**Synthesis, X-ray analysis and computational studies of two novel thiophene derivatives**

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|  |  |
| --- | --- |
|  |  |
| **Compound 8** | **Compound 7** |

**Fig. S1.** Optimized structures of compounds **7** and **8**.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  |  |  |  |
|  |  |  |  | **A** |
|  |  |  |  | **B** |
|  |  |  |  | **C** |
|  | **7** |  | **8** |  |

**Fig. S2.** Hirshfeld surfaces of compounds **7** and **8** mapped over A) dnorm, B) curvedness and C) shape index.

**Table S1. The crystal and experimental data of compounds 7** and **8**

|  |  |  |
| --- | --- | --- |
| **Crystal data** | **7** | **8** |
| Chemical formula | [C11H14O3S2](file:///C:\Users\ygaber\Downloads\a%20_chemical_formula_sum) | [C14H19NO3S2](file:///C:\Users\ygaber\Downloads\a_a%20_chemical_formula_sum) |
| *M*r | [258.34](file:///C:\Users\ygaber\Downloads\a%20_chemical_formula_weight) | [313.42](file:///C:\Users\ygaber\Downloads\a_a%20_chemical_formula_weight) |
| Crystal system, space group | [Monoclinic](file:///C:\Users\ygaber\Downloads\a%20_symmetry_cell_setting), [*P*21/*c*](file:///C:\Users\ygaber\Downloads\a%20_symmetry_space_group_name_H-M) | [Triclinic](file:///C:\Users\ygaber\Downloads\a_a%20_symmetry_cell_setting), [*P*](file:///C:\Users\ygaber\Downloads\a_a%20_symmetry_space_group_name_H-M)-1 |
| Temperature (K) | [296](file:///C:\Users\ygaber\Downloads\a%20_cell_measurement_temperature) | [296](file:///C:\Users\ygaber\Downloads\a_a%20_cell_measurement_temperature) |
| *a*, *b*, *c* (Å) | [5.6444 (2)](file:///C:\Users\ygaber\Downloads\a%20_cell_length_a), [26.9651 (8)](file:///C:\Users\ygaber\Downloads\a%20_cell_length_b), [8.0007 (2)](file:///C:\Users\ygaber\Downloads\a%20_cell_length_c) | [8.5051 (4)](file:///C:\Users\ygaber\Downloads\a_a%20_cell_length_a), [8.7406 (4)](file:///C:\Users\ygaber\Downloads\a_a%20_cell_length_b), [11.4925 (5)](file:///C:\Users\ygaber\Downloads\a_a%20_cell_length_c) |
| α, β, γ (°) | 90.0, [104.973 (1)](file:///C:\Users\ygaber\Downloads\a%20_cell_angle_beta), 90.0 | [77.363 (1)](file:///C:\Users\ygaber\Downloads\a_a%20_cell_angle_alpha), [68.514 (1)](file:///C:\Users\ygaber\Downloads\a_a%20_cell_angle_beta), [73.415 (2)](file:///C:\Users\ygaber\Downloads\a_a%20_cell_angle_gamma) |
| V (Å3) | [1176.38 (6)](file:///C:\Users\ygaber\Downloads\a%20_cell_volume) | [755.63 (6)](file:///C:\Users\ygaber\Downloads\a_a%20_cell_volume) |
| *Z* | [4](file:///C:\Users\ygaber\Downloads\a%20_cell_formula_units_Z) | [2](file:///C:\Users\ygaber\Downloads\a_a%20_cell_formula_units_Z) |
| Radiation type | [Mo *K*α](file:///C:\Users\ygaber\Downloads\a%20_diffrn_radiation_type) | [Mo *K*α](file:///C:\Users\ygaber\Downloads\a_a%20_diffrn_radiation_type) |
| µ (mm−1) | [0.44](file:///C:\Users\ygaber\Downloads\a%20_exptl_absorpt_coefficient_mu) | [0.36](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_absorpt_coefficient_mu) |
| Crystal size (mm) | [0.69](file:///C:\Users\ygaber\Downloads\a%20_exptl_crystal_size_max) × [0.21](file:///C:\Users\ygaber\Downloads\a%20_exptl_crystal_size_mid) × [0.18](file:///C:\Users\ygaber\Downloads\a%20_exptl_crystal_size_min) | [0.70](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_crystal_size_max) × [0.51](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_crystal_size_mid) × [0.19](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_crystal_size_min) |
