Supporting Information for

Solid-State 1D → 3D Transformation of Polynitrile-Based Coordination Polymers by Dehydration Reaction

Artem O. Dmitrienko,[a,b] Mikhail I. Buzin,[b] Zouaoui Setifi,[c,d] Eugeny V. Alexandrov,[e,f] Eugenia D. Voronova,[a] Fatima Setifi,[d] and Anna V. Vologzhanina[a,]*

a A. N. Nesmeyanov Institute of Organoelement Compounds, RAS. 28 Vavilova str. 119991 Moscow, Russia.

b Lomonosov Moscow State University. GSP1 Leninskie Gory 119991 Moscow, Russia.

c Département de Technologie, Faculté de Technologie, Université 20 Août 1955-Skikda, Skikda 21000, Algeria.

d Laboratoire de Chimie, Ingénierie Moléculaire et Nanostructures (LCIMN), Université Ferhat Abbas Sétif 1, Sétif 19000, Algeria.

e Samara Polytech, Molodogvardeyskaya str. 244, 443100 Samara, Russia.

f Samara Branch of P. N. Lebedev Physical Institute of the Russian Academy of Sciences, Novo-Sadovaya str. 221, 443011 Samara, Russia

Powder XRD data of **1** and **2**.

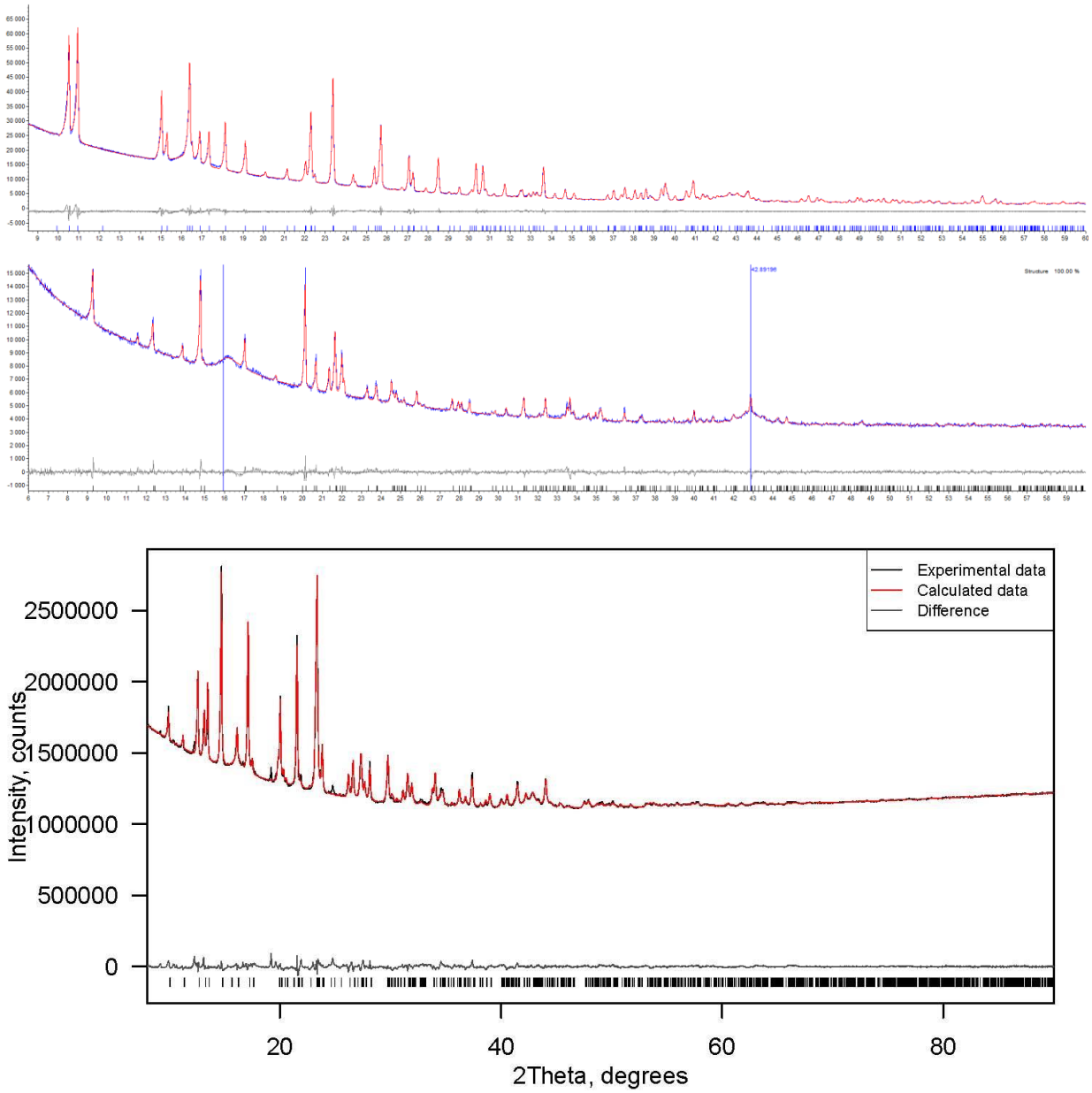

Figure S1. Observed (black), calculated (red) and difference profiles (gray) for the Rietveld refinement of (top) **1**, (middle) **2** and (bottom) **4**.

