STRUCTURAL CHEMISTRY

Volume 77 (2021)

Supporting information for article:

Crystal structure refinements of stoichiometric Ni3Se2 and NiSe

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Tables for deposit data

Deposit data 1. Chemical composition and average of measured points in Ni_3Se_2 and NiSe.

Ni_3Se_2	Ni	Se	Total
	52.53	47.36	99.89
	52.74	48.24	100.99
	52.19	47.28	99.46
	52.59	47.82	100.41
	52.31	46.87	99.18
	52.61	47.99	100.60
	52.67	46.93	99.61
	52.50	47.59	100.09
	52.45	47.41	99.86
	52.38	46.97	99.35
	52.09	46.95	99.04
	51.90	47.14	99.05
Average	52.41	47.38	99.79
S.D.	0.25	0.45	0.63

NiSe	Ni	Se	Total
	42.57	58.41	100.98
	42.50	57.92	100.41
	42.60	58.09	100.68
	42.62	57.74	100.36
	42.05	57.56	99.61
	42.06	57.54	99.60
	42.64	58.22	100.86
	42.63	56.97	99.60
	42.64	57.93	100.57
	42.21	56.92	99.13
	41.95	57.54	99.49
	42.00	57.29	99.28
Average	42.37	57.67	100.05
S.D.	0.29	0.47	0.66

****

Deposit data 2.

