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# Crystal growth, structure, and transport properties of the charge-transfer salt picene/2,3,5,6-tetrafluor--7,7,8,8-tetracyanoquinodimethane

Mahns B., Kataeva O., Islamov D., Hampel S., Steckel F., Hess C., Knupfer M., Büchner B., Himcinschi C., Hahn T., Renger R., Kortus J.
*Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

## Abstract

Single crystals of the charge-transfer salt picene/2,3,5,6-tetrafluoro-7,7, 8,8-tetracyanoquinodimethane have been grown using physical vapor transport. The crystal structure was determined using single-crystal X-ray diffraction. It was found that the crystals grow in a 1:1 molecular ratio and adopt a monoclinic structure with alternate stacking. Both X-ray data and Raman measurements show that the grown crystals are of good quality. From structure and infrared data, the charge transfer between acceptor and donor molecules was estimated to be approximately 0.14-0.19 electron. Transport measurements indicate a nonmetallic ground state with an activation energy of 0.6 eV. The supporting density functional theory calculations on molecular model systems as well as on crystalline structures confirm the amount of charge transfer and provide first insights into the electronic structure of the new material. 

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