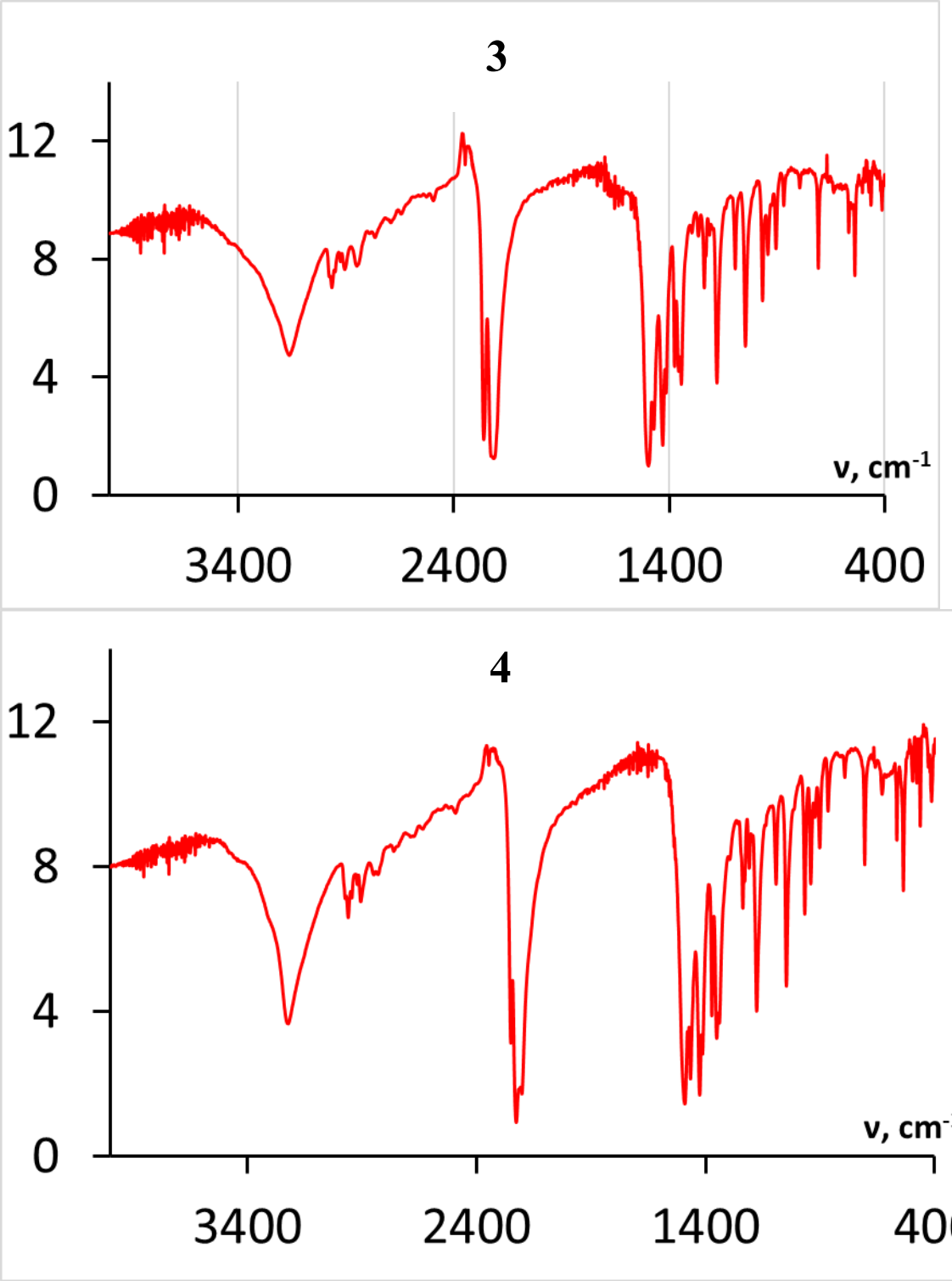

Figure S2. FT-IR spectra of studied compounds (top) **3** and (bottom) **4**.

TGA data

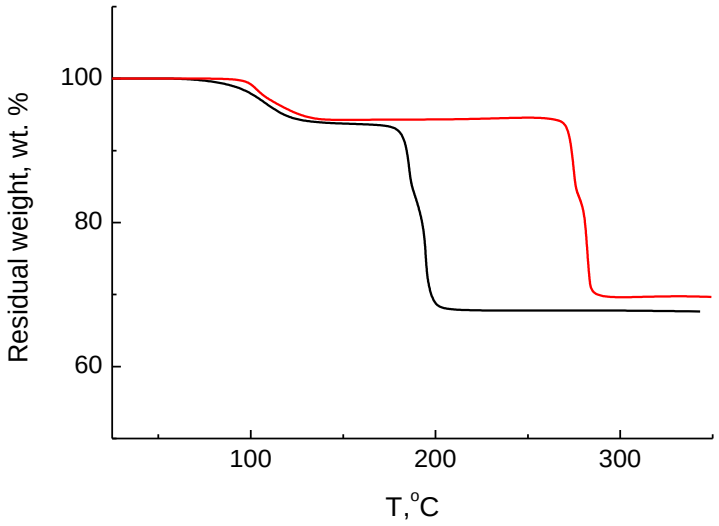

Figure S3. The thermal curves for (red) **1** and (black) **2**.

Analysis of subnet/supernet relations.

Notation of coordination modes and networks.

There is strong dependence between coordination modes of ligands at one hand, and theoretically possible nets and their occurrences in crystalline materials at the other.[S1-S4] Thus, there is need in notation of coordination modes that can be automatically processed to analyze and predict topology of underlying nets. We use notation described by some of us in Ref. [S5]. Within this notation the total denticity of a ligand is denoted as *M* for mono-, *B* for bi-, *T* for tri-, *K* for tetra-, *P* for penta-, *G* for hexa-, *H* for hepta-, *O* for octa-, *N* for nona- and *D* for decadenticity. The way in which *A* atoms surround the ligand is denoted by numerical superscripts (*mbtkpghond*). The superscripts define the `partial' denticity of the ligand with respect to any *A* atom (*m* – mono-, *b* – bi-, *t* – tri-, …, *d* – decadenticity). The number of *A* atoms with respect to the ligand that exhibits the corresponding partial denticity is denoted by the numerical value of the corresponding superscript. Then the coordination type of an *i*th ligand is given as $D_i^{mbtkpghond}$. This notation allows to calculate the total number of complexing atoms (*Z*) which surround the ligand, and the total number of chemical bonds that the ligand makes with the central atom (N_B). In the general case for a ligand with a $D_i^{mbtkpghond}$ coordination type

$Z = m + b + t + k + p + g + h + o + n + d,$

$N_B = 1m + 2b + 3t + 4k + 5p + 6g + 7h + 8o + 9n + 10d.$

Table S1 Potential contacts in the invironment of Co1 in structure of compound **1**

Atom	Symmetry code of edges	Distance, Å
N1	(-x-y-z)(-10-1); within unit cell	1.9902
N1	(-x-y-z)(00-1); (-100)	6.7929
N2	(-x-y-z)(-10-1); (00-1)	4.1737
N2	(-x-y-z)(-10-1); within unit cell	6.1161
N2	(-x-y-z)(-1-10); (0-1-1)	6.9115
N3	(-x-y-z); (-100)	4.6211
N3	(-x-y-z)(-100); (00-1)	4.4666
N4	(-x-y-z); (-10-1)	4.1849
N4	(-x-y-z)(0-10); (-11-1)	6.0434
O1	(-x-y-z)(00-1); (-100)	2.2903
O1	(-x-y-z)(-10-1); within unit cell	5.1537