CifFile: CIF data for a sample with another enantiomorph different from the Ni_3Se_2 sample in the text

```
data_shelx

_audit_creation_method                  'SHELXL-2018/3'
_shelx_SHELXL_version_number            '2018/3'
_chemical_name_systematic               ?
_chemical_name_common                   ?
_chemical_melting_point                 ?
_chemical_formula_moiety                'Ni3 Se2'
_chemical_formula_sum                   'Ni3 Se2'
_chemical_formula_weight                334.05

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'Ni'   'Ni'    0.3393    1.1124
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Se'   'Se'   -0.0929    2.2259
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting                  hexagonal
_space_group_IT_number                  155
_space_group_name_H-M_alt               'R 3 2 :H'
_space_group_name_Hall                  'R 3 2"'

_shelx_space_group_comment
;
The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
;

loop_
 _space_group_symop_operation_xyz
 'x, y, z'
 '-y, x-y, z'
 '-x+y, -x, z'
 'x-y, -y, -z'
 '-x, -x+y, -z'
 'y, x, -z'
 'x+2/3, y+1/3, z+1/3'
 '-y+2/3, x-y+1/3, z+1/3'
 '-x+y+2/3, -x+1/3, z+1/3'
```

```
 'x-y+2/3, -y+1/3, -z+1/3'
 '-x+2/3, -x+y+1/3, -z+1/3'
 'y+2/3, x+1/3, -z+1/3'
 'x+1/3, y+2/3, z+2/3'
 '-y+1/3, x-y+2/3, z+2/3'
 '-x+y+1/3, -x+2/3, z+2/3'
 'x-y+1/3, -y+2/3, -z+2/3'
 '-x+1/3, -x+y+2/3, -z+2/3'
 'y+1/3, x+2/3, -z+2/3'

_cell_length_a                    6.0286(4)
_cell_length_b                    6.0286(4)
_cell_length_c                    7.2500(5)
_cell_angle_alpha                 90
_cell_angle_beta                  90
_cell_angle_gamma                   120
_cell_volume                      228.19(3)
_cell_formula_units_Z             3
_cell_measurement_temperature     293(2)
_cell_measurement_reflns_used     958
_cell_measurement_theta_min       4.7880
_cell_measurement_theta_max       26.7610

_exptl_crystal_description        block
_exptl_crystal_colour               black
_exptl_crystal_density_meas       ?
_exptl_crystal_density_method     ?
_exptl_crystal_density_diffrn     7.293
_exptl_crystal_F_000                456
_exptl_crystal_size_max           0.142
_exptl_crystal_size_mid           0.058
_exptl_crystal_size_min           0.041
_exptl_absorpt_coefficient_mu     41.978
_exptl_absorpt_correction_type    gaussian
_exptl_absorpt_correction_T_min   0.052
_exptl_absorpt_correction_T_max   0.324
_exptl_absorpt_process_details
;
CrysAlisPro 1.171.40.53 (Rigaku Oxford Diffraction, 2019)
Numerical absorption correction based on gaussian integration over
                            a multifaceted crystal model
Empirical absorption correction using spherical harmonics,
  implemented in SCALE3 ABSPACK scaling algorithm.
;
_diffrn_ambient_temperature       293(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_source                      ?
_diffrn_measurement_device_type   'SuperNova, Single source at offset/far, HyPix3000'
_diffrn_measurement_method          '\w scans'
_diffrn_detector_area_resol_mean  10.0000
_diffrn_reflns_number               982
_diffrn_reflns_av_unetI/netI      0.0174
_diffrn_reflns_av_R_equivalents   0.0370
_diffrn_reflns_limit_h_min        -7
_diffrn_reflns_limit_h_max        7
_diffrn_reflns_limit_k_min        -7
```

```
_diffrn_reflns_limit_k_max              7
_diffrn_reflns_limit_l_min             -8
_diffrn_reflns_limit_l_max              9
_diffrn_reflns_theta_min                4.812
_diffrn_reflns_theta_max                26.730
_diffrn_reflns_theta_full               25.242
_diffrn_measured_fraction_theta_max     1.000
_diffrn_measured_fraction_theta_full    1.000
_diffrn_reflns_Laue_measured_fraction_max       1.000
_diffrn_reflns_Laue_measured_fraction_full      1.000
_diffrn_reflns_point_group_measured_fraction_max      0.991
_diffrn_reflns_point_group_measured_fraction_full     1.000
_reflns_number_total                    113
_reflns_number_gt                       110
_reflns_threshold_expression            'I > 2\s(I)'
_reflns_Friedel_coverage                0.548
_reflns_Friedel_fraction_max            0.976
_reflns_Friedel_fraction_full           1.000

_reflns_special_details
;
 Reflections were merged by SHELXL according to the crystal
 class for the calculation of statistics and refinement.

 _reflns_Friedel_fraction is defined as the number of unique
