

# Supporting Information

## **Superconductivity at 50 K of a Coordination Polymer System**

Jun He<sup>1\*</sup>, Zhiqing Liu<sup>1</sup>, Liangming Tang<sup>1</sup>, Xinhe Ye<sup>1</sup>, Jieying Hu<sup>1</sup> & Zhengtao Xu<sup>2\*</sup>

<sup>1</sup>School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou, China

<sup>2</sup>Department of Chemistry, City University of Hong Kong, Kowloon Tong, Kowloon, Hong Kong, China

\*Correspondence to: junhe@gdut.edu.cn; zhengtao@cityu.edu.hk

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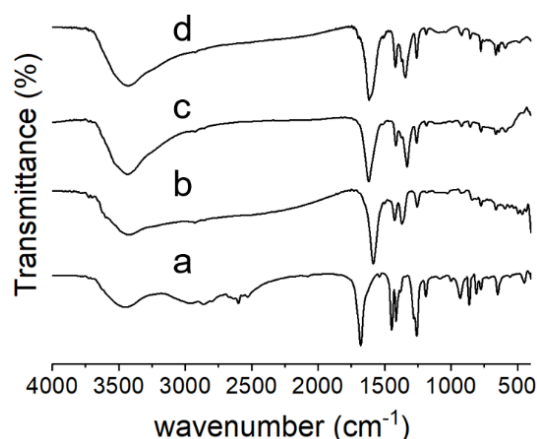
## General procedure

Unless specified, starting materials, reagents, and solvents were purchased from commercial sources (J&K, Zhengzhou Alfa and Acros) and used without further purification. Powder X-ray diffraction (PXRD) patterns were collected on a Rigaku Smart lab diffractometer with Cu K $\alpha$  radiation ( $\lambda = 1.5418 \text{ \AA}$ ) at room temperature. The X-ray tube was operated at a voltage of 40 kV and a current of 15 mA. FT-IR spectra in the range 400-4000  $\text{cm}^{-1}$  were recorded on a Nicolet Avatar 360 FT-IR spectrophotometer. Solution  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on a 400 MHz Bruker superconducting magnet high-field NMR spectrometer at room temperature, with tetramethylsilane (TMS) as the internal standard. Chemical shifts ( $\delta$ ) are expressed in ppm relative to the residual solvent (e.g., chloroform  $^1\text{H}$ : 7.26 ppm,  $^{13}\text{C}$ : 77.0 ppm) reference. Coupling constants are expressed in hertz. All of the magnetic and conductivity data were obtained using a physical property measurement system (PPMS, DynaCool, Quantum Design Inc; all five coordination polymer samples were left in air for twelve or more hours before testing). Thermogravimetric analyses (TGA) were carried out in a PerkinElmer thermal analysis equipment (STA 6000) under  $\text{O}_2$  or  $\text{N}_2$  with a heating rate of 10  $^\circ\text{C}$  per minute for  $\text{O}_2$  and 5  $^\circ\text{C}$  per minute for  $\text{N}_2$ . The organic molecule  $\text{H}_4\text{DMBD}$  was purchased from Jilin Chinese Academy of Sciences - Yanshen Technology Co., Ltd (吉林中科研伸科技有限公司), and the molecule  $\text{H}_4\text{dfdm}$  was prepared according to a recent work (*Chem. Commun.*, **2020**, 56, 3645-3648).

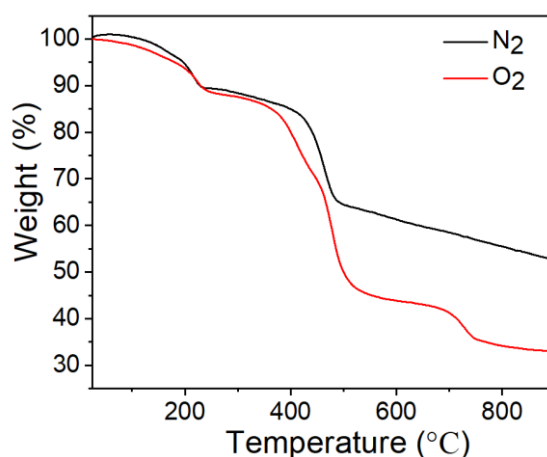
**Synthesis of Ni-dfdmt.**  $\text{H}_4\text{dfdm}$  (3.0 mg, 0.0113 mmol) and  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$  (3 mg, 0.0127 mol) was loaded into a glass tube (ID 6.0 mm, OD 8.0 mm). A DMF/ $\text{H}_2\text{O}$  (v/v 1:7, 1.6 mL) solvent mixture was then added and the tube was sealed with an oxyhydrogen flame. The glass tube was placed in an oven at 140  $^\circ\text{C}$  for 48 hours and then naturally cooled back to room temperature, affording the coordination network solid Ni-dfdmt as a black powder. For product collection, the reaction mixtures from multiple tubes were combined in a centrifuge tube for separating out the mother liquor, and for subsequent washing by DMF (1.0 mL x 3), methanol (1.0 mL x 3) and acetone (1.0 mL x 3) and then evacuated at room temperature (yield about 70% based on  $\text{H}_4\text{dfdm}$ ). The powder product was immediately placed under a  $\text{N}_2$  atmosphere for storage. Elemental analysis by atomic absorption spectroscopy (AAS) indicates a Ni content of 24.6% --cf 24.99% in the formula  $\text{Ni}(\text{C}_8\text{F}_2\text{S}_2\text{O}_4)(\text{H}_2\text{O})_2(\text{H}_2\text{O})_3$ . By using  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  and a 1:1  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}/\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  mixture respectively, the Co-dfdmt and CoNi-dfdmt samples were similarly prepared and characterized, e.g., with AAS elemental analysis indicating a 1:1 Co/Ni atomic ratio in CoNi-dfdmt, PXRD indicating the phase purity, and IR spectra featuring the carboxylate stretch at about 1600  $\text{cm}^{-1}$  (Figure S1). The black powder products were also immediately placed under a  $\text{N}_2$  atmosphere for storage.

**Synthesis of Co-DMBD.**  $\text{H}_4\text{DMBD}$  (2.0 mg, 0.0087 mmol) and  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  (3.0 mg, 0.0127 mmol) was loaded into a glass tube (ID 6.0 mm, OD 8.0 mm). A DMF/ $\text{H}_2\text{O}$  (v/v 1:5, 1.2 mL) solvent mixture was then added and the tube was sealed with an oxyhydrogen flame. The glass tube was placed in an oven at 140  $^\circ\text{C}$  for 48 hours and then naturally cooled back to room temperature, affording the coordination network solid Co-DMBD as a black powder. For product collection, the reaction mixtures from multiple tubes were combined in a centrifuge tube for separating out the mother liquor,

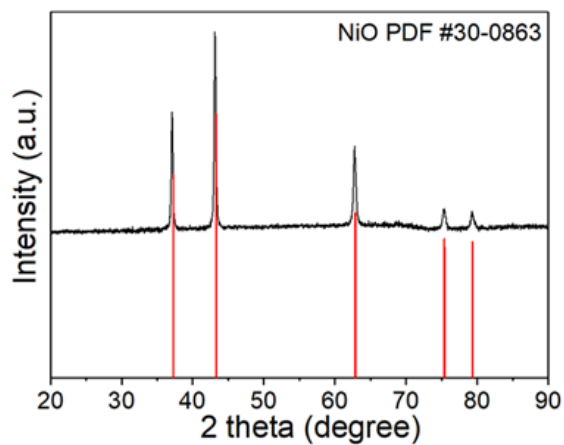
and for subsequent washing by DMF (1.0 mL x 3), methanol (1.0 mL x 3) and acetone (1.0 mL x 3) and then evacuated at room temperature. Yield from a 10-tube set: 22.0 mg, 91 % based on  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ . The powder product was immediately placed under a  $\text{N}_2$  atmosphere for storage. By using a molar 1:1  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}/\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  mixture, the CoNi-DMBD sample was similarly prepared and characterized: e.g., AAS elemental analysis indicates an 1:1 Co/Ni atomic ratio --13.1% Co and 13.65% Ni, cf 13.04% Co and 12.99% Ni in the formula  $\text{CoNi}(\text{C}_8\text{H}_2\text{S}_2\text{O}_4)(\text{H}_2\text{O})_2(\text{H}_2\text{O})_4$ ; PXRD indicates the phase purity, and IR spectra feature the carboxylate stretch at about  $1600\text{ cm}^{-1}$  (Figure S6). The black powder product of CoNi-DMBD was also immediately placed under a  $\text{N}_2$  atmosphere for storage.



