

# [(Z)-3-Dimethylamino-2-(1,3-dioxo-2,3-dihydro-1H-isoindol-2-yl)allylidene]dimethylammonium hexafluorophosphate

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## Key indicators

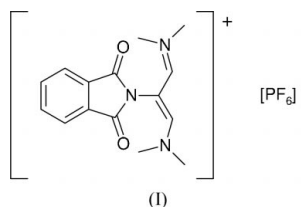
Single-crystal X-ray study  
T = 150 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
Disorder in solvent or counterion  
R factor = 0.045  
wR factor = 0.118  
Data-to-parameter ratio = 20.2

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

At 150 K, the asymmetric unit of the crystal structure of the title compound,  $\text{C}_{15}\text{H}_{18}\text{N}_3\text{O}_2^+\cdot\text{PF}_6^-$ , comprises two molecules. The geometric parameters for the two cations are similar, with the most significant difference being the magnitude of the dihedral angle between the two planar regions of each molecule.

## Comment

The title compound, (I), crystallizes with two molecules in the asymmetric unit (Fig. 1), but the bond lengths and angles for the two cations are very similar, and only cation 1 (Table 1) is discussed in detail below.



For cation 1 (C1–C15), the phthalimide (1,3-dioxo-2,3-dihydro-1H-isoindole) group is close to planar, the largest deviation from the least-squares plane being 0.047 (2) Å for atom C14. Similarly, the conjugated cationic 1,3-bis(dimethylamino)trimethinium group is planar, the largest deviation from the least-squares-plane being 0.109 (2) Å for the terminal methyl group C7. The most significant difference between the two cations is the magnitude of the dihedral angle between these two planar groups: 86.06 (4) and 83.29 (4)° for cations 1 and 2, respectively. The approximate symmetry of the bond distances in the trimethinium group, along with its planarity, confirm the delocalization of the positive charge over both N atoms. The  $[\text{PF}_6]^-$  anions occupy channels in the structure parallel to the crystallographic *a* axis (Fig. 2). Anion 2 (P2, *etc.*) is disordered over two orientations, with an occupancy ratio of 0.883 (2):0.117 (2).

## Experimental

The title compound, (I), was prepared according to the method of Davies *et al.* (2000). Suitable crystals were grown by recrystallization from methanol.

### Crystal data

$\text{C}_{15}\text{H}_{18}\text{N}_3\text{O}_2^+\cdot\text{F}_6\text{P}^-$   
 $M_r = 417.29$   
Triclinic,  $P\bar{1}$   
 $a = 9.2929$  (9) Å  
 $b = 10.8379$  (11) Å  
 $c = 18.7453$  (19) Å  
 $\alpha = 85.696$  (8)°  
 $\beta = 84.306$  (8)°  
 $\gamma = 83.175$  (8)°  
 $V = 1861.5$  (3) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.489$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 19784  
reflections  
 $\theta = 1.9\text{--}29.7^\circ$   
 $\mu = 0.22$  mm<sup>-1</sup>  
 $T = 150$  (2) K  
Lath, yellow  
0.60 × 0.25 × 0.10 mm

## Data collection

Stoe IPDS-II area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: none  
 41451 measured reflections  
 10507 independent reflections

5375 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.064$   
 $\theta_{\text{max}} = 29.7^\circ$   
 $h = -11 \rightarrow 12$   
 $k = -15 \rightarrow 15$   
 $l = -26 \rightarrow 26$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.118$   
 $S = 0.81$   
 10507 reflections  
 521 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.009$   
 $\Delta\rho_{\text{max}} = 0.52 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.36 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.0073 (7)