 Friedel pairs measured divided by the number that would be
 possible theoretically, ignoring centric projections and
 systematic absences.
;

_computing_data_collection              'CrysAlisPro 1.171.40.53 (Rigaku OD, 2019)'
_computing_cell_refinement              'CrysAlisPro 1.171.40.53 (Rigaku OD, 2019)'
_computing_data_reduction               'CrysAlisPro 1.171.40.53 (Rigaku OD, 2019)'
_computing_structure_solution           '<i>Olex2</i> (Dolomanov <i>et al.</i>, 2009) and SHELXL-2018/3
(Sheldrick, 2018)'
_computing_structure_refinement         'SHELXL-2018/3 (Sheldrick, 2018)'
_computing_molecular_graphics           ?
_computing_publication_material         ?
_refine_ls_structure_factor_coef        Fsqd
_refine_ls_matrix_type                  full
_refine_ls_weighting_scheme             calc
_refine_ls_weighting_details
'w=1/[\s^2^(Fo^2^)+(0.0234P)^2^] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_hydrogens          .
_refine_ls_hydrogen_treatment           undef
_refine_ls_extinction_method            none
_refine_ls_extinction_coef              .
_refine_ls_abs_structure_details
;
 Flack x determined using 39 quotients [(I+)-(I-)]/[(I+)+(I-)]
 (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
;
_refine_ls_abs_structure_Flack          -0.05(5)
_refine_ls_number_reflns                113
_refine_ls_number_parameters            9
_refine_ls_number_restraints            0
_refine_ls_R_factor_all                 0.0159
```

```
_refine_ls_R_factor_gt                 0.0156
_refine_ls_wR_factor_ref               0.0397
_refine_ls_wR_factor_gt                0.0396
_refine_ls_goodness_of_fit_ref         1.210
_refine_ls_restrained_S_all            1.210
_refine_ls_shift/su_max                0.000
_refine_ls_shift/su_mean               0.000

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_site_symmetry_order
  _atom_site_calc_flag
  _atom_site_refinement_flags_posn
  _atom_site_refinement_flags_adp
  _atom_site_refinement_flags_occupancy
  _atom_site_disorder_assembly
  _atom_site_disorder_group
Se1 Se 0.000000 0.000000 0.26014(11) 0.0086(3) Uani 1 3 d S T P . .
Ni2 Ni 0.24705(19) 0.000000 0.000000 0.0095(3) Uani 1 2 d S T P . .

loop_
  _atom_site_aniso_label
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_23
  _atom_site_aniso_U_13
  _atom_site_aniso_U_12
Se1 0.0081(4) 0.0081(4) 0.0096(5) 0.000 0.000 0.00404(19)
Ni2 0.0087(4) 0.0098(6) 0.0104(6) -0.0012(4) -0.0006(2) 0.0049(3)

_geom_special_details
;
  All esds (except the esd in the dihedral angle between two l.s. planes)
  are estimated using the full covariance matrix.    The cell esds are taken
  into account individually in the estimation of esds in distances, angles
  and torsion angles; correlations between esds in cell parameters are only
  used when they are defined by crystal symmetry.    An approximate (isotropic)
  treatment of cell esds is used for estimating esds involving l.s. planes.
;

loop_
  _geom_bond_atom_site_label_1
  _geom_bond_atom_site_label_2
  _geom_bond_distance
  _geom_bond_site_symmetry_2
  _geom_bond_publ_flag
Se1 Ni2 2.3739(7) 9 ?
Se1 Ni2 2.3739(7) 8_445 ?
Se1 Ni2 2.3740(7) 7_455 ?
```

```
Se1 Ni2 2.4032(9) 3 ?
Se1 Ni2 2.4032(9) 2 ?
Se1 Ni2 2.4032(8) . ?
Ni2 Ni2 2.5792(7) 9 ?
Ni2 Ni2 2.5792(7) 14_544 ?
Ni2 Ni2 2.580(2) 3 ?
Ni2 Ni2 2.580(2) 2 ?

loop_
  _geom_angle_atom_site_label_1
  _geom_angle_atom_site_label_2
  _geom_angle_atom_site_label_3
  _geom_angle
  _geom_angle_site_symmetry_1
  _geom_angle_site_symmetry_3
  _geom_angle_publ_flag
Ni2 Se1 Ni2 115.154(15) 9 8_445 ?
Ni2 Se1 Ni2 115.153(15) 9 7_455 ?
Ni2 Se1 Ni2 115.152(15) 8_445 7_455 ?
Ni2 Se1 Ni2 125.00(2) 9 3 ?
Ni2 Se1 Ni2 65.35(2) 8_445 3 ?
Ni2 Se1 Ni2 111.71(3) 7_455 3 ?
Ni2 Se1 Ni2 111.71(3) 9 2 ?
Ni2 Se1 Ni2 125.00(2) 8_445 2 ?
Ni2 Se1 Ni2 65.35(2) 7_455 2 ?
Ni2 Se1 Ni2 64.92(4) 3 2 ?
Ni2 Se1 Ni2 65.35(2) 9 . ?
Ni2 Se1 Ni2 111.71(3) 8_445 . ?
Ni2 Se1 Ni2 125.00(2) 7_455 . ?
Ni2 Se1 Ni2 64.92(4) 3 . ?
Ni2 Se1 Ni2 64.92(4) 2 . ?
Se1 Ni2 Se1 100.07(4) 10 13_544 ?
Se1 Ni2 Se1 125.00(2) 10 4 ?
Se1 Ni2 Se1 102.865(9) 13_544 4 ?
Se1 Ni2 Se1 102.865(9) 10 . ?
Se1 Ni2 Se1 125.00(2) 13_544 . ?
Se1 Ni2 Se1 103.40(5) 4 . ?
Se1 Ni2 Ni2 57.87(4) 10 9 ?
Se1 Ni2 Ni2 98.23(3) 13_544 9 ?
Se1 Ni2 Ni2 157.34(5) 4 9 ?
Se1 Ni2 Ni2 56.778(19) . 9 ?
Se1 Ni2 Ni2 98.23(3) 10 14_544 ?
Se1 Ni2 Ni2 57.87(4) 13_544 14_544 ?