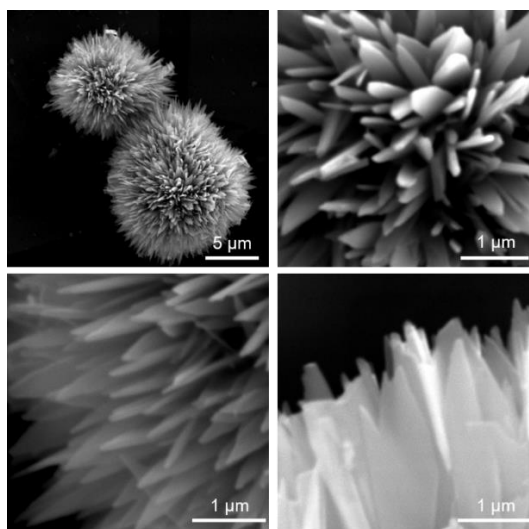
**Figure S1.** The IR spectra of a)  $\text{H}_4\text{dfdm}$ ; b)  $\text{Ni-dfdmt}$ ; c)  $\text{Co-dfdmt}$ ; d)  $\text{CoNi-dfdmt}$ .



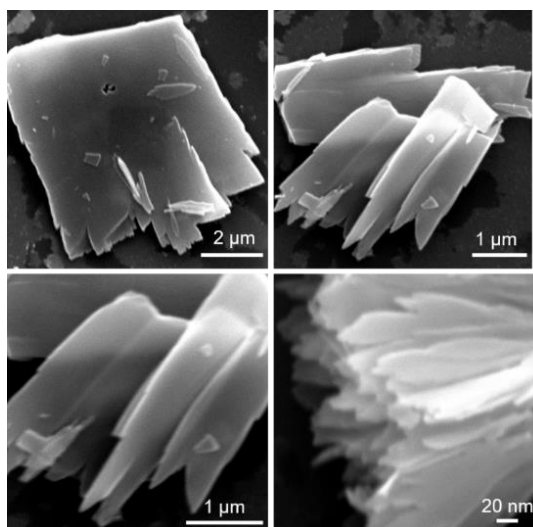
**Figure S2.** Plots for two thermogravimetric analyses (TGA) of  $\text{Ni-dfdmt}$ , one under  $\text{N}_2$ , the other under  $\text{O}_2$ . For the latter, the weight loss up to the inflection point at  $230\text{ }^\circ\text{C}$  can be ascribed to water and other guests physisorbed in the channels. The corresponding weight (89.0 %) afterward dropped all the way to 32.9 % at  $900\text{ }^\circ\text{C}$ . The ratio  $32.9/89.0 = 0.370$ , matches the  $\text{NiO}$  (mw 74.5) content in the formula  $\text{Ni}_2(\text{C}_8\text{F}_2\text{S}_2\text{O}_4)(\text{H}_2\text{O})_2$  (mw 416):  $74.5 \times 2/416 = 35.8\%$ .



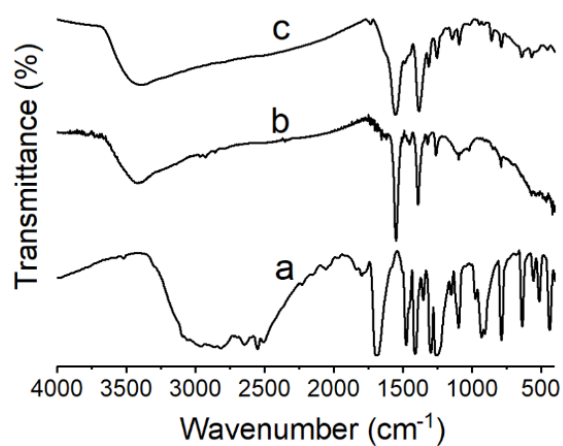
**Figure S3.** The PXRD pattern of the residue of Ni-dfdmt after TGA in an O<sub>2</sub> atmosphere, indicating the formation of NiO.



**Figure S4.** SEM images of Ni-dfdmt, consistent with the layered structure.



**Figure S5.** SEM images of CoNi-dfdmt.



**Figure S6.** The IR spectra of a) H<sub>4</sub>DMBD; b) Co-DMBD; c) CoNi-DMBD.

*The following is the cif data generated by MicroED studies on the powder sample of Ni-dfamt. The MicroED studies were conducted by ReadCrystal (苏州青云瑞晶生物科技有限公司; <https://www.readcrystal.com/>).*

data\_1\_a

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\_audit\_creation\_method

;

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(compiled 2018.05.29 svn.r3508 for OlexSys, GUI svn.r5506)

;

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\_audit\_contact\_author\_email ?

\_audit\_contact\_author\_name "

\_audit\_contact\_author\_phone ?

\_publ\_contact\_author\_id\_orcid ?

\_publ\_section\_references

;

Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H.

(2015). Acta Cryst. A71, 59-75.

Dolomanov, O.V., Bourhis, L.J., Gildea, R.J., Howard, J.A.K. & Puschmann, H.

(2009), J. Appl. Cryst. 42, 339-341.

Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

;

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\_chemical\_name\_systematic ?

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loop\_

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\_atom\_type\_description

\_atom\_type\_scatter\_dispersion\_real

\_atom\_type\_scatter\_dispersion\_imag

\_atom\_type\_scatter\_source

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'F' 'F' 0.0000 0.0000 'International Tables Vol C Tables 4.3.1.1'

'Ni' 'Ni' 0.0000 0.0000 'International Tables Vol C Tables 4.3.1.1'

'O' 'O' 0.0000 0.0000 'International Tables Vol C Tables 4.3.1.1'

'S' 'S' 0.0000 0.0000 'International Tables Vol C Tables 4.3.1.1'

\_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.

;

\_space\_group\_crystal\_system        'triclinic'

\_space\_group\_IT\_number                2

\_space\_group\_name\_H-M\_alt            'P -1'

\_space\_group\_name\_Hall                '-P 1'

loop\_

\_space\_group\_symop\_operation\_xyz

'x, y, z'

'-x, -y, -z'

\_cell\_length\_a                        3.3200(7)

\_cell\_length\_b                        8.4400(17)

\_cell\_length\_c                        9.6500(19)

|                                 |            |
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| _cell_angle_beta                | 84.29(3)   |
| _cell_angle_gamma               | 84.27(3)   |
| _cell_volume                    | 258.49(10) |
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| _cell_measurement_theta_min     | 0.178      |
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| _exptl_absorpt_correction_type  | none       |
| _exptl_absorpt_process_details  | ?          |
| _exptl_absorpt_special_details  | ?          |
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| _exptl_crystal_density_diffm    | 2.644      |
| _exptl_crystal_density_meas     | ?          |
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| _diffm_reflns_av_unetI/netI     | 0.1990     |

|                                                  |                       |
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| _diffn_reflns_limit_h_min                        | -4                    |
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| _diffn_reflns_limit_k_min                        | -10                   |
| _diffn_reflns_limit_l_max                        | 10                    |
| _diffn_reflns_limit_l_min                        | -10                   |
| _diffn_reflns_number                             | 2539                  |
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| _diffn_reflns_theta_full                         | 0.862                 |
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| _diffn_reflns_theta_min                          | 0.089                 |
| _diffn_ambient_temperature                       | 100(2)                |
| _diffn_detector_area_resol_mean                  | ?                     |
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| _diffn_measured_fraction_theta_max               | 0.636                 |
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| _diffn_measurement_method                        | 'Continuous Rotation' |
| _diffn_radiation_monochromator                   | None                  |
| _diffn_radiation_type                            | Electron              |
| _diffn_radiation_wavelength                      | 0.02508               |
| _diffn_source                                    | LaB6                  |
| _diffn_standards_number                          | 0                     |
| _reflns_Friedel_coverage                         | 0.000                 |
| _reflns_Friedel_fraction_full                    | .                     |
| _reflns_Friedel_fraction_max                     | .                     |
| _reflns_number_gt                                | 470                   |
| _reflns_number_total                             | 647                   |

\_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.

;

|                                 |                                      |
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| _computing_data_collection      | ?                                    |
| _computing_data_reduction       | ?                                    |
| _computing_molecular_graphics   | 'Olex2 (Dolomanov et al., 2009)'     |
| _computing_publication_material | 'Olex2 (Dolomanov et al., 2009)'     |
| _computing_structure_refinement | 'ShelXL (Sheldrick, 2015)'           |
| _computing_structure_solution   | 'olex2.solve (Bourhis et al., 2015)' |
| _refine_diff_density_max        | 0.434                                |
| _refine_diff_density_min        | -0.455                               |
| _refine_diff_density_rms        | 0.101                                |
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| _refine_ls_extinction_method    | none                                 |
| _refine_ls_goodness_of_fit_ref  | 1.976                                |
| _refine_ls_hydrogen_treatment   | undef                                |
| _refine_ls_matrix_type          | full                                 |
| _refine_ls_number_parameters    | 39                                   |
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| _refine_ls_number_restraints    | 3                                    |
| _refine_ls_R_factor_all         | 0.2972                               |

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_refine_ls_weighting_details

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_olex2_refinement_description

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# 1. Others

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Fixed Z: Ni00(0.5) Ni1(1)