| **Data collection** | | |
| Diffractometer | [Bruker APEX-II D8 venture  diffractometer](file:///C:\Users\ygaber\Downloads\a_a%20_diffrn_measurement_device_type) | [Bruker APEX-II D8 venture  diffractometer](file:///C:\Users\ygaber\Downloads\a_a%20_diffrn_measurement_device_type) |
| Absorption correction | [Multi-scan](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_absorpt_correction_type) [SADABS Bruker 2014](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_absorpt_process_details) | [Multi-scan](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_absorpt_correction_type) [SADABS Bruker 2014](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_absorpt_process_details) |
| Tmin, Tmax | [0.751](file:///C:\Users\ygaber\Downloads\a%20_exptl_absorpt_correction_T_min), [0.923](file:///C:\Users\ygaber\Downloads\a%20_exptl_absorpt_correction_T_max) | [0.788](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_absorpt_correction_T_min), [0.936](file:///C:\Users\ygaber\Downloads\a_a%20_exptl_absorpt_correction_T_max) |
| No. of measured, independent and observed [[I](file:///C:\Users\ygaber\Downloads\a_a%20_reflns_threshold_expression) [> 2σ(I)](file:///C:\Users\ygaber\Downloads\a_a%20_reflns_threshold_expression)] reflections | [37967](file:///C:\Users\ygaber\Downloads\a%20_diffrn_reflns_number), [4491](file:///C:\Users\ygaber\Downloads\a%20_reflns_number_total), [4016](file:///C:\Users\ygaber\Downloads\a%20_reflns_number_gt) | [11701](file:///C:\Users\ygaber\Downloads\a_a%20_diffrn_reflns_number), [2658](file:///C:\Users\ygaber\Downloads\a_a%20_reflns_number_total), [2367](file:///C:\Users\ygaber\Downloads\a_a%20_reflns_number_gt) |
| Rint | [0.030](file:///C:\Users\ygaber\Downloads\a%20_diffrn_reflns_av_R_equivalents) | [0.071](file:///C:\Users\ygaber\Downloads\a_a%20_diffrn_reflns_av_R_equivalents) |
| **Refinement** | | |
| R[*F2*> 2σ( *F2*)], wR( *F2*), S | [0.028](file:///C:\Users\ygaber\Downloads\a%20_refine_ls_R_factor_gt), [0.072](file:///C:\Users\ygaber\Downloads\a%20_refine_ls_wR_factor_ref), [1.04](file:///C:\Users\ygaber\Downloads\a%20_refine_ls_goodness_of_fit_ref) | [0.080](file:///C:\Users\ygaber\Downloads\a_a%20_refine_ls_R_factor_gt), [0.223](file:///C:\Users\ygaber\Downloads\a_a%20_refine_ls_wR_factor_ref), [1.15](file:///C:\Users\ygaber\Downloads\a_a%20_refine_ls_goodness_of_fit_ref) |
| No. of reflections | [4491](file:///C:\Users\ygaber\Downloads\a%20_refine_ls_number_reflns) | [2658](file:///C:\Users\ygaber\Downloads\a_a%20_refine_ls_number_reflns) |
| No. of parameters | [148](file:///C:\Users\ygaber\Downloads\a%20_refine_ls_number_parameters) | [176](file:///C:\Users\ygaber\Downloads\a_a%20_refine_ls_number_parameters) |
| H-atom treatment | [H atoms treated by a mixture of independent and constrained refinement](file:///C:\Users\ygaber\Downloads\a%20_refine_ls_hydrogen_treatment) | [H atoms treated by a mixture of independent and constrained refinement](file:///C:\Users\ygaber\Downloads\a_a%20_refine_ls_hydrogen_treatment) |
| Δρmax, Δρmin (e Å−3) | [0.45](file:///C:\Users\ygaber\Downloads\a%20_refine_diff_density_max), [−0.35](file:///C:\Users\ygaber\Downloads\a%20_refine_diff_density_min) | [0.96](file:///C:\Users\ygaber\Downloads\a_a%20_refine_diff_density_max), [−1.33](file:///C:\Users\ygaber\Downloads\a_a%20_refine_diff_density_min) |
| CCDC number | 1551320 | 1555388 |