Se1 Ni2 Ni2 56.779(19) 4 14_544 ?
Se1 Ni2 Ni2 157.35(5) . 14_544 ?
Ni2 Ni2 Ni2 144.78(7) 9 14_544 ?
Se1 Ni2 Ni2 157.34(2) 10 3 ?
Se1 Ni2 Ni2 100.94(2) 13_544 3 ?
Se1 Ni2 Ni2 57.54(2) 4 3 ?
Se1 Ni2 Ni2 57.54(2) . 3 ?
Ni2 Ni2 Ni2 110.45(4) 9 3 ?
Ni2 Ni2 Ni2 100.059(19) 14_544 3 ?
Se1 Ni2 Ni2 100.94(2) 10 2 ?
Se1 Ni2 Ni2 157.34(2) 13_544 2 ?
Se1 Ni2 Ni2 57.54(2) 4 2 ?
Se1 Ni2 Ni2 57.54(2) . 2 ?
Ni2 Ni2 Ni2 100.058(19) 9 2 ?
```

```
Ni2 Ni2 Ni2 110.45(4) 14_544 2 ?
Ni2 Ni2 Ni2 60.0 3 2 ?

_refine_diff_density_max        0.680
_refine_diff_density_min       -0.500
_refine_diff_density_rms        0.179

_shelx_res_file
;
TITL NiSe12 in R32 #155
      shelx.res
      created by SHELXL-2018/3 at 13:27:26 on 02-Jun-2020
REM reset to R32 #155
CELL 0.71073 6.02856 6.02856 7.250038 90 90 120
ZERR 3 0.000355 0.000355 0.000518 0 0 0
LATT -3
SYMM -Y,+X-Y,+Z
SYMM +Y-X,-X,+Z
SYMM -Y+X,-Y,-Z
SYMM -X,-X+Y,-Z
SYMM +Y,+X,-Z
SFAC Ni Se
UNIT 9 6

L.S. 4
PLAN    5
fmap 2
ACTA
REM <olex2.extras>
REM <HklSrc "%.\\NiSe12.hkl">
REM </olex2.extras>

WGHT        0.023400
FVAR            0.62925
SE1     2       0.000000        0.000000        0.260137        10.33333        0.00809         0.00809 =
             0.00958        0.00000         0.00000         0.00404
NI2     1       0.247053        0.000000        0.000000        10.50000        0.00866         0.00979 =
             0.01042       -0.00118        -0.00059         0.00489
HKLF 4




REM    NiSe12 in R32 #155
REM wR2 = 0.0397, GooF = S = 1.210, Restrained GooF = 1.210 for all data
REM R1 = 0.0156 for 110 Fo > 4sig(Fo) and 0.0159 for all 113 data
REM 9 parameters refined using 0 restraints

END

WGHT           0.0234           0.0000

REM Highest difference peak    0.680,    deepest hole -0.500,    1-sigma level    0.179
Q1        1    -0.0919 -0.1621    0.3271    11.00000    0.05        0.68
Q2        1    -0.1502 -0.0837    0.2193    11.00000    0.05        0.55
Q3        1     0.1956    0.1040 -0.1167    11.00000    0.05        0.52
Q4        1     0.0018 -0.1584    0.1387    11.00000    0.05        0.48
```

```
Q5       1      0.3478 -0.0795 -0.1016    11.00000    0.05        0.48
;
_shelx_res_checksum      58391

_shelx_hkl_file
;
     0     0    -3 18916.2 348.521      4
     0     0     3 19781.0 359.128      2
     0     0     3 18465.7 331.078     11
     0     0    -3 19264.0 313.761      9
     0     0    -3 17731.5 345.480      2
     0     0     3 18504.2 351.873      4
     0     0    -3 19047.2 308.701     10
     0     0     3 18339.5 306.447     10
     0     0     6 260.653 31.1200      2
     0     0    -6 227.893 27.6373      3
     0     0     6 264.486 39.5168      4
     0     0     9 610.816 66.2101      4
     0     1     8 3953.89 157.147      4
    -1     0     8 4014.99 168.650      4
     1    -1     8 3859.96 159.951      4
     1     0    -5 44.6285 17.2131      5
     1     0    -5 45.2514 20.0221      8
     0    -1    -5 49.7303 16.9252      2
     0    -1    -5 41.5842 18.7732      4
     1    -1     5 49.6792 18.7311      4
     0    -1    -5 54.9538 15.7979      3
     0     1     5 61.1158 19.6193      4
     0    -1    -5 53.8041 13.5500     10
     0     1     5 43.1954 16.5065      2
     1    -1     5 44.8499 12.1847     10
     1     0    -5 50.1100 17.7689      2
     1    -1     5 36.0199 12.1240      2
     1     0    -5 71.6173 17.1396      3
    -1     1    -5 48.4995 13.1596      9
    -1     0     5 46.9706 20.0533      4
    -1     0     5 38.4964 11.6826     11
    -1     1    -5 51.9873 13.5932     10
     1     0    -5 36.0070 17.3793      4
     1    -1     5 64.4725 19.6391     11
    -1     1    -2 3721.96 92.9832      9
     0    -1    -2 3645.55 88.9052      3
    -1     0     2 3430.01 70.2791      9
     1     0    -2 3660.01 93.2194      5
    -1     0     2 3733.69 75.9272      6
     1     0    -2 3601.76 97.0665      4
     0     1     2 3615.37 119.801      2
     1     0    -2 3655.66 93.6912      8
     1     0    -2 3549.25 75.9005      6
    -1     0     2 3469.64 84.9845     11
     0    -1    -2 3365.41 77.2742      6
    -1     1    -2 3410.39 84.2756     10
    -1     1    -2 3505.71 79.5231      1
    -1     0     2 3950.05 95.5933      8
     0    -1    -2 3318.48 85.8808     10
     1    -1     2 4040.26 93.9957      1
     0    -1    -2 3523.20 92.7998      4
```