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_atom_site_fract_y
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_atom_site_fract_z
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_atom_site_adp_type
```

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_atom_site_occupancy
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\_atom\_site\_symmetry\_order

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\_atom\_site\_refinement\_flags\_adp

\_atom\_site\_refinement\_flags\_occupancy

\_atom\_site\_disorder\_assembly

\_atom\_site\_disorder\_group

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C004 C 0.420(5) 1.0021(19) 0.361(2) 0.006(4) Uiso 1 1 d D . . . .

O005 O 0.887(4) 0.5765(19) 0.681(2) 0.010(4) Uiso 1 1 d . . . . .

F006 F 0.328(5) 1.007(2) 0.237(3) 0.020(4) Uiso 1 1 d . . . . .

C007 C 0.506(6) 0.854(2) 0.464(3) 0.012(5) Uiso 1 1 d D . . . .

O008 O 0.506(5) 0.687(2) 0.828(3) 0.015(4) Uiso 1 1 d . . . . .

C009 C 0.650(7) 0.695(3) 0.709(3) 0.024(6) Uiso 1 1 d D . . . .

C00A C 0.571(5) 0.848(2) 0.594(2) 0.006(4) Uiso 1 1 d D . . . .

Ni1 Ni 0.500000 0.500000 1.000000 0.034(3) Uiso 1 2 d S . P . .

O1 O 0.053(7) 0.387(3) 0.926(4) 0.039(6) Uiso 1 1 d . . . . .

\_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\_

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 Ni00 O005 2.012(19) . ?  
 Ni00 O005 2.012(19) 2\_766 ?  
 S002 C007 1.76(2) . ?  
 C004 F006 1.26(3) . ?  
 C004 C007 1.395(17) . ?  
 C004 C00A 1.45(3) 2\_676 ?  
 O005 C009 1.28(3) . ?  
 C007 C00A 1.29(3) . ?  
 O008 C009 1.18(4) . ?  
 O008 Ni1 1.96(2) . ?  
 C009 C00A 1.478(18) . ?  
 Ni1 O1 2.11(3) 2\_667 ?  
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S002 Ni00 S002 88.4(4) 2\_766 1\_655 ?

S002 Ni00 S002 91.6(4) 2\_766 2\_666 ?

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O005 Ni00 S002 89.2(6) . 2\_766 ?

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Ni00 S002 Ni00 91.6(4) . 1\_455 ?

C007 S002 Ni00 115.3(8) . 1\_455 ?

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C009 O005 Ni00 131(2) . . ?

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C00A C007 S002 125.7(15) . . ?

C00A C007 C004 122.6(19) . . ?

C009 O008 Ni1 130.4(16) . . ?

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 C007 C00A C004 120.5(17) . 2\_676 ?  
 C007 C00A C009 125(2) . . ?  
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 O008 Ni1 O1 86.9(10) . 2\_667 ?  
 O008 Ni1 O1 87.5(9) 2\_667 1\_655 ?  
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 O008 Ni1 O1 92.5(10) 2\_667 2\_567 ?  
 O008 Ni1 O1 87.5(9) . 2\_567 ?  
 O008 Ni1 O1 86.9(10) 2\_667 . ?  
 O008 Ni1 O1 92.5(10) . 1\_655 ?  
 O1 Ni1 O1 102.9(11) . 1\_655 ?  
 O1 Ni1 O1 102.9(11) 2\_667 2\_567 ?  
 O1 Ni1 O1 77.1(11) 2\_667 1\_655 ?  
 O1 Ni1 O1 180.0 1\_655 2\_567 ?  
 O1 Ni1 O1 77.1(11) . 2\_567 ?  
 O1 Ni1 O1 180.0 2\_667 . ?  
 Ni1 O1 Ni1 102.9(11) . 1\_455 ?

loop\_

\_geom\_torsion\_atom\_site\_label\_1  
 \_geom\_torsion\_atom\_site\_label\_2  
 \_geom\_torsion\_atom\_site\_label\_3  
 \_geom\_torsion\_atom\_site\_label\_4  
 \_geom\_torsion  
 \_geom\_torsion\_site\_symmetry\_1  
 \_geom\_torsion\_site\_symmetry\_2  
 \_geom\_torsion\_site\_symmetry\_3

\_geom\_torsion\_site\_symmetry\_4

\_geom\_torsion\_publ\_flag

Ni00 S002 C007 C004 -116.6(13) 1\_455 . . . ?

Ni00 S002 C007 C004 144.3(12) . . . . ?

Ni00 S002 C007 C00A -36.7(18) . . . . ?

Ni00 S002 C007 C00A 62.4(19) 1\_455 . . . ?

Ni00 O005 C009 O008 151(2) . . . . ?

Ni00 O005 C009 C00A -32(3) . . . . ?

S002 C007 C00A C004 177.8(15) . . . 2\_676 ?

S002 C007 C00A C009 -1(3) . . . . ?

C004 C007 C00A C004 -3(3) . . . 2\_676 ?

C004 C007 C00A C009 177.9(18) . . . . ?

O005 C009 C00A C004 -136(2) . . . 2\_676 ?

O005 C009 C00A C007 43(3) . . . . ?

F006 C004 C007 S002 4(2) . . . . ?

F006 C004 C007 C00A -174.9(18) . . . . ?

O008 C009 C00A C004 40(3) . . . 2\_676 ?

O008 C009 C00A C007 -141(3) . . . . ?

C00A C004 C007 S002 -177.7(14) 2\_676 . . . ?

C00A C004 C007 C00A 3(3) 2\_676 . . . ?

Ni1 O008 C009 O005 -10(4) . . . . ?

Ni1 O008 C009 C00A 173.2(14) . . . . ?

\_shelx\_res\_file

;

TITL 1\_a.res in P-1

1\_a.res

created by SHELXL-2018/3 at 11:53:25 on 26-Jan-2022

REM Old TITL 1 in P-1

REM SHELXT solution in P-1: R1 0.324, Rweak 0.186, Alpha 0.388

REM <I/s> 0.000 for 0 systematic absences, Orientation as input  
 REM Formula found by SHELXT: C9 O2 F7 S3  
 CELL 0.02508 3.32 8.44 9.65 74.48 84.29 84.27  
 ZERR 1 0.0007 0.0017 0.0019 0.03 0.03 0.03  
 LATT 1  
 SFAC C 0.731 36.995 1.195 11.297 0.456 2.814 0.125 0.346 0 0 0 0 0.77 12.011  
 SFAC F 0.369 20.239 0.811 6.609 0.475 1.931 0.146 0.279 0 0 0 0 0.72 18.998  
 SFAC Ni 2.210 58.727 2.134 13.553 1.689 2.609 0.524 0.339 0 0 0 0 1.15 58.693  
 SFAC O 0.455 23.78 0.917 7.622 0.472 2.144 0.138 0.296 0 0 0 0 0.73 15.999  
 SFAC S 1.659 36.65 2.386 11.488 0.79 2.469 0.321 0.34 0 0 0 0 1.02 32.066  
 UNIT 8 2 2 6 2  
 DFIX 1.5 C00A C009  
 DFIX 1.39 C007 C004  
 DANG 2.408 C004 C00A  
 L.S. 50  
 PLAN 5  
 CONF  
 LIST 6  
 fmap 2  
 acta  
 MORE -1  
 REM <olex2.extras>  
 REM <HklSrc "%\\1\_a.hkl">  
 REM </olex2.extras>  
 WGHT 0.200000  
 FVAR 6.66023  
 NI00 3 1.000000 0.500000 0.500000 10.50000 0.00977

|      |   |          |          |          |          |         |
|------|---|----------|----------|----------|----------|---------|
| S002 | 5 | 0.502595 | 0.683301 | 0.392601 | 11.00000 | 0.00696 |
| C004 | 1 | 0.420069 | 1.002102 | 0.361261 | 11.00000 | 0.00560 |
| O005 | 4 | 0.886768 | 0.576472 | 0.681391 | 11.00000 | 0.00951 |
| F006 | 2 | 0.328287 | 1.007308 | 0.236778 | 11.00000 | 0.02006 |
| C007 | 1 | 0.505597 | 0.853941 | 0.463807 | 11.00000 | 0.01236 |
| O008 | 4 | 0.505905 | 0.686748 | 0.827848 | 11.00000 | 0.01467 |
| C009 | 1 | 0.649576 | 0.695146 | 0.709307 | 11.00000 | 0.02441 |
| C00A | 1 | 0.571001 | 0.847801 | 0.594285 | 11.00000 | 0.00636 |
| NI1  | 3 | 0.500000 | 0.500000 | 1.000000 | 10.50000 | 0.03435 |
| O1   | 4 | 0.053473 | 0.386930 | 0.926493 | 11.00000 | 0.03886 |

HKLF 4

REM 1\_a.res in P-1

REM wR2 = 0.5906, GooF = S = 1.976, Restrained GooF = 1.976 for all data

REM R1 = 0.2634 for 470 Fo > 4sig(Fo) and 0.2972 for all 647 data

REM 39 parameters refined using 3 restraints

END

WGHT 0.2000 0.0000

REM Highest difference peak 0.434, deepest hole -0.455, 1-sigma level 0.101

|    |   |         |        |        |          |      |      |
|----|---|---------|--------|--------|----------|------|------|
| Q1 | 1 | 1.0128  | 0.5411 | 0.4197 | 11.00000 | 0.05 | 0.43 |
| Q2 | 1 | 0.8639  | 1.0001 | 0.3594 | 11.00000 | 0.05 | 0.35 |
| Q3 | 1 | 0.0325  | 0.7015 | 0.4021 | 11.00000 | 0.05 | 0.34 |
| Q4 | 1 | 0.5737  | 0.7228 | 0.3169 | 11.00000 | 0.05 | 0.32 |