Table S2 Potential contacts in the invironment of Ni1 in structure of compound **2**

Atom	Symmetry code of edges	Distance, Å
N1	(-x-y-z)(-100); (0-10)	2.1023
N1	(-x-y-z); (-1-10)	6.6732
N2	(-x-y-z)(0-10); (-100)	2.0907
N2	(-x-y-z)(-100); (0-10)	6.9348
N2	(-x-y-z); (-1-10)	6.8607
N3	(-x-y-z)(-100); (0-10)	3.9255
N3	(-x-y-z); (-1-10)	5.326
N3	(-x-y-z)(0-10); (-100)	6.1484
N4	(-x-y-z)(00-1); (-1-11)	5.1559
N4	(-x-y-z); (-1-10)	5.6816
N4	(-x-y-z)(-100); (0-10)	6.4896
O3	(-x-y-z)(-100); (0-10)	3.9473
O3	(-x-y-z)(-10-1); (0-11)	6.5739

Table S3. Supercells used for screening of the network transitions in structure of compound **1**, number of transitions (*N*), and their distribution over 3,6-c underlying nets with tridentate ligands.

Supercell	*N*	1D	2D				3D					
		3,6C1	3,6L60	3,6L64	3,6L66	3,6L83	**kgd**	**alb**-3,6-*C2/c*	**alb**-3,6-*P4$_2$/mnm*	**ant**	**flu**-3,6-*C2/c*	**rtl**	**sit**
(2a,b,c)	27225			208			311	156			698	342	
(2a,b,c; ½,0,0)	74613				8		1709			2268			
(-a,2b+2c,-c)	74613				184	360	1599			1150			
(-a,2b+2c,-c; 0,½,0)	27225			28			863	116	40		568	192	
(a,b,2b+2c)	27225			204			331	84	72		954	396	
(a,b,2b+2c; 0,0,½)	74613				4	8	1599			2374			
(a+c,-a-b+c,a-c)	27225			4			519	72			1000	324	
(a+c,-a-b+c,a-c; ½,0,0)	74613	216	448				663			1530			13
(-a-b,-b-c,2a)	74613	196	1272				637			1408			32
(-a-b,-b-c,2a; ½,0,0)	27225			24			499	44			928	214	
(2b,-a-b,c)	74613				8		1709			2268			
(2b,-a-b,c; ½,0,0)	27225			180			339	40			802	192	
(-a,-b-c,-2b)	74613				24	48	1233			2044			
(-a,-b-c,-2b; 0,½,0)	74613			184			391	112	44	894		250	

Unit cells that contain two independent metal atoms and two anions are marked with gray.

Table S4. Supercells used for screening of the network transitions in structure of compound **2**, number of transitions (*N*), and their distribution over 3,6-c underlying nets with tridentate ligands.

Supercell	*N*	**kgd**	**ant**	**flu**-3,6-C2/c	**rtl**
(-b,2a-2c,-a+2c)	230230	1009	1164		
(-b,2a-2c,-a+2c; 0,0,½)	81796	1009		1164	
(2a-b,2a-b-c,b)	81796	1009		1536	
(2a-b,2a-b-c,b; ½,0,0)	230230	1009	1536		
(-a,a-2b,-a-b+c)	230230	2005	1716		
(-a,a-2b,-a-b+c; 0,½,0)	81796	1009			996
(a+c,b-c,2c)	230230	1009	1692		
(a+c,b-c,2c; ½,0,0)	81796	1009		1692	
(a-2b,2b,c)	81796	1009		1032	
(a-2b,2b,c; 0,½,0)	230230	1009	1032		
(a-b,a-b-c,a+b)	81796	1009			864
(a-b,a-b-c,a+b; ½,0,0)	230230	1873	1848		
(-a-b+c,-b+2c,-a+b-c)	230230	1861	1860		
(-a-b+c,-b+2c,-a+b-c; ½,0,0)	81796	1009			852

Unit cells that contain two independent metal atoms and two anions are marked with gray.

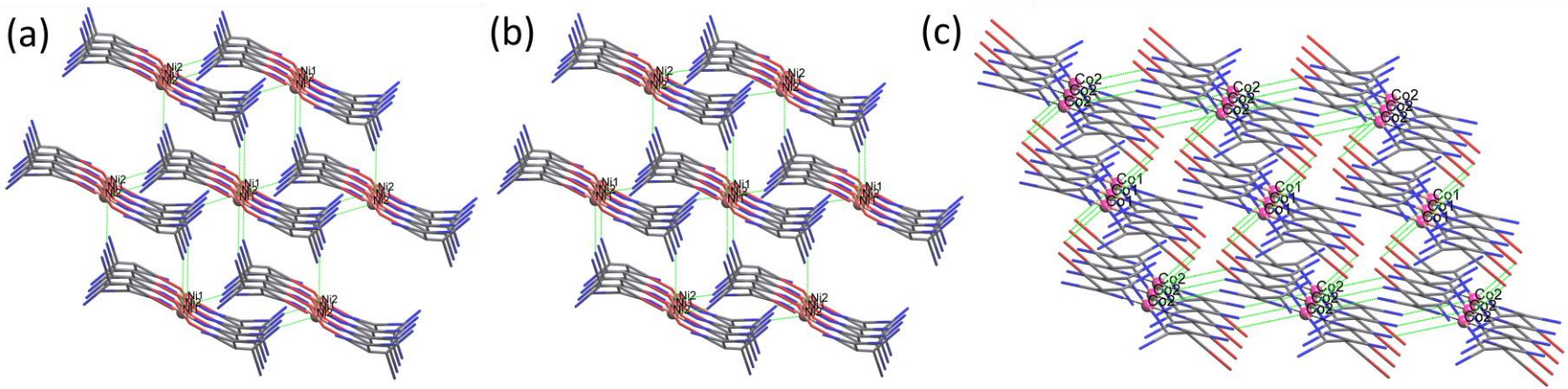

Figure S4. Closest neighborhood of metal atoms forming novel coordination bonds.

References:

S1. T. G. Mitina and V. A. Blatov *Cryst Growth & Des.*, 2013, **13**, 1655.

S2. E. V. Alexandrov, A. V. Virovets, V. A. Blatov and E. V. Peresypkina *Chem. Rev.* 2015, **115**, 12286.

