8.9937	-0.1412	-14.3700	-1.5576
0.500	9.1288	0.4570	-13.9206	-1.7323
0.600	9.1446	0.8138	-13.6631	-1.8377
0.700	9.1039	1.1361	-13.4795	-1.9265
0.800	9.0498	1.3559	-13.3709	-1.9778
0.900	9.0586	1.1042	-13.6434	-1.9258

	C02	C03	C05	C07	F08
Reference	0.002(1)	0.006(2)	-0.006(2)	-0.011(2)	-0.007(2)
$t = 0.000$	0.014	0.000	-0.020	-0.009	-0.009
0.100	0.027	0.003	-0.007	0.019	-0.025
0.200	0.030	0.022	0.004	0.029	-0.044
0.300	0.025	0.038	-0.013	0.020	-0.062
0.400	0.019	0.028	-0.037	0.008	-0.057
0.500	0.004	-0.001	-0.031	-0.005	-0.017
0.600	-0.019	-0.019	0.003	-0.024	0.031
0.700	-0.034	-0.014	0.027	-0.047	0.053
0.800	-0.029	0.000	0.018	-0.057	0.040
0.900	-0.007	0.004	-0.007	-0.042	0.013

**Table s5:**

Torsion angles as function of the phase of the modulation  $t$  describing the variation of the molecular conformation of the 4-fluorobenzoate anion.

	O09-C01- -C02-C06	O10-C01- -C02-C04	O09-C01- -C02-C04	O10-C01- -C02-C06
Reference	0.8 (3)	0.7 (2)	181.2 (1)	180.3 (2)
$t = 0.000$	-0.2 (4)	2.6 (3)	183.0 (3)	179.4 (3)
0.100	-10.7 (4)	-5.8 (3)	175.5 (3)	168.0 (3)
0.200	-15.6 (4)	-9.8 (3)	171.2 (3)	163.5 (3)
0.300	-12.6 (4)	-6.7 (3)	173.1 (3)	167.6 (3)
0.400	-5.2 (4)	-0.6 (3)	179.0 (3)	175.2 (3)
0.500	2.6 (4)	3.0 (3)	183.6 (3)	182.0 (3)
0.600	9.5 (4)	3.6 (3)	185.2 (3)	187.9 (3)
0.700	14.2 (4)	5.1 (3)	186.3 (3)	193.0 (3)
0.800	14.6 (4)	8.1 (3)	188.1 (3)	194.7 (3)
0.900	9.6 (4)	8.4 (3)	188.0 (3)	190.1 (3)
Average	0.6 (4)	0.8 (3)	181.2 (3)	180.1 (3)
Minimum	-15.6 (4)	-9.7 (3)	171.2 (2)	163.5 (3)
Maximum	15.1 (4)	8.9 (3)	188.1 (3)	194.7 (3)

## supplementary material

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**Table s6:**

Absolute values of the torsion angles between the fluorophenyl and the carboxylate group, corresponding to O09-C01-C02-C06 and O10-C01-C02-C04, as found *via* a search in the CAMBRIDGE STRUCTURAL DATABASE (CSD) VERSION 5.34, update November 2012 (Allen; 2002). Given are the CSD codes, the temperature (K) and the two torsion angles ( $^{\circ}$ ).

4-fluorobenzoate anion,  $\text{C}_7\text{H}_4\text{FO}_2^-$

EQOQOR	295	16.2 (6)	20.6 (6)	Ji et al. (2010)
FUVCII	295	10.0 (4)	11.3 (4)	Karipides et al. (1988)
ISEHUK	295	7.8 (6)	14.3 (6)	Shi et al. (2011)
OVUMEY	294	4.2 (5)	5.9 (6)	Sridhar and Ravikumar (2011)
EYOXEV	293	17.4 (11)	19.3 (12)	Qu et al. (2004)
IYUZIL	293	2.2 (10)	4.1 (10)	Liu et al. (2004)
UCIWIN	293	1.0 (10)	3.7 (10)	Qu et al. (2005)
OBOTIK	290	6.4 (11)	6.5 (10)	Li et al. (2011)
WABMAP	290	15.9 (6)	21.3 (6)	Zhang et al. (2010)
TAPWIR	180	2.0 (2)	2.0 (2)	Sharma et al. (2005)

4-fluorobenzoate anion,  $\text{C}_7\text{H}_4\text{FO}_2^-$ , “coordinated to metal cation”

FUVCII	295	4.7 (4)	7.8 (4)	Karipides et al. (1988)
ISEHUK	295	17.2 (6)	21.1 (6)	Shi et al. (2011)
OBOTIK	290	9.5 (9)	10.8 (10)	Li et al. (2011)
TAPWIR	180	8.2 (3)	9.5 (3)	Sharma et al. (2005)
TAPWIR	180	13.6 (2)	13.6 (2)	Sharma et al. (2005)
UTUPIJ	123	0.3 (14)	0.9 (15)	Arlin et al. (2011)
UTUPIJ	123	10.4 (16)	11.6 (16)	Arlin et al. (2011)

4-fluorobenzoic acid,  $\text{C}_7\text{H}_5\text{FO}_2$

ISEHUK	295	2.5 (8)	7.2 (8)	Shi et al. (2011)
OVUMEY	294	0.3 (6)	3.9 (6)	Sridhar and Ravikumar (2011)

$R - 4$ -fluorobenzoate,  $R-\text{C}_7\text{H}_4\text{FO}_2$ , “covalently bound to  $R$ ”

DUTPEO	296	1.5 (5)	6.3 (5)	Xu et al. (2010)
HICFII	295	0.9 (10)	7.1 (10)	Shibakami and Sekiya (1995)
YASJEI	294	9.5 (6)	14.7 (6)	Li et al. (2005)
COZCOS	273	1.8 (7)	5.9 (6)	Wan et al. (2008)
YAFROE	273	1.9 (5)	2.6 (5)	Yousuf et al. (2012)
PONVEU	174	1.3 (3)	1.9 (3)	You et al. (2009)

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## supplementary material

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