| Q5 | 1 | -0.0985 | 0.4977 | 0.9718 | 11.00000 | 0.05 | 0.30 |

;

\_shelx\_res\_checksum            67046

\_shelx\_hkl\_file

;

0 -1 0 2201.88 591.24

0 2 1 495.85 125.99

0 2 1 517.15 186.78

0 2 1 287.07 93.59

0 -2 -1 453.45 164.08

0 -2 -1 187.58 64.19

0 -2 -1 429.06 109.69

0 2 0 1201.58 329.57

0 -2 0 1337.87 365.66

0 -3 -2 4099.49 979.90

0 -3 -2 2393.16 720.63

0 3 1 160.98 62.19

0 3 1 475.65 145.99

0 -3 -1 222.08 77.69

0 -3 -1 480.65 147.79

0 -3 0 1757.62 478.65

0 4 3 1963.10 476.15

0 4 3 6587.64 1779.52

0 -4 -3 1907.91 468.15

0 -4 -3 4271.57 1154.08

0 4 2 5125.29 1221.68

0 4 2 3618.04 1291.57

0 4 2 4661.83 1395.56

0 -4 -2 2915.71 1043.40

0 -4 -2 4221.48 1267.37

0 -4 -2 5049.59 1203.58

|   |    |    |         |        |
|---|----|----|---------|--------|
| 0 | 4  | 1  | 255.67  | 86.49  |
| 0 | -4 | -1 | 190.68  | 59.79  |
| 0 | -4 | -1 | 120.99  | 55.19  |
| 0 | 4  | 0  | 2454.85 | 665.83 |
| 0 | -4 | 0  | 2178.78 | 592.94 |
| 0 | 4  | -1 | 125.59  | 60.79  |
| 0 | 5  | 5  | 122.69  | 48.60  |
| 0 | 5  | 4  | 1378.86 | 391.46 |
| 0 | -5 | -4 | 477.65  | 136.49 |
| 0 | 5  | 3  | 154.18  | 69.39  |
| 0 | 5  | 3  | 97.29   | 39.50  |
| 0 | 5  | 3  | -5.80   | 23.90  |
| 0 | -5 | -3 | 149.88  | 55.29  |
| 0 | -5 | -3 | 63.99   | 37.90  |
| 0 | -5 | -3 | 55.29   | 46.20  |
| 0 | -5 | -3 | 273.87  | 94.29  |
| 0 | 5  | 2  | 831.62  | 212.48 |
| 0 | 5  | 2  | 1448.26 | 528.35 |
| 0 | 5  | 2  | 791.02  | 226.78 |
| 0 | -5 | -2 | 984.20  | 299.17 |
| 0 | -5 | -2 | 940.11  | 235.48 |
| 0 | -5 | -2 | 797.32  | 229.28 |
| 0 | 5  | 1  | 102.89  | 43.10  |
| 0 | 5  | 1  | 138.89  | 55.09  |
| 0 | -5 | -1 | 200.18  | 66.69  |
| 0 | -5 | -1 | 133.29  | 56.09  |
| 0 | 5  | 0  | 1112.89 | 310.67 |
| 0 | -5 | 0  | 1085.89 | 305.67 |
| 0 | 5  | -1 | 698.93  | 202.98 |
| 0 | -5 | 1  | 688.83  | 202.08 |

|   |    |    |         |        |
|---|----|----|---------|--------|
| 0 | 6  | 6  | 124.39  | 48.70  |
| 0 | 6  | 5  | 1382.76 | 396.16 |
| 0 | -6 | -5 | 1266.27 | 360.66 |
| 0 | -6 | -4 | 676.53  | 180.38 |
| 0 | -6 | -4 | 351.26  | 121.59 |
| 0 | 6  | 3  | 581.24  | 177.08 |
| 0 | 6  | 3  | 393.56  | 109.49 |
| 0 | 6  | 3  | 203.98  | 69.09  |
| 0 | 6  | 3  | 245.08  | 93.59  |
| 0 | -6 | -3 | 286.27  | 109.79 |
| 0 | -6 | -3 | 194.28  | 79.09  |
| 0 | -6 | -3 | 441.16  | 120.79 |
| 0 | 6  | 2  | 2162.08 | 590.34 |
| 0 | 6  | 2  | 2131.29 | 518.85 |
| 0 | 6  | 2  | 2393.16 | 719.23 |
| 0 | -6 | -2 | 1946.41 | 472.85 |
| 0 | -6 | -2 | 2459.95 | 741.73 |
| 0 | -6 | -2 | 2854.11 | 776.52 |
| 0 | 6  | 1  | 948.41  | 268.77 |
| 0 | -6 | -1 | 895.61  | 255.87 |
| 0 | 6  | 0  | 1553.54 | 428.66 |
| 0 | -6 | 0  | 837.92  | 222.38 |
| 0 | -6 | 0  | 1530.45 | 424.86 |
| 0 | 6  | -1 | 1612.54 | 445.86 |
| 0 | -6 | 1  | 1898.91 | 524.25 |
| 0 | 7  | 7  | 77.49   | 37.00  |
| 0 | 7  | 6  | 94.79   | 43.10  |
| 0 | 7  | 6  | 184.28  | 82.29  |
| 0 | -7 | -6 | 8.50    | 30.40  |
| 0 | -7 | -6 | 244.88  | 92.99  |

|   |    |    |         |         |
|---|----|----|---------|---------|
| 0 | 7  | 5  | 65.49   | 38.00   |
| 0 | 7  | 5  | 270.67  | 110.19  |
| 0 | -7 | -5 | 54.09   | 47.70   |
| 0 | -7 | -5 | 108.39  | 76.59   |
| 0 | 7  | 4  | 1145.09 | 331.37  |
| 0 | 7  | 4  | 372.96  | 121.89  |
| 0 | -7 | -4 | 1312.17 | 329.17  |
| 0 | -7 | -4 | 1390.46 | 392.86  |
| 0 | 7  | 3  | 1351.96 | 379.36  |
| 0 | 7  | 3  | 1018.70 | 370.76  |
| 0 | 7  | 3  | 991.90  | 302.37  |
| 0 | 7  | 3  | 1063.59 | 265.17  |
| 0 | -7 | -3 | 1658.83 | 604.34  |
| 0 | -7 | -3 | 1108.99 | 279.87  |
| 0 | -7 | -3 | 824.92  | 255.47  |
| 0 | -7 | -3 | 1215.48 | 341.27  |
| 0 | 7  | 2  | 3779.82 | 1023.10 |
| 0 | 7  | 2  | 5941.91 | 1421.26 |
| 0 | 7  | 2  | 4803.02 | 1444.36 |
| 0 | -7 | -2 | 7383.66 | 1765.32 |
| 0 | -7 | -2 | 4130.29 | 1241.68 |
| 0 | -7 | -2 | 3937.71 | 1065.99 |
| 0 | 7  | 1  | 1684.43 | 416.36  |
| 0 | 7  | 1  | 1323.67 | 369.76  |
| 0 | -7 | -1 | 1883.51 | 467.85  |
| 0 | -7 | -1 | 1556.04 | 434.46  |
| 0 | 7  | 0  | 1414.86 | 393.36  |
| 0 | -7 | 0  | 820.82  | 219.38  |
| 0 | -7 | 0  | 1348.07 | 378.96  |
| 0 | 7  | -1 | 167.68  | 64.89   |

|   |    |    |         |        |
|---|----|----|---------|--------|
| 0 | -7 | 1  | 154.48  | 69.09  |
| 0 | 8  | 8  | 60.39   | 32.00  |
| 0 | 8  | 7  | 79.89   | 43.10  |
| 0 | 8  | 7  | 26.70   | 33.70  |
| 0 | -8 | -7 | -4.10   | 21.50  |
| 0 | -8 | -7 | 131.59  | 66.99  |
| 0 | 8  | 6  | 143.69  | 73.79  |
| 0 | -8 | -6 | 177.98  | 80.99  |
| 0 | 8  | 5  | 28.80   | 27.20  |
| 0 | 8  | 5  | 5.60    | 24.60  |
| 0 | -8 | -5 | 239.68  | 91.99  |
| 0 | 8  | 4  | 126.29  | 52.79  |
| 0 | 8  | 4  | 844.92  | 217.88 |
| 0 | 8  | 4  | 785.52  | 234.68 |
| 0 | -8 | -4 | 806.02  | 210.18 |
| 0 | 8  | 3  | 97.29   | 40.90  |
| 0 | 8  | 3  | 93.59   | 46.90  |
| 0 | 8  | 3  | 189.78  | 64.99  |
| 0 | 8  | 2  | 2041.40 | 563.54 |
| 0 | 8  | 2  | 1201.08 | 366.56 |
| 0 | -8 | -2 | 2796.32 | 678.33 |
| 0 | 8  | 1  | 192.38  | 70.79  |
| 0 | 8  | 1  | 174.88  | 66.49  |
| 0 | -8 | -1 | 330.07  | 107.09 |
| 0 | -8 | -1 | 192.08  | 73.19  |
| 0 | 8  | 0  | 493.75  | 152.18 |
| 0 | -8 | 0  | 235.38  | 81.09  |
| 0 | -8 | 0  | 494.65  | 156.38 |
| 0 | 8  | -1 | 206.48  | 76.19  |
| 0 | -8 | 1  | 150.38  | 65.49  |

|   |    |    |         |        |
|---|----|----|---------|--------|
| 0 | 8  | -2 | 136.49  | 60.59  |
| 0 | 9  | 8  | 24.90   | 26.00  |
| 0 | 9  | 8  | 15.20   | 27.40  |
| 0 | 9  | 7  | 447.46  | 127.29 |
| 0 | 9  | 6  | 21.30   | 24.50  |
| 0 | -9 | -6 | 59.69   | 35.10  |
| 0 | 9  | 5  | 325.37  | 113.99 |
| 0 | 9  | 5  | 84.49   | 42.00  |
| 0 | -9 | -5 | 261.37  | 102.69 |
| 0 | -9 | -5 | 266.67  | 83.59  |
| 0 | -9 | -5 | 40.90   | 52.39  |
| 0 | 9  | 4  | 193.58  | 75.89  |
| 0 | 9  | 4  | 179.98  | 59.49  |
| 0 | 9  | 4  | 182.28  | 63.19  |
| 0 | -9 | -4 | 166.28  | 67.29  |
| 0 | -9 | -4 | 48.10   | 34.20  |
| 0 | 9  | 3  | 7.10    | 15.70  |
| 0 | 9  | 3  | 35.90   | 18.80  |
| 0 | -9 | -3 | 120.69  | 46.50  |
| 0 | -9 | -3 | 52.49   | 29.90  |
| 0 | 9  | 2  | 505.95  | 136.79 |
| 0 | -9 | -2 | 609.44  | 188.08 |
| 0 | 9  | 1  | 12.80   | 25.40  |
| 0 | 9  | 1  | 156.88  | 62.29  |
| 0 | -9 | -1 | 32.10   | 30.60  |
| 0 | 9  | 0  | 239.58  | 86.59  |
| 0 | -9 | 0  | 132.99  | 54.89  |
| 0 | 9  | -1 | 108.79  | 51.59  |
| 0 | 9  | -2 | 1018.30 | 292.87 |
| 0 | 10 | 6  | 387.06  | 109.99 |

|    |     |    |        |        |
|----|-----|----|--------|--------|
| 0  | -10 | -6 | 201.48 | 81.79  |
| 0  | -10 | -6 | 162.58 | 64.29  |
| 0  | 10  | 5  | 41.70  | 29.10  |
| 0  | 10  | 5  | 157.28 | 67.79  |
| 0  | -10 | -5 | 47.70  | 30.80  |
| 0  | 10  | 4  | 14.00  | 22.40  |
| 0  | 10  | 4  | 63.39  | 30.90  |
| 0  | -10 | -4 | 29.50  | 24.60  |
| 0  | 10  | 3  | 382.26 | 108.09 |
| 0  | 10  | 3  | 132.49 | 56.09  |