**Table S2.** Experimental and calculated geometric parameters (Å, º) of compounds **7** and **8**.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compound 8** | **Calc** | **exp** | **Compound 7** | **calc** | **exp** |
| R(1-17) | 1.783 | 1.765 | R(1-6) | 1.740 | 1.722 |
| R(1-23) | 1.778 | 1.762 | R(1-10) | 1.745 | 1.724 |
| R(2-23) | 1.744 | 1.721 | R(2-10) | 1.763 | 1.747 |
| R(2-26) | 1.740 | 1.724 | R(2-23) | 1.835 | 1.809 |
| R(3-18) | 1.229 | 1.231 | R(3-15) | 1.221 | 1.219 |
| R(4-32) | 1.219 | 1.209 | R(4-15) | 1.354 | 1.341 |
| R(5-32) | 1.356 | 1.349 | R(4-16) | 1.446 | 1.453 |
| R(5-33) | 1.445 | 1.446 | R(5-26) | 1.214 | 1.217 |
| R(6-7) | 1.461 | 1.471 | R(6-8) | 1.363 | 1.362 |
| R(6-11) | 1.460 | 1.464 | R(8-9) | 1.450 | 1.447 |
| R(6-15) | 1.344 | 1.319 | R(8-11) | 1.506 | 1.502 |
| R(15-17) | 1.380 | 1.378 | R(9-10) | 1.393 | 1.392 |
| R(17-18) | 1.491 | 1.470 | R(9-15) | 1.470 | 1.467 |
| R(18-19) | 1.519 | 1.505 | R(16-19) | 1.516 | 1.505 |
| R(23-24) | 1.391 | 1.395 | R(23-26) | 1.526 | 1.510 |
| R(24-25) | 1.452 | 1.445 | R(26-27) | 1.517 | 1.503 |
| R(24-32) | 1.474 | 1.465 | A(6-1-10) | 91.8 | 92.1 |
| R(25-26) | 1.363 | 1.358 | A(1-6-8) | 112.8 | 113.0 |
| R(25-28) | 1.505 | 1.503 | A(1-10-2) | 123.6 | 122.9 |
| R(33-36) | 1.516 | 1.505 | A(1-10-9) | 110.5 | 110.8 |
| R(3-16) | 2.190 | 2.264 | A(10-2-23) | 99.5 | 99.7 |
| A(17-1-23) | 103.1 | 102.3 | A(2-10-9) | 125.9 | 126.3 |
| A(1-17-15) | 125.2 | 124.2 | A(2-23-26) | 109.6 | 110.0 |
| A(1-17-18) | 119.8 | 120.1 | A(3-15-4) | 122.4 | 122.9 |
| A(1-23-2) | 120.1 | 119.8 | A(3-15-9) | 123.7 | 123.6 |
| A(1-23-24) | 128.9 | 129.0 | A(15-4-16) | 115.4 | 115.6 |
| A(23-2-26) | 91.4 | 91.7 | A(4-15-9) | 113.9 | 113.5 |
| A(2-23-24) | 111.0 | 111.2 | A(4-16-19) | 107.6 | 107.0 |
| A(2-26-25) | 113.1 | 113.3 | A(5-26-23) | 121.9 | 121.6 |
| A(3-18-17) | 121.2 | 121.7 | A(5-26-27) | 122.4 | 123.3 |
| A(3-18-19) | 119.8 | 118.8 | A(6-8-9) | 111.7 | 111.3 |
| A(4-32-5) | 122.3 | 122.9 | A(6-8-11) | 122.0 | 122.2 |
| A(4-32-24) | 125.1 | 125.0 | A(9-8-11) | 126.3 | 126.5 |
| A(32-5-33) | 115.8 | 115.0 | A(8-9-10) | 113.2 | 112.8 |
| A(5-32-24) | 112.5 | 112.1 | A(8-9-15) | 127.5 | 127.5 |
| A(5-33-36) | 107.8 | 107.7 | A(10-9-15) | 119.3 | 119.6 |
| A(7-6-11) | 115.2 | 114.6 | A(23-26-27) | 115.8 | 115.1 |
| A(7-6-15) | 125.3 | 125.3 |  |  |  |
| A(11-6-15) | 119.3 | 120.1 |  |  |  |
| A(6-15-17) | 134.3 | 133.9 |  |  |  |
| A(15-17-18) | 114.4 | 115.3 |  |  |  |
| A(17-18-19) | 118.9 | 119.5 |  |  |  |
| A(23-24-25) | 112.9 | 112.4 |  |  |  |
| A(23-24-32) | 125.5 | 124.8 |  |  |  |
| A(25-24-32) | 121.6 | 122.8 |  |  |  |
| A(24-25-26) | 111.6 | 111.3 |  |  |  |
| A(24-25-28) | 125.5 | 125.7 |  |  |  |
| A(26-25-28) | 122.9 | 122.9 |  |  |  |

