Supplementary materials

Responses for the Checkcif level A Alerts:

Compound 1

_vrf_PLAT430_ALERT_2_A

Problem: Short Inter D...A Contact S11 ... S26 ... 2.87 Ang.

Response: The S11 and S26 atoms do not correspond the same part of the disordered ET molecule. ALERT is generated because S11 belongs to both parts of the disordered molecule. As carbon atoms of the lower fraction of the twin generated disorder cannot be placed, the S26 S11 short distance is considered as intermolecular contact instead of intra-molecular one.

Compound 2

_vrf_REFLT03_ALERT_3_A

Problem: Reflection count <85% complete (theta max?)
From the CIF: _diffrn_reflns_theta_max 23.35
From the CIF: _diffrn_reflns_theta_full 23.35
From the CIF: _reflns_number_total 3379
TEST2: Reflns within _diffrn_reflns_theta_max
Count of symmetry unique reflns 4995
Completeness (_total/calc) 67.65%.

Response: The low quality and size of the single crystal of this compound did not allow the collection of enough observed data for precise refinements.

_vrf_RFACR01_ALERT_3_A

Problem: The value of the weighted R factor is 0.45; Weighted R factor given 0.474.

Response: The low quality and size of the single crystal of this compound did not allow the collection of enough observed data for precise refinements.

_vrf_PLAT022_ALERT_3_A

Problem: Ratio Unique/Expected Reflections (too) Low ... 0.676.

Response: The low quality and size of the single crystal of this compound did not allow the collection of enough observed data for precise refinements.

_vrf_PLAT029_ALERT_3_A

Problem: _diffrn_measured_fraction_theta_full Low ... 0.676.
Response: The low quality and size of the single crystal of this compound did not allow the collection of enough observed data for precise refinements.

_vrf_PLAT084_ALERT_2_A

Problem: High wR2 Value ... 0.47.

Response: The low quality and size of the single crystal of this compound did not allow the collection of enough observed data for precise refinements.

_vrf_PLAT201_ALERT_2_A

Problem: Isotropic non-H Atoms in Main Residue(s) ... 26.

Response: The crystal structure of this compound have been determined and refined with an anisotropic/isotropic mixed model in order to reduce the number of parameters as the number of observed data was too low.

_vrf_PLAT241_ALERT_2_A

Problem: Check High Ueq as Compared to Neighbors for S7A.

Problem: Check High Ueq as Compared to Neighbors for C8A.

Response: These atoms correspond to a disordered region of the ET molecule (see isostructural compound 1) that has not been solved due to the poor quality of the data.

Compound 3

_vrf_REFLT03_ALERT_3_A

Problem: Reflection count <85% complete (theta max?)

From the CIF: _diffrn_reflns_theta_max 31.78

From the CIF: _diffrn_reflns_theta_full 31.78

From the CIF: _reflns_number_total 42071

TEST2: Reflns within _diffrn_reflns_theta_max

Count of symmetry unique reflns 51928

Completeness (_total/calc) 81.02%.

Response: The low quality and size of the single crystal of this compound did not allow the collection of enough observed data for precise refinements.

_vrf_PLAT026_ALERT_3_A

Problem: Ratio Observed/Unique Reflections too Low ... 10 Perc.

Response: The low quality and size of the single crystal of this compound did not allow the collection of enough observed data for precise refinements.

_vrf_PLAT029_ALERT_3_A

Problem: _diffrn_measured_fraction_theta_full Low ... 0.810.

Response: The low quality and size of the single crystal of this compound did not allow the collection of enough observed data for precise refinements

_vrf_PLAT201_ALERT_2_A

Problem: Isotropic non-H Atoms in Main Residue(s) ... 116.

Response: The crystal structure of this compound have been determined and refined with an anisotropic/isotropic mixed model in order to reduce the number of parameters as the number of observed data was too low.

_vrf_PLAT312_ALERT_2_A

Problem: Strange C-O-H Geometry (C-O .LT. 1.25 Ang) ... O2.

Response: O2 anisotropic displacement parameters show a strong elongation along one direction suggesting a 2 positions disorder that could not been solved due to the poor quality of the data.

_vrf_PLAT360_ALERT_2_A

Problem: Short C(sp3)-C(sp3) Bond C38–C39 ... 1.23 Ang.

Response: These atoms correspond to a disordered region of the tcnoetOH anion that could not been solved due to the poor quality of the data.