| 0  | 10  | 3  | 330.87 | 108.39 |
| 0  | 10  | 2  | 125.49 | 48.20  |
| 0  | 10  | 2  | 170.38 | 71.59  |
| 0  | -10 | -2 | 129.39 | 50.49  |
| 0  | 10  | 1  | 88.29  | 43.50  |
| 0  | -10 | -1 | 64.99  | 37.40  |
| 0  | 10  | 0  | 511.55 | 160.58 |
| 0  | -10 | 0  | 150.38 | 59.89  |
| 1  | -9  | 1  | 33.00  | 41.30  |
| -1 | 9   | -1 | 9.60   | 30.50  |
| 1  | -9  | 0  | 154.48 | 66.99  |
| -1 | 9   | 0  | 242.88 | 85.69  |
| -1 | 9   | 0  | 170.78 | 71.59  |
| 1  | -9  | -1 | 453.05 | 147.79 |
| -1 | 9   | 1  | 456.45 | 137.69 |
| -1 | 9   | 1  | 9.00   | 36.30  |
| 1  | -9  | -2 | 74.69  | 44.70  |
| -1 | 9   | 2  | 146.59 | 65.79  |
| -1 | 9   | 2  | 120.69 | 58.19  |
| -1 | 9   | 2  | 56.69  | 57.89  |

|    |    |    |        |        |
|----|----|----|--------|--------|
| 1  | -9 | -3 | 61.49  | 56.99  |
| -1 | 9  | 3  | 120.09 | 65.09  |
| -1 | 9  | 3  | 124.59 | 55.99  |
| -1 | 9  | 3  | 53.79  | 39.70  |
| 1  | -9 | -4 | 140.49 | 72.89  |
| 1  | -9 | -4 | 91.29  | 50.19  |
| -1 | 9  | 4  | 169.78 | 73.79  |
| -1 | 9  | 4  | 147.89 | 73.69  |
| 1  | -9 | -5 | 216.98 | 102.09 |
| 1  | -9 | -5 | 169.88 | 72.99  |
| -1 | 9  | 5  | 137.99 | 68.29  |
| 1  | -9 | -6 | 120.79 | 72.99  |
| 1  | -9 | -6 | 36.70  | 38.20  |
| -1 | 9  | 6  | 122.59 | 55.09  |
| -1 | 9  | 6  | 10.00  | 23.90  |
| -1 | 8  | -4 | 19.00  | 31.80  |
| 1  | -8 | 3  | 44.40  | 41.60  |
| -1 | 8  | -3 | 179.08 | 75.79  |
| -1 | 8  | -2 | 17.10  | 37.00  |
| 1  | -8 | 1  | 241.28 | 95.79  |
| -1 | 8  | -1 | 235.08 | 90.79  |
| 1  | -8 | 0  | 427.96 | 139.99 |
| -1 | 8  | 0  | 441.06 | 135.99 |
| -1 | 8  | 0  | 357.46 | 121.89 |
| 1  | -8 | -1 | 204.88 | 87.59  |
| 1  | -8 | -1 | 119.99 | 62.79  |
| 1  | -8 | -1 | 8.10   | 40.00  |
| -1 | 8  | 1  | 134.29 | 60.99  |
| -1 | 8  | 1  | 30.40  | 41.00  |
| -1 | 8  | 1  | 73.09  | 50.39  |

|    |    |    |         |        |
|----|----|----|---------|--------|
| 1  | -8 | -2 | 22.90   | 33.10  |
| 1  | -8 | -2 | 18.70   | 41.40  |
| 1  | -8 | -2 | 22.90   | 33.00  |
| 1  | -8 | -2 | 35.70   | 53.99  |
| -1 | 8  | 2  | 135.29  | 60.99  |
| -1 | 8  | 2  | 7.60    | 24.50  |
| -1 | 8  | 2  | 41.90   | 40.30  |
| 1  | -8 | -3 | 104.99  | 50.99  |
| 1  | -8 | -3 | 171.28  | 99.19  |
| 1  | -8 | -3 | 92.79   | 54.39  |
| 1  | -8 | -3 | 83.89   | 49.10  |
| -1 | 8  | 3  | 141.99  | 68.39  |
| -1 | 8  | 3  | 150.68  | 63.99  |
| 1  | -8 | -4 | 490.55  | 147.79 |
| 1  | -8 | -4 | 426.76  | 171.78 |
| -1 | 8  | 4  | 295.77  | 98.09  |
| -1 | 8  | 4  | 268.77  | 98.59  |
| -1 | 8  | 4  | 384.36  | 137.89 |
| 1  | -8 | -5 | 692.83  | 196.58 |
| 1  | -8 | -5 | 66.29   | 45.60  |
| 1  | -8 | -5 | 30.40   | 40.80  |
| -1 | 8  | 5  | 1064.09 | 281.47 |
| -1 | 8  | 5  | 100.29  | 67.69  |
| 1  | -8 | -6 | 130.59  | 71.59  |
| 1  | -8 | -6 | 143.69  | 88.69  |
| -1 | 8  | 6  | 301.97  | 102.09 |
| -1 | 8  | 6  | -8.00   | 42.70  |
| -1 | 8  | 6  | 227.68  | 95.59  |
| 1  | -8 | -7 | 848.12  | 344.27 |
| 1  | -8 | -7 | 553.44  | 174.78 |

|    |    |    |         |        |
|----|----|----|---------|--------|
| -1 | 8  | 7  | 557.04  | 191.28 |
| -1 | 8  | 7  | 774.02  | 216.88 |
| -1 | 8  | 7  | 948.21  | 302.57 |
| 1  | -8 | -8 | 36.80   | 42.20  |
| -1 | 8  | 8  | -3.40   | 21.50  |
| -1 | 8  | 8  | 8.30    | 26.80  |
| -1 | 7  | -4 | 17.30   | 34.20  |
| 1  | -7 | 2  | 137.39  | 70.09  |
| -1 | 7  | -2 | 139.59  | 67.39  |
| 1  | -7 | 1  | 36.10   | 59.19  |
| 1  | -7 | 1  | 16.00   | 44.20  |
| -1 | 7  | -1 | 21.40   | 42.80  |
| 1  | -7 | 0  | 222.38  | 91.19  |
| 1  | -7 | 0  | 405.46  | 135.29 |
| -1 | 7  | 0  | 359.66  | 123.19 |
| -1 | 7  | 0  | 394.16  | 131.99 |
| 1  | -7 | -1 | 1601.04 | 425.66 |
| 1  | -7 | -1 | 1778.22 | 505.45 |
| -1 | 7  | 1  | 1721.73 | 441.26 |
| -1 | 7  | 1  | 2074.79 | 578.14 |
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| 1  | -6 | 2  | 289.87  | 105.79 |

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| 1  | -6 | -5  | 133.49 | 83.09  |
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| 1  | -6 | -6  | 131.69 | 70.29  |
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| 1  | -6 | -6  | 101.69 | 74.69  |
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| -2 | 4  | -2 | 1891.21 | 496.85 |

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| -2 | 4  | -1 | 1539.45 | 442.36 |
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| -2 | 3  | -3 | 901.21  | 266.77 |
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| 2  | -3 | 1  | 704.83  | 208.28 |
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| 2  | -2 | -3 | 2228.88 | 623.84 |
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| 2  | -1 | -2 | 498.75  | 223.88 |
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| 2  | -1 | -4 | 500.85  | 192.38 |
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| 2  | 0  | 1  | 572.14  | 178.48  |
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| 2  | 0  | 0  | 4334.47 | 1176.78 |

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| 2  | 0 | 0  | 4955.80 | 1202.28 |
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| 2  | 0 | -2 | 2183.88 | 608.14  |
| 2  | 0 | -2 | 2655.13 | 664.53  |
| 2  | 0 | -2 | 2792.52 | 863.31  |
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| 2  | 0 | -3 | 663.63  | 281.27  |
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 -2 -2 0 1783.32 500.95  
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| -2 | -3 | -3 | 941.51  | 250.87 |
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| 2  | 3  | 2  | 51.29   | 87.79  |
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| 2  | 3  | 1  | 513.05  | 152.48 |
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| -2 | -3 | 0  | 859.91  | 225.38 |
| 2  | 3  | -1 | 160.28  | 76.89  |
| 2  | 3  | -1 | 195.58  | 106.29 |
| 2  | 3  | -1 | 242.88  | 102.19 |

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| -2 | -3 | 1  | 219.28  | 92.29  |
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| 2  | 3  | -2 | 923.51  | 366.86 |
| 2  | 3  | -2 | 861.41  | 288.27 |
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| -2 | -3 | 2  | 702.53  | 234.28 |
| 2  | 3  | -3 | 442.96  | 214.68 |
| 2  | 3  | -3 | 149.99  | 97.39  |
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| -2 | -3 | 4  | 1110.59 | 368.36 |
| -2 | -3 | 5  | 746.13  | 206.08 |
| 2  | 3  | -6 | 299.27  | 148.79 |
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| 2  | 4  | 4  | 721.03  | 326.77 |
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| 2  | 4  | 3  | 408.56  | 117.39 |
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| 2  | 4  | 2  | 1683.23 | 416.76 |
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| 2  | 4  | 1  | 649.04  | 177.18 |