S3. E. V. Alexandrov, A. P. Shevchenko, A. A. Asiri and V. A. Blatov *CrystEngComm*, 2015, **17**, 2913.

S4. E. V. Alexandrov, A. P. Shevchenko and V. A. Blatov *Cryst Growth & Des.*, 2019, **19**, 2604.

S5. V. N. Serezhkin, A. V. Vologzhanina, L. B. Serezhkina, E. S. Smirnova, E. V. Grachova, P. V. Ostrova and M. Yu. Antipin, *Acta Crystallogr., Sect. B*, 2009, **65**, 45.

CIF files of **1** and **2** in doubled unit cells with removed water molecules and a corrected connectivity of atoms identical with that of, respectively, **3** and **4**.

```
data_1-TOPOS_f31_start/P-1->P-1(a+c,-a-b+c,a-c)[Ind=2];Bondsets:1,6,10,17,19,21
_audit_creation_date              2020-04-09
_audit_creation_method            ToposPro
_chemical_formula_structural      'f31_start/P -1->P -1 (a+c,-a-b+c,a-c)[Ind=2];Bond sets:
1,6,10,17,19,21'
_chemical_name_systematic
;
?.
;
_chemical_formula_sum             'C20 H18 N8 Ni1 O6'
_citation_special_details
;
Temperature: 296(2). Experiment details: ?. Experiment details: ?. Fi
le: f31.cif.
CENTAT: Ni1 Ni2
LIGAND: C10H7N4O2[T3] C10H7N4O2[T3] H
2O[0D] H2O[0D]
ATOMLIG: H2#1 H12#1 O5#1 H3#2 H11#2 O2#2 H1#3 H4#3 H5
#3 H6#3 H7#3 H8#3 H9#3 H10#4 H13#4 H14#4 H15#4 H16#4 H17#4 H18#4 C1#3
 C2#3 C3#3 C4#3 C5#3 C6#3 C7#3 C8#3 C9#3 C10#3 C11#4 C12#4 C13#4 C14#
4 C15#4 C16#4 C17#4 C18#4 C19#4 C20#4 N1#3 N2#3 N3#3 N4#3 N5#4 N6#4 N
7#4 N8#4 O1#3 O3#3 O4#4 O6#4
SIMPPAR: METH=Stand; INTRA=V
;
_cell_length_a                    9.1887
_cell_length_b                    12.5105
_cell_length_c                    11.88307
_cell_angle_alpha                 107.5305
_cell_angle_beta                  67.40137
_cell_angle_gamma                 107.8335
_cell_volume                      1174.072
_cell_formula_units_Z             2
_symmetry_space_group_name_H-M    'P -1'
_symmetry_Int_Tables_number       2
_refine_ls_R_factor_all           0.0344
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
loop_
_atom_site_label
_atom_site_type_symbol
```

_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 2 0.53710 0.25630 0.18430 1.0000
H2 H 2 0.23440 0.54200 0.57530 1.0000
H3 H 2 0.32380 0.08985 0.96935 1.0000
H4 H 2 0.73600 0.31715 0.91885 1.0000
H5 H 2 0.92450 0.36015 0.86605 1.0000
H6 H 2 0.86840 0.19490 0.94080 1.0000
H7 H 2 0.95850 0.29885 0.01925 1.0000
H8 H 2 0.71270 0.31365 0.17945 1.0000
H9 H 2 0.75270 0.19355 0.15345 1.0000
H10 H 2 0.53710 0.75630 0.68430 1.0000
H11 H 2 0.23440 0.04200 0.07530 1.0000
H12 H 2 0.32380 0.58985 0.46935 1.0000
H13 H 2 0.73600 0.81715 0.41885 1.0000
H14 H 2 0.92450 0.86015 0.36605 1.0000
H15 H 2 0.86840 0.69490 0.44080 1.0000
H16 H 2 0.95850 0.79885 0.51925 1.0000
H17 H 2 0.71270 0.81365 0.67945 1.0000
H18 H 2 0.75270 0.69355 0.65345 1.0000
C1 C 2 0.64973 0.57276 0.24337 1.0000
C2 C 2 0.69596 0.60680 0.12942 1.0000
C3 C 2 0.68129 0.71773 0.13306 1.0000
C4 C 2 0.66909 0.60074 0.89076 1.0000
C5 C 2 0.77735 0.54655 0.89981 1.0000
C6 C 2 0.90694 0.52086 0.79014 1.0000
C7 C 2 0.76530 0.53477 0.01686 1.0000
C8 C 2 0.83419 0.34824 0.94102 1.0000
C9 C 2 0.85785 0.26693 0.00067 1.0000
C10 C 2 0.72408 0.24215 0.11885 1.0000
C11 C 2 0.64973 0.07276 0.74337 1.0000
C12 C 2 0.69596 0.10680 0.62942 1.0000
C13 C 2 0.68129 0.21773 0.63306 1.0000
C14 C 2 0.66909 0.10074 0.39076 1.0000
C15 C 2 0.77735 0.04655 0.39981 1.0000
C16 C 2 0.90694 0.02086 0.29013 1.0000
C17 C 2 0.76530 0.03477 0.51686 1.0000
C18 C 2 0.83419 0.84824 0.44102 1.0000
C19 C 2 0.85785 0.76693 0.50067 1.0000
C20 C 2 0.72408 0.74215 0.61885 1.0000
N1 N 2 0.61285 0.54633 0.33619 1.0000
N2 N 2 0.67413 0.80766 0.13270 1.0000
N3 N 2 0.57732 0.64193 0.88436 1.0000