**XYZ coordinates of the optimized geometry of 7**

S 0.888819000 2.240770000 0.000291000

S 1.442959000 -0.799663000 -0.000014000

O -1.106528000 -1.852519000 -0.000201000

O -3.059846000 -0.719537000 -0.000313000

O 3.987499000 -2.122314000 0.000190000

C -0.747498000 2.831682000 0.000216000

H -0.927271000 3.897802000 0.000214000

C -1.671494000 1.830022000 -0.000169000

C -1.043680000 0.522502000 -0.000245000

C 0.348086000 0.582179000 -0.000045000

C -3.150937000 2.109060000 -0.000394000

H -3.329055000 3.187725000 -0.001213000

H -3.639572000 1.676245000 0.876785000

H -3.639591000 1.674785000 -0.876747000

C -1.707322000 -0.789281000 -0.000258000

C -3.746456000 -1.992484000 -0.000239000

H -3.435191000 -2.561791000 0.880981000

H -3.436362000 -2.561248000 -0.882234000

C -5.236271000 -1.709539000 0.000795000

H -5.790883000 -2.652973000 0.000383000

H -5.529018000 -1.139752000 -0.885816000

H -5.528075000 -1.141058000 0.888549000

C 3.050487000 0.086248000 0.000019000

H 3.145877000 0.731478000 -0.882141000

H 3.145949000 0.731326000 0.882298000

C 4.192176000 -0.926009000 -0.000008000

C 5.592048000 -0.340986000 -0.000120000

H 6.322674000 -1.150538000 -0.000964000

H 5.744388000 0.291689000 0.881572000

H 5.743835000 0.293197000 -0.880806000

**XYZ coordinates of the optimized geometry of 8**

S 0.431191000 0.882713000 0.327294000

S 0.337692000 -2.150637000 0.014733000

O 3.689771000 -0.341203000 2.254218000

O -4.054842000 0.152895000 -0.289250000

O -2.292114000 1.532183000 -0.000865000

N 3.150573000 0.442112000 -1.649215000

C 1.995497000 0.671275000 -2.514160000

H 2.265723000 0.373343000 -3.530658000

H 1.696115000 1.725263000 -2.525396000

H 1.148319000 0.071090000 -2.188277000

C 4.449311000 0.531950000 -2.310379000

H 4.616779000 1.539742000 -2.711326000

H 4.504808000 -0.181323000 -3.140336000

H 5.245343000 0.306569000 -1.599960000

C 3.099995000 0.267111000 -0.317498000

H 4.066434000 0.041883000 0.131095000

C 2.088364000 0.293182000 0.620511000

C 2.529467000 -0.017018000 2.010995000

C 1.519678000 0.080617000 3.141636000

H 1.135014000 1.100748000 3.239288000

H 2.015713000 -0.215342000 4.066488000

H 0.656425000 -0.567642000 2.961689000

C -0.488619000 -0.615557000 0.065239000

C -1.856434000 -0.778483000 -0.128931000

C -2.238072000 -2.167074000 -0.315420000

C -1.158289000 -2.996281000 -0.259932000

H -1.149630000 -4.072999000 -0.360423000

C -3.639235000 -2.665647000 -0.543172000

H -4.297253000 -2.398837000 0.287931000

H -3.636141000 -3.753379000 -0.657208000

H -4.082093000 -2.218085000 -1.436978000

C -2.853676000 0.306964000 -0.150843000

C -3.210376000 2.648015000 0.005562000

H -3.948095000 2.492323000 0.798716000

H -3.752281000 2.663090000 -0.945402000

C -2.401032000 3.912125000 0.220593000

H -3.068404000 4.779626000 0.230715000

H -1.668584000 4.050584000 -0.579611000

H -1.866332000 3.877261000 1.173698000