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| 2  | 4  | 1  | 534.45  | 241.48 |
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| 2  | 5  | 4  | 283.37  | 87.19  |
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| -2 | -6 | -3 | 621.54  | 257.67 |
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| 2  | 6  | 2  | 621.64  | 162.68 |
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| 2  | 6  | 1  | 644.54  | 219.38 |
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| 2  | 6  | 0  | 228.38  | 127.59 |
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| 2  | 7  | 0  | 106.69 | 57.69  |
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| 2  | 7  | -2 | 293.77 | 114.59 |
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| 2  | 8  | 4  | 243.78 | 127.09 |
| 2  | 8  | 4  | 174.78 | 77.79  |
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| 2  | 8  | 3  | 106.99 | 74.99  |
| 2  | 8  | 3  | 161.38 | 51.29  |
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| 2  | 8  | 2  | 189.28 | 110.59 |
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| 2  | 8  | 1  | 28.40  | 46.90  |

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| -2 | -8 | -1 | 120.39 | 84.39  |
| -2 | -8 | -1 | 239.88 | 95.89  |
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| 2  | 8  | 0  | 19.50  | 51.39  |
| 2  | 8  | 0  | 99.99  | 63.09  |
| -2 | -8 | 0  | 22.00  | 19.50  |
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| 2  | 8  | -1 | 184.78 | 125.79 |
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| 2  | 9  | 5  | 168.88 | 107.69 |
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| 2  | 9  | 1  | -4.20  | 23.30  |
| 2  | 9  | 1  | 18.30  | 25.90  |
| -2 | -9 | -1 | 32.10  | 41.20  |

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| -2 | -9 | -1 | 15.60  | 17.40  |
| 2  | 9  | 0  | 139.99 | 68.59  |
| -2 | -9 | 0  | 25.30  | 33.50  |
| 3  | -6 | 1  | 33.00  | 78.49  |
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| -3 | 6  | 1  | 3.10   | 47.70  |
| 3  | -6 | -2 | 353.56 | 179.78 |
| 3  | -6 | -2 | 662.23 | 248.58 |
| -3 | 6  | 2  | 873.61 | 263.67 |
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| -3 | 6  | 2  | 366.16 | 140.89 |
| 3  | -6 | -3 | 53.49  | 70.89  |
| 3  | -6 | -3 | 16.40  | 47.90  |
| -3 | 6  | 3  | 45.30  | 56.69  |
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| 3  | -5 | 2  | 122.59 | 105.89 |
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| -3 | 5  | -1 | 99.09  | 67.19  |
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| 3  | -5 | 0  | 274.07 | 170.28 |
| 3  | -5 | 0  | 82.19  | 90.39  |
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| -3 | 5  | 0  | 81.89  | 73.49  |
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| -3 | 5  | 1  | 450.55 | 155.38 |
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| 3  | -5 | -2 | 571.84 | 256.77 |
| 3  | -5 | -2 | 609.74 | 232.68 |
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| 3  | -5 | -3 | 365.16 | 174.88 |
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| 3  | -5 | -5 | 86.99  | 73.79  |

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| -3 | 5  | 5  | 84.29   | 63.59  |
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| -3 | 4  | 1  | 995.70  | 305.67 |

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| 3  | -4 | -2 | 227.98 | 121.09 |
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| 3  | -4 | -3 | 623.24 | 272.27 |
| 3  | -4 | -3 | 239.58 | 120.69 |
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| -3 | 4  | 5  | 373.76 | 169.08 |
| -3 | 4  | 5  | 37.10  | 46.40  |
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| 3  | -4 | -6 | 47.30  | 59.09  |
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| -3 | 3  | -3 | 256.37 | 137.49 |
| -3 | 3  | -3 | 131.99 | 96.49  |
| -3 | 3  | -3 | 154.58 | 78.99  |
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| 3  | -3 | 2  | 32.80  | 101.89 |
| 3  | -3 | 2  | 16.40  | 56.09  |
| -3 | 3  | -2 | 3.20   | 40.00  |
| -3 | 3  | -2 | 34.20  | 55.69  |
| 3  | -3 | 1  | 577.14 | 276.57 |
| 3  | -3 | 1  | 95.19  | 70.99  |
| 3  | -3 | 1  | 207.38 | 126.59 |
| -3 | 3  | -1 | 464.95 | 215.78 |
| -3 | 3  | -1 | 86.39  | 77.29  |
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| 3  | -3 | 0  | 218.48 | 155.78 |
| 3  | -3 | 0  | -4.80  | 45.40  |
| -3 | 3  | 0  | 92.79  | 84.49  |
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| -3 | 3  | 0  | 73.99  | 62.89  |
| -3 | 3  | 0  | 23.90  | 51.59  |
| 3  | -3 | -1 | 538.85 | 176.58 |
| 3  | -3 | -1 | 630.74 | 283.77 |
| 3  | -3 | -1 | 745.73 | 277.17 |
| -3 | 3  | 1  | 696.63 | 212.88 |
| -3 | 3  | 1  | 598.44 | 215.48 |
| -3 | 3  | 1  | 454.15 | 175.48 |
| 3  | -3 | -2 | 182.18 | 93.19  |
| 3  | -3 | -2 | 277.87 | 153.08 |
| 3  | -3 | -2 | 102.69 | 82.59  |

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| -3 | 3  | 2  | 191.68 | 100.99 |
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| 3  | -3 | -3 | 152.48 | 103.19 |
| -3 | 3  | 3  | 156.28 | 90.29  |
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| -3 | 3  | 3  | 214.38 | 100.79 |
| -3 | 3  | 3  | 64.09  | 63.29  |
| 3  | -3 | -4 | 721.53 | 303.37 |
| -3 | 3  | 4  | 802.72 | 320.97 |
| -3 | 3  | 4  | 319.87 | 121.29 |
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| 3  | -3 | -5 | 189.98 | 110.69 |
| 3  | -3 | -5 | 83.39  | 69.29  |
| -3 | 3  | 5  | 250.87 | 130.79 |
| -3 | 3  | 5  | 80.09  | 56.59  |
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| 3  | -3 | -6 | 67.49  | 67.69  |
| 3  | -3 | -6 | 6.30   | 50.19  |
| -3 | 3  | 6  | 14.80  | 69.19  |
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| 3  | -2 | 3  | 786.52  | 233.58 |
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| 3  | -2 | 1  | 586.34  | 194.68 |
| 3  | -2 | 1  | 856.11  | 395.46 |
| 3  | -2 | 1  | 698.53  | 217.38 |
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| -3 | 2  | -1 | 776.22  | 336.67 |
| -3 | 2  | -1 | 554.64  | 183.08 |
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| 3  | -2 | -1 | 393.16  | 141.89 |

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| 3  | -2 | -1 | 617.64 | 239.28 |
| -3 | 2  | 1  | 577.84 | 200.78 |
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| 3  | -2 | -2 | 225.18 | 135.19 |
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| 3  | -2 | -4 | 328.47 | 133.39 |
| 3  | -2 | -4 | 53.29  | 64.89  |
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| -3 | 2  | 6  | 124.69 | 74.39  |

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| 3  | -2 | -7 | 238.38  | 129.29 |
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| 3  | -1 | 2  | 694.23  | 212.78 |
| 3  | -1 | 2  | 889.51  | 323.27 |
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| 3  | -1 | 0  | 445.66 | 220.08 |