0	-1	-2	3518.00	109.771	2
0	1	2	3368.04	88.7217	4
1	-1	2	3575.70	75.7936	2
1	0	-2	3751.14	76.9388	9
0	1	2	3580.34	88.3650	3
1	-1	2	3386.37	81.1543	10
1	0	-2	3474.90	86.7514	11
-1	0	2	3667.52	100.520	4
-1	1	-2	3691.18	82.0798	7
1	-1	-1	2080.48	58.9493	1
0	1	-1	2003.29	51.1534	5
0	1	-1	1859.23	47.4674	8
0	-1	1	1998.60	53.2505	9
0	-1	1	1996.80	45.8339	7
1	0	1	1920.88	51.9800	10
0	-1	1	1846.86	53.4194	4
1	-1	-1	2007.91	61.2857	2
0	-1	1	1927.83	49.0573	8
-1	1	1	2153.16	61.5183	1
-1	1	1	2007.57	58.3732	3
1	0	1	1937.05	49.3756	6
-1	1	1	1938.85	50.9647	7
-1	0	-1	1851.45	52.4154	10
0	-1	1	1974.85	49.9845	5
1	-1	-1	1900.70	52.4733	7
1	-1	-1	1871.64	55.8508	3
0	-1	1	1808.99	69.1618	11
0	1	-1	1938.83	55.8068	9
0	-1	1	1905.55	61.0721	6
0	1	-1	1837.09	69.9330	11
0	1	-1	1967.49	48.9425	7
-1	0	-1	1968.35	48.3251	6
1	-1	-1	2147.56	53.9231	8
0	1	-4	14104.8	283.919	8
1	-1	-4	13074.2	265.656	3
1	0	4	13218.6	288.437	2
0	1	-4	11880.8	248.968	2
0	1	-4	14370.7	269.180	9
1	-1	-4	11649.4	274.278	2
1	0	4	13104.7	248.136	10
0	-1	4	13399.5	293.403	4
1	0	4	12487.3	210.801	1
-1	1	4	13334.4	285.447	4
0	-1	4	13128.3	286.733	11
1	-1	-4	13036.0	222.274	9
0	-1	4	13183.8	224.223	10
1	0	4	12452.2	273.577	4
1	-1	-4	12698.7	230.924	10
-1	1	4	15014.2	309.584	2
-1	0	-4	12805.1	242.650	3
1	-1	-4	11968.8	279.239	8
0	1	-4	13791.3	276.076	5
0	-1	4	12965.5	214.097	6
-1	0	-4	12719.4	250.796	10
1	0	4	12433.7	203.447	6
1	-1	-4	12998.8	278.559	4
0	-1	7	2377.96	121.525	4