N4 N 2 0.01461 0.50542 0.70168 1.0000
N5 N 2 0.61285 0.04634 0.83618 1.0000
N6 N 2 0.67413 0.30766 0.63270 1.0000
N7 N 2 0.57732 0.14194 0.38436 1.0000
N8 N 2 0.01461 0.00542 0.20168 1.0000
O1 O 2 0.57275 0.18658 0.09733 1.0000
O2 O 2 0.30128 0.02980 0.00004 1.0000
O3 O 2 0.82347 0.45605 0.03195 1.0000
O4 O 2 0.57275 0.68659 0.59733 1.0000
O5 O 2 0.30128 0.52980 0.50004 1.0000
O6 O 2 0.82347 0.95605 0.53195 1.0000
Ni1 Ni 1 0.50000 0.00000 0.00000 1.0000
Ni2 Ni 1 0.50000 0.50000 0.50000 1.0000
loop_
_topol_link.node_label_1
_topol_link.node_label_2
_topol_link.distance
_topol_link.site_symmetry_symop_1
_topol_link.site_symmetry_translation_1_x
_topol_link.site_symmetry_translation_1_y
_topol_link.site_symmetry_translation_1_z
_topol_link.site_symmetry_symop_2
_topol_link.site_symmetry_translation_2_x
_topol_link.site_symmetry_translation_2_y
_topol_link.site_symmetry_translation_2_z
_topol_link.type
_topol_link.multiplicity
_topol_link.voronoi_solidangle
H1 O1 1.1436 1 0 0 0 1 0 0 0 V 2 27.75
H1 H8 1.5382 1 0 0 0 1 0 0 0 W 2 17.67
H1 C10 1.6323 1 0 0 0 1 0 0 0 W 2 5.21
H1 N3 2.3446 1 0 0 0 2 1 1 1 W 2 14.90
H1 H10 1.4806 1 0 0 0 2 1 1 1 W 2 23.04
H2 O5 0.8681 1 0 0 0 1 0 0 0 V 2 32.38
H2 N1 2.6613 1 0 0 0 2 1 1 1 W 2 8.65
H2 H15 2.7920 1 0 0 0 2 1 1 1 W 2 6.39
H2 H8 3.0613 1 0 0 0 2 1 1 1 W 2 7.95
H2 O4 3.1468 1 0 0 0 1 0 0 0 W 2 2.50
H2 N4 2.0151 1 0 0 0 1 0 0 0 H 2 24.17
H3 O2 0.8672 1 0 0 0 1 0 0 1 V 2 32.70
H3 N5 2.6441 1 0 0 0 1 0 0 0 W 2 9.23
H3 O1 2.9799 1 0 0 0 1 0 0 1 W 2 5.50
H3 N3 3.3074 1 0 0 0 2 1 1 2 W 2 5.56
H3 N8 4.0433 1 0 0 0 2 0 0 1 W 2 2.37
H3 N2 2.0047 1 0 0 0 2 1 1 1 H 2 25.03
H4 C8 0.9699 1 0 0 0 1 0 0 0 V 2 28.45

H4 O1 2.7491 1 0 0 0 1 0 0 1 W 2 7.27
H4 C5 2.8441 1 0 0 0 1 0 0 0 W 2 5.67
H4 N3 3.0044 1 0 0 0 2 1 1 2 W 2 8.92
H4 N5 3.1977 1 0 0 0 1 0 0 0 W 2 3.75
H4 C11 3.2046 1 0 0 0 1 0 0 0 W 2 5.61
H4 C13 3.4230 1 0 0 0 1 0 0 0 W 2 5.05
H4 N2 3.8222 1 0 0 0 2 1 1 1 W 2 2.84
H4 C3 3.9880 1 0 0 0 2 1 1 1 W 2 1.87
H5 C8 0.9698 1 0 0 0 1 0 0 0 V 2 28.24
H5 C6 2.5071 1 0 0 0 1 0 0 0 W 2 10.40
H5 O3 3.0555 1 0 0 0 2 2 1 1 W 2 6.29
H5 H15 3.3687 1 0 0 0 2 2 1 1 W 2 5.93
H5 C2 3.4036 1 0 0 0 2 2 1 1 W 2 3.06
H5 H14 3.4568 1 0 0 0 2 2 1 1 W 2 5.77
H5 C1 3.5267 1 0 0 0 2 2 1 1 W 2 3.67
H6 C9 0.9705 1 0 0 0 1 0 0 1 V 2 27.91
H6 H11 2.7920 1 0 0 0 2 1 0 1 W 2 6.39
H6 N8 2.8281 1 0 0 0 2 1 0 1 W 2 11.21
H6 O2 2.9139 1 0 0 0 2 1 0 1 W 2 3.27
H6 N5 2.9482 1 0 0 0 1 0 0 0 W 2 7.18
H6 H14 3.3687 1 0 0 0 2 2 1 1 W 2 5.93
H7 C9 0.9701 1 0 0 0 1 0 0 0 V 2 27.85
H7 C7 2.7246 1 0 0 0 2 2 1 0 W 2 7.29
H7 C5 2.8906 1 0 0 0 2 2 1 1 W 2 5.38
H7 C6 3.0188 1 0 0 0 2 2 1 1 W 2 7.28
H7 C2 3.0405 1 0 0 0 2 2 1 0 W 2 2.89
H7 C3 3.1408 1 0 0 0 2 2 1 0 W 2 6.15
H8 C10 0.9701 1 0 0 0 1 0 0 0 V 2 26.55
H8 O3 2.5848 1 0 0 0 1 0 0 0 W 2 10.05
H8 N1 3.1370 1 0 0 0 1 0 0 0 W 2 5.29
H8 N4 3.2737 1 0 0 0 2 1 1 1 W 2 5.63
H8 C1 3.2783 1 0 0 0 1 0 0 0 W 2 2.20
H9 C10 0.9693 1 0 0 0 1 0 0 0 V 2 27.83
H9 N7 2.7523 1 0 0 0 1 0 0 0 W 2 10.57
H9 O2 2.8560 1 0 0 0 2 1 0 0 W 2 10.38
H9 C16 3.8823 1 0 0 0 1 0 0 0 W 2 3.45
H10 O4 1.1436 1 0 0 0 1 0 0 0 V 2 27.75
H10 H17 1.5382 1 0 0 0 1 0 0 0 W 2 17.67
H10 C20 1.6323 1 0 0 0 1 0 0 0 W 2 5.21
H10 N7 2.3446 1 0 0 0 2 1 1 1 W 2 14.90
H11 O2 0.8681 1 0 0 0 1 0 0 0 V 2 32.38
H11 N5 2.6613 1 0 0 0 2 1 0 1 W 2 8.65
H11 H17 3.0613 1 0 0 0 2 1 1 1 W 2 7.95
H11 O1 3.1468 1 0 0 0 1 0 0 0 W 2 2.50
H11 N8 2.0151 1 0 0 0 1 0 0 0 H 2 24.17
H12 O5 0.8672 1 0 0 0 1 0 0 0 V 2 32.70