| 3  | -1 | 0  | 243.28 | 102.89 |
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| -3 | 1  | 2  | 41.50  | 55.09  |
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| 3  | -1 | -3 | 577.74 | 193.08 |
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| 3  | -1 | -7 | 183.18 | 122.99 |
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| -3 | 1  | 7  | 23.30  | 51.29  |
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| 3  | 0  | 4  | 369.26 | 139.29 |
| 3  | 0  | 4  | 772.62 | 345.97 |
| 3  | 0  | 4  | 441.16 | 157.28 |
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| 3  | 0  | 3  | 12.80  | 61.09  |

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| 3  | 0 | 1  | 205.68  | 151.58 |
| 3  | 0 | 1  | 146.99  | 73.09  |
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| 3  | 0 | 0  | 721.93  | 222.08 |
| 3  | 0 | 0  | 672.13  | 206.68 |
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| -3 | 0 | 0  | 1566.34 | 590.44 |
| -3 | 0 | 0  | 833.42  | 285.97 |
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| 3  | 0 | -1 | 100.79  | 79.19  |
| 3  | 0 | -1 | 142.69  | 103.19 |
| 3  | 0 | -1 | 49.60   | 82.59  |
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| 3  | 0 | -2 | 660.33 | 279.77 |
| 3  | 0 | -2 | 753.62 | 236.48 |
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| -3 | 0 | 2  | 718.23 | 291.97 |
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| -3 | 0 | 2  | 596.34 | 220.28 |
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| 3  | 0 | -3 | 617.54 | 200.08 |
| 3  | 0 | -3 | 430.36 | 187.18 |
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| 3  | 0 | -6 | 49.90  | 64.89  |
| 3  | 0 | -6 | 5.80   | 39.40  |
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| 3  | 1  | 6  | 179.08 | 88.19  |
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| 3  | 1  | 5  | 296.07 | 122.29 |
| 3  | 1  | 5  | 61.39  | 48.50  |
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| -3 | -1 | -5 | 238.28 | 95.59  |
| 3  | 1  | 4  | 258.57 | 176.18 |
| 3  | 1  | 4  | 68.59  | 61.69  |
| 3  | 1  | 4  | 139.09 | 97.79  |
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| -3 | -1 | -4 | 85.49  | 81.19  |
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| 3  | 1  | 3  | 59.59  | 49.80  |
| 3  | 1  | 3  | 61.29  | 117.79 |
| 3  | 1  | 3  | 51.39  | 90.69  |
| 3  | 1  | 3  | 36.50  | 58.89  |
| -3 | -1 | -3 | 58.09  | 86.79  |
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| 3  | 1  | 1  | 181.28 | 75.49  |

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| 3  | 1  | 1  | 144.69  | 93.59  |
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| 3  | 1  | 0  | 73.09   | 47.70  |
| 3  | 1  | 0  | 103.29  | 92.59  |
| 3  | 1  | 0  | 76.69   | 89.19  |
| 3  | 1  | 0  | 41.20   | 55.89  |
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| 3  | 1  | -1 | 792.82  | 285.07 |
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| -3 | -1 | 1  | 1061.49 | 337.57 |
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| 3  | 1  | -2 | 1511.15 | 575.84 |
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| -3 | -1 | 3  | 763.52 | 221.08 |
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| 3  | 1  | -5 | 349.57 | 171.78 |
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| 3  | 1  | -6 | 37.60  | 62.39  |
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| 3  | 2  | 5  | 351.16 | 198.78 |
| 3  | 2  | 5  | 32.60  | 53.39  |
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| 3  | 2  | 4  | 24.20  | 114.39 |
| 3  | 2  | 4  | -2.80  | 50.49  |
| 3  | 2  | 4  | 35.40  | 49.60  |
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| 3  | 2  | 3  | 361.76 | 116.29 |
| 3  | 2  | 3  | 561.44 | 176.28 |
| 3  | 2  | 3  | 470.95 | 194.78 |
| 3  | 2  | 3  | 410.96 | 232.48 |
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| -3 | -2 | -3 | 461.85 | 179.98 |

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| 3  | 2  | 2  | 119.29  | 115.69 |
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| 3  | 2  | 2  | 51.69   | 84.59  |
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| -3 | -2 | -2 | 38.70   | 69.39  |
| -3 | -2 | -2 | 55.69   | 50.49  |
| 3  | 2  | 1  | 387.76  | 133.19 |
| 3  | 2  | 1  | 524.45  | 162.68 |
| -3 | -2 | -1 | 1063.79 | 421.56 |
| -3 | -2 | -1 | 551.34  | 173.58 |
| -3 | -2 | -1 | 470.05  | 157.18 |
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| 3  | 2  | 0  | 268.47  | 133.19 |
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| 3  | 2  | -1 | 172.08  | 86.59  |
| 3  | 2  | -1 | 311.27  | 160.08 |
| 3  | 2  | -1 | 228.88  | 91.29  |
| 3  | 2  | -1 | 113.09  | 83.39  |
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| -3 | -2 | 2  | 245.88  | 95.39  |
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| 3  | 2  | -3 | 315.17  | 133.19 |

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| 3  | 2  | -3 | 176.18 | 104.99 |
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| 3  | 2  | -4 | 38.40  | 68.69  |
| -3 | -2 | 4  | 7.90   | 36.70  |
| -3 | -2 | 4  | 22.20  | 59.69  |
| 3  | 2  | -5 | 152.68 | 107.59 |
| 3  | 2  | -5 | 48.70  | 63.29  |
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| 3  | 2  | -6 | 14.00  | 45.10  |
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| -3 | -2 | 6  | 11.90  | 32.30  |
| 3  | 3  | 6  | 109.99 | 63.99  |
| -3 | -3 | -6 | 85.89  | 53.89  |
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| 3  | 3  | 5  | 221.58 | 141.59 |
| 3  | 3  | 5  | 9.30   | 50.49  |
| 3  | 3  | 5  | -12.10 | 32.60  |
| -3 | -3 | -5 | 196.48 | 149.09 |
| -3 | -3 | -5 | 8.10   | 38.50  |
| 3  | 3  | 4  | 654.23 | 199.18 |
| -3 | -3 | -4 | 518.15 | 163.08 |
| -3 | -3 | -4 | 473.15 | 185.28 |
| 3  | 3  | 3  | 151.28 | 63.29  |
| 3  | 3  | 3  | 123.29 | 68.69  |
| 3  | 3  | 3  | 155.18 | 106.79 |
| 3  | 3  | 3  | 200.08 | 146.29 |

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| -3 | -3 | -3 | 169.08 | 104.29 |
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| 3  | 3  | 2  | 350.26 | 124.59 |
| 3  | 3  | 2  | 572.24 | 256.37 |
| 3  | 3  | 2  | 254.17 | 85.59  |
| 3  | 3  | 2  | 19.80  | 55.89  |
| -3 | -3 | -2 | 251.47 | 95.59  |
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| -3 | -3 | -2 | 270.17 | 128.29 |
| -3 | -3 | -2 | 247.68 | 99.79  |
| 3  | 3  | 1  | 667.13 | 197.68 |
| 3  | 3  | 1  | 951.60 | 382.56 |
| 3  | 3  | 1  | 901.91 | 314.27 |
| -3 | -3 | -1 | 622.34 | 257.67 |
| -3 | -3 | -1 | 673.53 | 238.28 |
| -3 | -3 | -1 | 769.72 | 209.78 |
| 3  | 3  | 0  | 187.68 | 92.79  |
| 3  | 3  | 0  | 24.70  | 62.69  |
| -3 | -3 | 0  | 619.64 | 265.87 |
| -3 | -3 | 0  | 164.98 | 78.49  |
| -3 | -3 | 0  | 140.29 | 87.29  |
| 3  | 3  | -1 | 151.98 | 79.59  |
| 3  | 3  | -1 | 349.87 | 173.48 |