0	1	-7	1811.31	95.4084	5
-1	1	7	2357.31	120.027	4
1	0	7	2025.85	106.954	4
-2	1	0	12161.3	215.000	3
1	-2	0	15437.7	297.850	1
1	-2	0	11978.8	220.092	9
1	-2	0	11690.8	224.623	7
-2	1	0	11715.2	211.456	7
1	1	0	12073.1	190.629	4
1	1	0	12349.1	229.070	6
1	-2	0	14565.5	249.842	2
1	1	0	12057.6	222.147	11
1	1	3	5652.61	138.386	10
1	1	-3	5460.44	149.264	4
1	1	-3	5704.26	143.130	5
1	1	3	5502.10	152.145	2
1	1	-3	5489.85	140.172	9
1	1	3	5321.92	121.120	6
1	-2	3	5679.38	119.114	7
1	-2	-3	5122.47	164.647	2
1	-2	3	5465.33	135.759	9
1	-2	3	5459.22	183.585	11
1	1	-3	5651.12	136.730	6
1	1	-3	5589.79	139.770	8
1	-2	-3	5790.43	144.234	4
1	1	3	5364.52	135.670	4
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-3	7	2	965.704	71.2662	3
7	-4	2	1060.93	78.7539	6
-4	7	-2	1146.97	80.3404	9
-4	-3	2	1116.84	78.1389	8
7	-3	1	113.681	29.8799	6
7	-4	-1	112.357	32.3059	6
-4	7	1	109.632	29.5499	3

```
   -3     7    -1 97.0176 28.7219      9
   -4     7     1 79.7113 29.6884      1
   -3    -4     1 122.593 30.1428      8
   -3     7    -1 119.084 35.5112      1
    7    -2    -3 1030.74 74.4220      6
    7    -5     3 1052.71 79.4427      6
   -5     7    -3 1078.85 78.5833      9
   -2     7     3 901.073 78.9318      1
   -5     7    -3 768.298 70.4293      1
    7    -2     0 1840.91 103.805      6
   -5     7     0 1827.56 103.779      3
    7    -5     0 2119.41 127.189      6
   -5    -2     0 2073.65 110.365      8
   -2     7     0 1858.94 127.647      1
    7    -2     3 942.641 71.0300      6
   -2     7    -3 956.066 85.8878      1
   -5     7     3 800.596 68.9824      1
   -1    -6    -1 1476.69 95.4881     10
   -1    -6    -1 1414.46 95.2297      7
    0     0     0        0.00        0.00      0

TITL NiSe12 in R32
REM R32 (#155 in standard setting)
CELL 0.71073      6.028560      6.028560      7.250038    90.0000    90.0000 120.0000
ZERR        3.00      0.000355      0.000355      0.000518      0.0000      0.0000      0.0000
LATT -3
SYMM -y, x-y, z
SYMM -x+y,-x, z
SYMM    y, x,-z
SYMM    x-y,-y,-z
SYMM -x,-x+y,-z
SFAC Ni Se
UNIT 9.00 6.00
TREF
HKLF 4
END
;
_shelx_hkl_checksum      61895
```