H12 N1 2.6441 1 0 0 0 1 0 0 0 W 2 9.23
H12 O4 2.9799 1 0 0 0 1 0 0 0 W 2 5.50
H12 N7 3.3074 1 0 0 0 2 1 1 1 W 2 5.56
H12 N4 4.0433 1 0 0 0 2 0 1 1 W 2 2.37
H12 N6 2.0047 1 0 0 0 2 1 1 1 H 2 25.03
H13 C18 0.9699 1 0 0 0 1 0 0 0 V 2 28.45
H13 O4 2.7491 1 0 0 0 1 0 0 0 W 2 7.27
H13 C15 2.8441 1 0 0 0 1 0 1 0 W 2 5.67
H13 N7 3.0044 1 0 0 0 2 1 1 1 W 2 8.92
H13 N1 3.1977 1 0 0 0 1 0 0 0 W 2 3.75
H13 C1 3.2046 1 0 0 0 1 0 0 0 W 2 5.61
H13 C3 3.4230 1 0 0 0 1 0 0 0 W 2 5.05
H13 N6 3.8222 1 0 0 0 2 1 1 1 W 2 2.84
H13 C13 3.9880 1 0 0 0 2 1 1 1 W 2 1.87
H14 C18 0.9698 1 0 0 0 1 0 0 0 V 2 28.24
H14 C16 2.5071 1 0 0 0 1 0 1 0 W 2 10.40
H14 O6 3.0555 1 0 0 0 2 2 2 1 W 2 6.29
H14 C12 3.4036 1 0 0 0 2 2 1 1 W 2 3.06
H14 C11 3.5267 1 0 0 0 2 2 1 1 W 2 3.67
H15 C19 0.9705 1 0 0 0 1 0 0 0 V 2 27.91
H15 N4 2.8281 1 0 0 0 2 1 1 1 W 2 11.21
H15 O5 2.9139 1 0 0 0 2 1 1 1 W 2 3.27
H15 N1 2.9482 1 0 0 0 1 0 0 0 W 2 7.18
H16 C19 0.9701 1 0 0 0 1 0 0 0 V 2 27.85
H16 C17 2.7246 1 0 0 0 2 2 1 1 W 2 7.29
H16 C15 2.8906 1 0 0 0 2 2 1 1 W 2 5.38
H16 C16 3.0188 1 0 0 0 2 2 1 1 W 2 7.28
H16 C12 3.0405 1 0 0 0 2 2 1 1 W 2 2.89
H16 C13 3.1408 1 0 0 0 2 2 1 1 W 2 6.15
H17 C20 0.9701 1 0 0 0 1 0 0 0 V 2 26.55
H17 O6 2.5848 1 0 0 0 1 0 0 0 W 2 10.05
H17 N5 3.1370 1 0 0 0 1 0 1 0 W 2 5.29
H17 N8 3.2737 1 0 0 0 2 1 1 1 W 2 5.63
H17 C11 3.2783 1 0 0 0 1 0 1 0 W 2 2.20
H18 C20 0.9693 1 0 0 0 1 0 0 0 V 2 27.83
H18 N3 2.7523 1 0 0 0 1 0 0 0 W 2 10.57
H18 O5 2.8560 1 0 0 0 2 1 1 1 W 2 10.38
H18 C6 3.8823 1 0 0 0 1 0 0 0 W 2 3.45
C1 N1 1.1421 1 0 0 0 1 0 0 0 V 2 34.12
C1 C2 1.4107 1 0 0 0 1 0 0 0 V 2 28.57
C1 O3 2.6698 1 0 0 0 1 0 0 0 W 2 6.88
C1 N3 3.2274 1 0 0 0 2 1 1 1 W 2 6.00
C1 N6 3.3606 1 0 0 0 2 1 1 1 W 2 5.27
C2 C7 1.4063 1 0 0 0 1 0 0 0 V 2 27.20
C2 C3 1.4212 1 0 0 0 1 0 0 0 V 2 28.91
C2 N3 3.3524 1 0 0 0 2 1 1 1 W 2 1.79

C3 N2 1.1483 1 0 0 0 1 0 0 0 V 2 34.87
C3 C4 2.8380 1 0 0 0 1 0 0 -1 W 2 7.39
C3 N6 3.3801 1 0 0 0 2 1 1 1 W 2 6.32
C4 N3 1.1496 1 0 0 0 1 0 0 0 V 2 34.56
C4 C5 1.4142 1 0 0 0 1 0 0 0 V 2 29.34
C4 C4 3.9616 1 0 0 0 2 1 1 2 W 1 2.44
C4 N6 4.0089 1 0 0 0 1 0 0 0 W 2 2.05
C5 C7 1.4013 1 0 0 0 1 0 0 1 V 2 27.38
C5 C6 1.4174 1 0 0 0 1 0 0 0 V 2 27.98
C6 N4 1.1474 1 0 0 0 1 1 0 0 V 2 34.63
C6 N6 3.4301 1 0 0 0 1 0 0 0 W 2 5.81
C7 O3 1.3380 1 0 0 0 1 0 0 0 V 2 27.70
C7 N3 3.2613 1 0 0 0 2 1 1 1 W 2 4.21
C8 O3 1.4553 1 0 0 0 1 0 0 1 V 2 20.79
C8 C9 1.5076 1 0 0 0 1 0 0 1 V 2 17.83
C9 C10 1.5104 1 0 0 0 1 0 0 0 V 2 17.84
C10 O1 1.4340 1 0 0 0 1 0 0 0 V 2 17.86
C11 N5 1.1421 1 0 0 0 1 0 0 0 V 2 34.12
C11 C12 1.4107 1 0 0 0 1 0 0 0 V 2 28.57
C11 O6 2.6698 1 0 0 0 1 0 -1 0 W 2 6.88
C11 N7 3.2274 1 0 0 0 2 1 0 1 W 2 6.00
C11 N2 3.3606 1 0 0 0 2 1 1 1 W 2 5.27
C12 C17 1.4063 1 0 0 0 1 0 0 0 V 2 27.20
C12 C13 1.4212 1 0 0 0 1 0 0 0 V 2 28.91
C12 N7 3.3524 1 0 0 0 2 1 0 1 W 2 1.79
C13 N6 1.1483 1 0 0 0 1 0 0 0 V 2 34.87
C13 C14 2.8380 1 0 0 0 1 0 0 0 W 2 7.39
C13 N2 3.3801 1 0 0 0 2 1 1 1 W 2 6.32
C14 N7 1.1496 1 0 0 0 1 0 0 0 V 2 34.56
C14 C15 1.4142 1 0 0 0 1 0 0 0 V 2 29.34
C14 C14 3.9616 1 0 0 0 2 1 0 1 W 1 2.44
C14 N2 4.0089 1 0 0 0 1 0 -1 0 W 2 2.05
C15 C17 1.4013 1 0 0 0 1 0 0 0 V 2 27.38
C15 C16 1.4174 1 0 0 0 1 0 0 0 V 2 27.98
C16 N8 1.1474 1 0 0 0 1 1 0 0 V 2 34.63
C16 N2 3.4301 1 0 0 0 1 0 -1 0 W 2 5.81
C17 O6 1.3380 1 0 0 0 1 0 -1 0 V 2 27.70
C17 N7 3.2613 1 0 0 0 2 1 0 1 W 2 4.21
C18 O6 1.4553 1 0 0 0 1 0 0 0 V 2 20.79
C18 C19 1.5076 1 0 0 0 1 0 0 0 V 2 17.83
C19 C20 1.5104 1 0 0 0 1 0 0 0 V 2 17.84
C20 O4 1.4340 1 0 0 0 1 0 0 0 V 2 17.86
N1 Ni2 1.9902 1 0 0 0 1 0 0 0 V 2 17.27
N1 O5 2.7615 1 0 0 0 1 0 0 0 W 2 1.78
N1 O4 3.0136 1 0 0 0 1 0 0 0 W 2 3.44
N1 Ni1 6.7929 1 0 0 0 1 0 0 0 N 2 0.00