Table 1

 Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O1—C8	1.205 (2)	N2—C2	1.313 (2)
O2—C9	1.204 (2)	N3—C3	1.304 (2)
N1—C8	1.406 (2)	C1—C2	1.397 (3)
N1—C9	1.413 (2)	C1—C3	1.406 (2)
N1—C1	1.421 (2)		
C8—N1—C9	111.69 (13)	C2—C1—N1	123.21 (16)
C8—N1—C1	124.06 (14)	C3—C1—N1	122.30 (16)
C9—N1—C1	124.07 (14)	N2—C2—C1	131.96 (16)
C2—C1—C3	114.43 (15)	N3—C3—C1	131.78 (16)
C8—N1—C1—C2	98.2 (2)	C28—N21—C21—C23	-101.8 (2)
C9—N1—C1—C2	-86.9 (2)	C29—N21—C21—C23	83.2 (2)
C8—N1—C1—C3	-84.7 (2)	C28—N21—C21—C22	81.3 (2)
C9—N1—C1—C3	90.1 (2)	C29—N21—C21—C22	-93.6 (2)
C3—C1—C2—N2	-176.71 (19)	C23—C21—C22—N22	-177.07 (19)
N1—C1—C2—N2	0.6 (3)	N21—C21—C22—N22	0.0 (3)
C2—C1—C3—N3	178.06 (19)	C22—C21—C23—N23	178.97 (19)
N1—C1—C3—N3	0.8 (3)	N21—C21—C23—N23	1.9 (3)

All H atoms were initially located in a difference Fourier map. All C—H atoms were then placed in geometrically idealized positions, with C—H distances of 0.95–0.98  $\text{\AA}$  and  $U_{\text{iso}}(\text{H})$  values set at  $1.2U_{\text{eq}}(\text{C})$ .

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2001); program(s) used to solve structure: *X-STEP32* (Stoe & Cie, 2001) and *WinGX* (Farrugia, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX*.

## References

Davies, I. W., Marcoux, J. F., Wu, J., Palucki, M., Corley, E. G., Robbins, M. A., Tsou, N., Ball, R. G., Dormer, P., Larsen, R. D. & Reider, P. J. (2000). *J. Org. Chem.* **65**, 4571–4574.

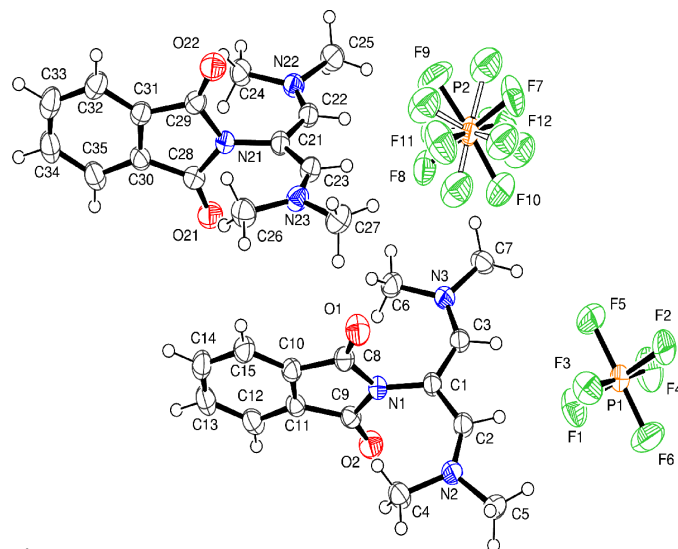


Figure 1

View of the asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size. Both disorder components are shown; the F-atom labels of the minor component (hollow bonds) have been omitted for clarity.

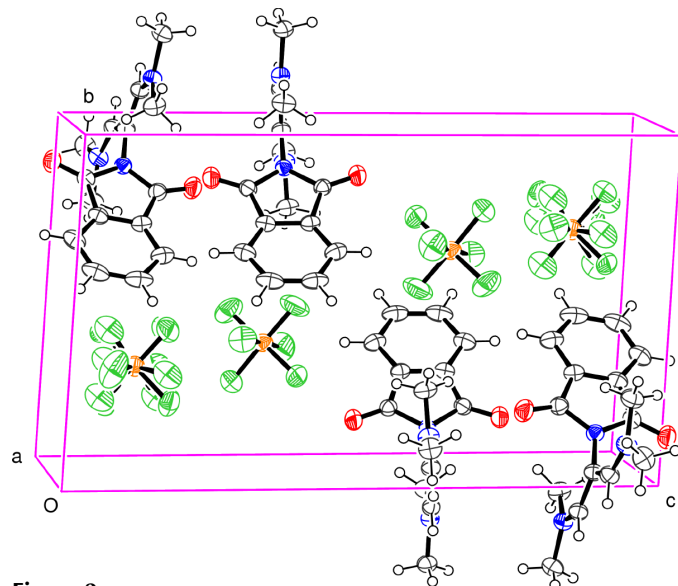


Figure 2

The packing of (I).

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