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Supplementary Information:

Influence of lattice dynamics on charge transport in dianthra[2,3-b:2',3'-f]-thieno[3,2-b]thiophene organic crystal from a theoretical study

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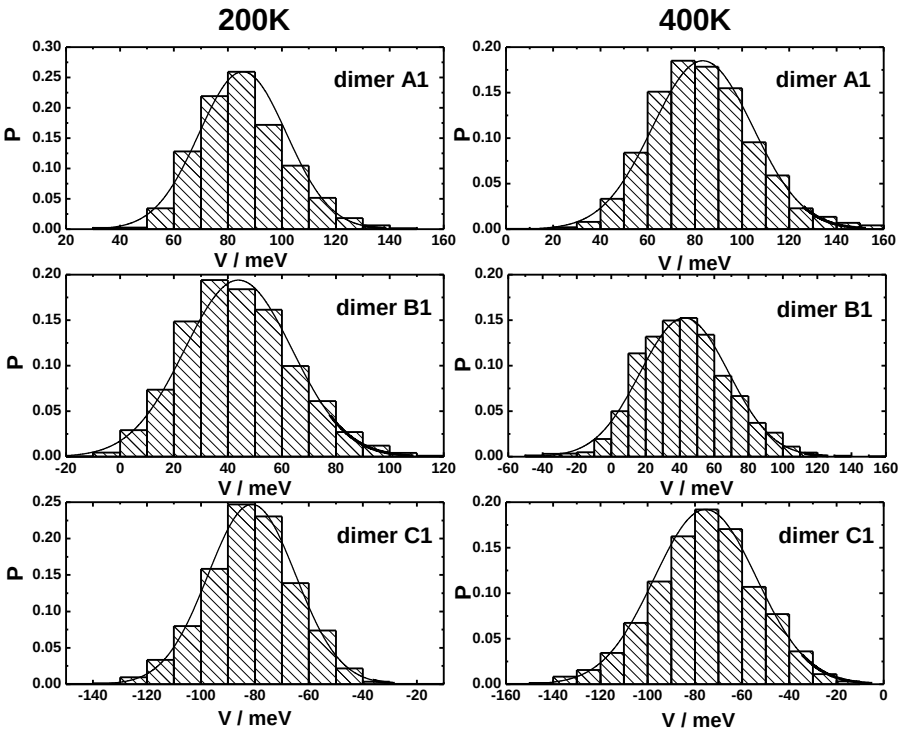

Figure S1. The normalized probability distributions of transfer integrals for nearest-neighboring dimers A1, B1 and C1 in the *ab* plane of DATT at 200K and 400K.

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Table S1. The intermolecular distances (R_0) and the transfer integrals (V_0) with the equilibrium geometry at the COMPASS molecular mechanics level for the nearest-neighboring dimers of pentacene in Fig. 1(b).

Dimers	R_0 (Å)	V_0 (meV)
A1	6.239	35.6
A2	6.239	35.5
B1	4.689	90.8
B2	4.689	90.8
C1	5.160	-51.7
C2	5.160	-51.7