N2 N3 3.3167 1 0 0 0 1 0 0 -1 W 2 2.85
N2 N8 3.5481 1 0 0 0 1 1 1 0 W 2 4.63
N2 Ni1 4.1737 1 0 0 0 1 0 1 0 N 2 0.00
N2 Ni2 6.1161 1 0 0 0 1 0 0 0 N 2 0.00
N2 Ni1 6.9115 1 0 0 0 1 1 1 0 N 2 0.00
N3 Ni2 4.6211 1 0 0 0 1 0 0 0 V 2 0.00
N3 O3 3.3480 1 0 0 0 2 1 1 1 W 2 1.94
N3 Ni1 4.4666 1 0 0 0 1 0 1 1 N 2 0.00
N4 N6 3.5481 1 0 0 0 1 -1 0 0 W 2 4.63
N4 Ni2 4.1849 1 0 0 0 1 0 0 0 N 2 0.00
N4 Ni2 6.0434 1 0 0 0 1 -1 0 0 N 2 0.00
N5 Ni1 1.9902 1 0 0 0 1 0 0 1 V 2 17.27
N5 O2 2.7615 1 0 0 0 1 0 0 1 W 2 1.78
N5 O1 3.0136 1 0 0 0 1 0 0 1 W 2 3.44
N5 Ni2 6.7929 1 0 0 0 1 0 -1 0 N 2 0.00
N6 N7 3.3167 1 0 0 0 1 0 0 0 W 2 2.85
N6 Ni2 4.1737 1 0 0 0 1 0 0 0 N 2 0.00
N6 Ni1 6.1161 1 0 0 0 1 0 0 1 N 2 0.00
N6 Ni2 6.9115 1 0 0 0 1 1 0 0 N 2 0.00
N7 O6 3.3480 1 0 0 0 2 1 1 1 W 2 1.94
N7 Ni1 4.6211 1 0 0 0 1 0 0 0 N 2 0.00
N7 Ni2 4.4666 1 0 0 0 1 0 0 0 N 2 0.00
N8 Ni1 4.1849 1 0 0 0 1 0 0 0 V 2 0.00
N8 Ni1 6.0434 1 0 0 0 1 -1 0 0 N 2 0.00
O1 Ni1 2.2903 1 0 0 0 1 0 0 0 V 2 13.76
O1 O2 3.0016 1 0 0 0 2 1 0 0 W 2 2.10
O1 Ni2 5.1537 1 0 0 0 1 0 0 0 N 2 0.00
O2 Ni1 1.9721 1 0 0 0 1 0 0 0 S 2 15.96
O3 O3 2.9555 1 0 0 0 2 2 1 0 W 1 6.36
O4 Ni2 2.2903 1 0 0 0 1 0 0 0 V 2 13.76
O4 O5 3.0016 1 0 0 0 2 1 1 1 W 2 2.10
O4 Ni1 5.1537 1 0 0 0 1 0 1 1 N 2 0.00
O5 Ni2 1.9721 1 0 0 0 1 0 0 0 S 2 15.96
O6 O6 2.9555 1 0 0 0 2 2 2 1 W 1 6.36
#End of data_1-TOPOS_f31_start/P-1->P-1(a+c,-a-b+c,a-c)[Ind=2];Bondsets:1,6,10,17,19,21

data_1-TOPOS_f31_start/P-1->P-1(2b,-a-b,c;1/2,0,0)[Ind=2];Bondsets:1,4,8,10,19,21
_audit_creation_date 2020-04-09
_audit_creation_method ToposPro
_chemical_formula_structural 'f31_start/P -1->P -1 (2b,-a-b,c; 1/2,0,0)[Ind=2];Bond sets: 1,4,8,10,19,21'
_chemical_name_systematic
;
?.
;
_chemical_formula_sum 'C20 H18 N8 Ni1 O6'

```
_citation_special_details
;
Temperature: 296(2). Experiment details: ?. Experiment details: ?. Fi
le: f31.cif.
CENTAT: Ni1 Ni2
LIGAND: C10H7N4O2[T3] C10H7N4O2[T3] H
2O[0D] H2O[0D]
ATOMLIG: H7#1 H8#1 O2#1 H11#2 H12#2 O5#2 H1#3 H2#3 H3
#3 H4#3 H5#3 H6#3 H9#3 H10#4 H13#4 H14#4 H15#4 H16#4 H17#4 H18#4 C1#3
 C2#3 C3#3 C4#3 C5#3 C6#3 C7#3 C8#3 C9#3 C10#3 C11#4 C12#4 C13#4 C14#
4 C15#4 C16#4 C17#4 C18#4 C19#4 C20#4 N1#4 N2#3 N3#3 N4#3 N5#4 N6#4 N
7#4 N8#3 O1#3 O3#3 O4#4 O6#4
SIMPPAR: METH=Stand; INTRA=V
;
_cell_length_a                 11.96771
_cell_length_b                 11.38943
_cell_length_c                 9.8397
_cell_angle_alpha               67.7645
_cell_angle_beta                107.1662
_cell_angle_gamma                103.7474
_cell_volume                   1174.072
_cell_formula_units_Z           2
_symmetry_space_group_name_H-M     'P -1'
_symmetry_Int_Tables_number       2
_refine_ls_R_factor_all          0.0344
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 2 0.79985 0.04715 0.04010 1.0000
H2 H 2 0.85290 0.14020 0.13420 1.0000
H3 H 2 0.88830 0.92980 0.27960 1.0000
H4 H 2 0.75205 0.88365 0.25410 1.0000
H5 H 2 0.82535 0.90085 0.49410 1.0000
H6 H 2 0.73600 0.00000 0.39830 1.0000
H7 H 2 0.44150 0.11770 0.12050 1.0000
H8 H 2 0.42585 0.19145 0.96670 1.0000
```