| 3  | 3  | -1 | 383.16 | 157.68 |
| -3 | -3 | 1  | 200.18 | 119.29 |
| -3 | -3 | 1  | 203.08 | 112.19 |
| 3  | 3  | -2 | 7.20   | 53.39  |
| -3 | -3 | 2  | 5.60   | 31.80  |
| 3  | 3  | -3 | 44.40  | 62.09  |

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| 3  | 3  | -3 | 14.90  | 54.49  |
| -3 | -3 | 3  | 39.50  | 44.50  |
| 3  | 3  | -4 | 107.39 | 82.89  |
| 3  | 3  | -4 | 62.59  | 58.19  |
| -3 | -3 | 4  | 92.89  | 79.69  |
| 3  | 3  | -5 | 53.89  | 71.79  |
| 3  | 3  | -5 | 18.00  | 48.50  |
| -3 | -3 | 5  | 40.10  | 40.80  |
| 3  | 4  | 6  | 221.18 | 157.78 |
| 3  | 4  | 6  | 147.19 | 71.29  |
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| 3  | 4  | 5  | 71.49  | 102.99 |
| 3  | 4  | 5  | 87.79  | 61.99  |
| 3  | 4  | 5  | 52.29  | 41.80  |
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| 3  | 4  | 4  | 12.00  | 30.80  |
| 3  | 4  | 4  | 291.17 | 175.98 |
| 3  | 4  | 4  | 1.60   | 50.59  |
| -3 | -4 | -4 | 122.49 | 107.09 |
| -3 | -4 | -4 | 1.70   | 36.20  |
| -3 | -4 | -4 | 20.30  | 24.20  |
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| 3  | 4  | 3  | 428.16 | 216.98 |
| 3  | 4  | 3  | 239.28 | 74.59  |
| 3  | 4  | 3  | 226.08 | 127.49 |
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| -3 | -4 | -3 | 318.77 | 106.99 |
| 3  | 4  | 2  | 403.16 | 205.18 |
| 3  | 4  | 2  | 72.89  | 74.59  |
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| 3  | 4  | 1  | 1100.39 | 311.77 |
| 3  | 4  | 1  | 1197.28 | 324.67 |
| 3  | 4  | 1  | 1303.17 | 433.86 |
| 3  | 4  | 1  | 1305.77 | 505.45 |
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| 3  | 4  | 0  | 644.04  | 187.28 |
| 3  | 4  | 0  | 583.44  | 249.08 |
| 3  | 4  | 0  | 451.45  | 179.08 |
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| -3 | -4 | 0  | 497.25  | 177.58 |
| -3 | -4 | 0  | 389.66  | 126.49 |
| 3  | 4  | -1 | 258.37  | 104.09 |
| -3 | -4 | 1  | 160.08  | 67.79  |
| 3  | 4  | -2 | 228.58  | 102.99 |
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| 3  | 5  | 6  | 549.05  | 256.27 |
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| 3  | 5  | 5  | 816.02  | 228.78 |

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| -3 | -5 | -5 | 819.52 | 222.38 |
| -3 | -5 | -5 | 559.54 | 163.78 |
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| 3  | 5  | 4  | 232.38 | 84.69  |
| 3  | 5  | 4  | 253.17 | 158.08 |
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| 3  | 5  | 3  | 104.19 | 53.49  |
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| 3  | 5  | 2  | 62.39  | 70.69  |
| 3  | 5  | 2  | -0.10  | 47.90  |
| 3  | 5  | 2  | 36.30  | 24.70  |
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| 3  | 5  | 1  | 72.09  | 51.09  |
| 3  | 5  | 1  | 40.70  | 68.19  |
| -3 | -5 | -1 | 117.79 | 79.79  |
| 3  | 5  | 0  | 272.57 | 139.79 |
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| 3  | 5  | -1 | 88.49  | 68.89  |
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| 3  | 5  | -2 | 74.89  | 69.79  |
| -3 | -5 | 2  | 113.49 | 56.99  |
| -3 | -5 | 2  | 16.10  | 48.90  |
| 3  | 5  | -3 | 44.80  | 58.79  |
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| -3 | -5 | 3  | 1.20   | 44.80  |

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| 3  | 5  | -4 | 50.19  | 71.39  |
| -3 | -5 | 4  | 29.10  | 34.00  |
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| 3  | 6  | 4  | 203.38 | 62.59  |
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| 3  | 6  | 3  | 173.88 | 55.59  |
| 3  | 6  | 3  | 290.67 | 152.28 |
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| -3 | -7 | -6 | 181.38 | 69.89  |

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| 3  | 7  | 5  | 51.29  | 76.79  |
| -3 | -7 | -5 | 76.89  | 65.39  |
| 3  | 7  | 4  | 84.09  | 80.29  |
| 3  | 7  | 4  | 19.90  | 11.10  |
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| 3  | 7  | 3  | 90.59  | 31.80  |
| 3  | 7  | 3  | 85.69  | 87.19  |
| -3 | -7 | -3 | 18.10  | 29.10  |
| -3 | -7 | -3 | 6.90   | 49.50  |
| 3  | 7  | 2  | 100.19 | 81.69  |
| -3 | -7 | -2 | 98.39  | 46.60  |
| -3 | -7 | -2 | 105.89 | 72.39  |
| 3  | 7  | 1  | 71.19  | 65.69  |
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| 3  | 7  | 0  | 49.70  | 55.19  |
| -3 | -7 | 0  | 21.20  | 25.10  |
| -4 | 1  | -2 | 22.00  | 34.60  |
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| -4 | 1  | 0  | 160.98 | 90.19  |
| -4 | 1  | 0  | 151.78 | 98.99  |
| 4  | 0  | 3  | 27.10  | 45.90  |
| 4  | 0  | 3  | 24.80  | 74.79  |
| -4 | 0  | -3 | 24.80  | 67.19  |
| -4 | 0  | -3 | 83.59  | 73.19  |
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| 4  | 0  | 2  | 187.68 | 92.69  |

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| -4 | 0  | -2 | 288.97 | 119.59 |
| -4 | 0  | -2 | 167.68 | 100.89 |
| 4  | 0  | 1  | 225.48 | 137.09 |
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| 4  | 0  | -1 | 33.20  | 65.29  |
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| 4  | 1  | 3  | 137.69 | 125.89 |
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| -4 | -1 | -3 | 190.78 | 83.89  |
| 4  | 1  | 2  | 534.15 | 175.98 |
| 4  | 1  | 2  | 528.45 | 264.87 |
| -4 | -1 | -2 | 677.73 | 221.38 |
| -4 | -1 | -2 | 754.72 | 284.67 |
| -4 | -1 | -2 | 556.44 | 180.28 |
| 4  | 1  | 1  | 94.49  | 83.19  |
| 4  | 1  | 1  | 30.90  | 38.30  |
| 4  | 1  | 0  | 101.39 | 70.69  |
| 4  | 1  | 0  | 120.39 | 94.19  |
| -4 | -1 | 0  | 747.33 | 272.87 |
| -4 | -1 | 0  | 300.87 | 122.29 |
| -4 | -1 | 0  | 132.59 | 83.19  |
| 4  | 1  | -1 | 42.90  | 57.79  |
| 4  | 1  | -1 | 132.79 | 85.69  |
| -4 | -1 | 1  | -6.80  | 52.79  |

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| 4  | 2  | 3  | 13.80  | 36.80  |
| -4 | -2 | -3 | 22.50  | 34.10  |
| 4  | 2  | 2  | 142.29 | 79.39  |
| 4  | 2  | 2  | 98.59  | 88.89  |
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| -4 | -2 | -2 | 289.17 | 143.69 |
| -4 | -2 | -2 | 220.18 | 91.59  |
| 4  | 2  | 1  | 10.20  | 29.90  |
| -4 | -2 | -1 | 32.60  | 42.70  |
| -4 | -2 | -1 | 84.29  | 72.29  |
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| 4  | 2  | 0  | 17.10  | 44.70  |
| -4 | -2 | 0  | 63.59  | 60.59  |
| -4 | -2 | 0  | 172.58 | 112.39 |
| -4 | -2 | 0  | 37.60  | 44.20  |
| -4 | -3 | -3 | 81.59  | 91.49  |
| 4  | 3  | 2  | 62.09  | 73.99  |
| -4 | -3 | -2 | 66.09  | 67.69  |
| -4 | -3 | -2 | 136.79 | 110.79 |
| 4  | 3  | 1  | 17.40  | 51.19  |
| -4 | -3 | -1 | 104.89 | 66.89  |
| -4 | -3 | -1 | 104.79 | 77.59  |
| -4 | -3 | -1 | -1.70  | 20.70  |
| 0  | 0  | 0  | 0.00   | 0.00   |

\_computing\_structure\_solution 'SHELXT 2018/2 (Sheldrick, 2018)'

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\_shelx\_hkl\_checksum 3872

\_olex2\_submission\_special\_instructions 'No special instructions were received'