H9 H 2 0.73885 0.20175 0.07200 1.0000
H10 H 2 0.76115 0.29825 0.92800 1.0000
H11 H 2 0.07415 0.30855 0.03330 1.0000
H12 H 2 0.05850 0.38230 0.87950 1.0000
H13 H 2 0.76400 0.50000 0.60170 1.0000
H14 H 2 0.67465 0.59915 0.50590 1.0000
H15 H 2 0.74795 0.61635 0.74590 1.0000
H16 H 2 0.61170 0.57020 0.72040 1.0000
H17 H 2 0.64710 0.35980 0.86580 1.0000
H18 H 2 0.70015 0.45285 0.95990 1.0000
C1 C 2 0.79254 0.06846 0.12330 1.0000
C2 C 2 0.81273 0.95487 0.26626 1.0000
C3 C 2 0.81173 0.97754 0.40722 1.0000
C4 C 2 0.90846 0.14316 0.51791 1.0000
C5 C 2 0.85897 0.95203 0.73073 1.0000
C6 C 2 0.86186 0.08450 0.64674 1.0000
C7 C 2 0.83029 0.16121 0.70998 1.0000
C8 C 2 0.01604 0.33476 0.58467 1.0000
C9 C 2 0.96609 0.27013 0.47739 1.0000
C10 C 2 0.98293 0.33320 0.32939 1.0000
C11 C 2 0.51707 0.16680 0.67061 1.0000
C12 C 2 0.53391 0.22987 0.52261 1.0000
C13 C 2 0.48396 0.16524 0.41533 1.0000
C14 C 2 0.66971 0.33879 0.29002 1.0000
C15 C 2 0.63814 0.41550 0.35326 1.0000
C16 C 2 0.64103 0.54797 0.26927 1.0000
C17 C 2 0.59154 0.35684 0.48209 1.0000
C18 C 2 0.68827 0.52246 0.59278 1.0000
C19 C 2 0.68727 0.54513 0.73374 1.0000
C20 C 2 0.70746 0.43154 0.87670 1.0000
N1 N 2 0.36085 0.34624 0.80374 1.0000
N2 N 2 0.80181 0.22449 0.75757 1.0000
N3 N 2 0.05725 0.38311 0.67496 1.0000
N4 N 2 0.99769 0.38484 0.21015 1.0000
N5 N 2 0.50231 0.11517 0.78985 1.0000
N6 N 2 0.44275 0.11689 0.32504 1.0000
N7 N 2 0.69819 0.27551 0.24243 1.0000
N8 N 2 0.13915 0.15376 0.19626 1.0000
O1 O 2 0.90574 0.08226 0.42410 1.0000
O2 O 2 0.41556 0.11428 0.02976 1.0000
O3 O 2 0.67833 0.10559 0.08925 1.0000
O4 O 2 0.82167 0.39441 0.91075 1.0000
O5 O 2 0.08444 0.38572 0.97024 1.0000
O6 O 2 0.59426 0.41774 0.57590 1.0000
Ni1 Ni 1 0.50000 0.00000 0.00000 1.0000
Ni2 Ni 1 0.00000 0.50000 0.00000 1.0000

```
loop_
_topol_link.node_label_1
_topol_link.node_label_2
_topol_link.distance
_topol_link.site_symmetry_symop_1
_topol_link.site_symmetry_translation_1_x
_topol_link.site_symmetry_translation_1_y
_topol_link.site_symmetry_translation_1_z
_topol_link.site_symmetry_symop_2
_topol_link.site_symmetry_translation_2_x
_topol_link.site_symmetry_translation_2_y
_topol_link.site_symmetry_translation_2_z
_topol_link.type
_topol_link.multiplicity
_topol_link.voronoi_solidangle
H1 C1 0.9693 1 0 0 0 1 0 0 0 V 2 27.83
H1 N2 2.7523 1 0 0 0 1 0 0 -1 W 2 10.57
H1 O2 2.8560 1 0 0 0 2 1 0 0 W 2 10.38
H1 C5 3.8823 1 0 0 0 1 0 -1 -1 W 2 3.45
H2 C1 0.9701 1 0 0 0 1 0 0 0 V 2 26.55
H2 H9 1.5382 1 0 0 0 1 0 0 0 W 2 17.67
H2 O1 2.5848 1 0 0 0 1 0 0 0 W 2 10.05
H2 H11 3.0613 1 0 0 0 1 1 0 0 W 2 7.95
H2 N4 3.1370 1 0 0 0 1 0 0 0 W 2 5.29
H2 N8 3.2737 1 0 0 0 1 1 0 0 W 2 5.63
H2 C10 3.2783 1 0 0 0 1 0 0 0 W 2 2.20
H3 C2 0.9701 1 0 0 0 1 0 0 0 V 2 27.85
H3 C4 2.7246 1 0 0 0 2 2 1 1 W 2 7.29
H3 C6 2.8906 1 0 0 0 2 2 1 1 W 2 5.38
H3 C5 3.0188 1 0 0 0 2 2 2 1 W 2 7.28
H3 C9 3.0405 1 0 0 0 2 2 1 1 W 2 2.89
H3 C8 3.1408 1 0 0 0 2 1 1 1 W 2 6.15
H4 C2 0.9705 1 0 0 0 1 0 0 0 V 2 27.91
H4 H8 2.7920 1 0 0 0 2 1 1 1 W 2 6.39
H4 N1 2.8281 1 0 0 0 2 1 1 1 W 2 11.21
H4 O2 2.9139 1 0 0 0 2 1 1 0 W 2 3.27
H4 N5 2.9482 1 0 0 0 2 1 1 1 W 2 7.18
H4 H14 3.3687 1 0 0 0 1 0 0 0 W 2 5.93
H5 C3 0.9698 1 0 0 0 1 0 0 0 V 2 28.24
H5 C5 2.5071 1 0 0 0 1 0 0 0 W 2 10.40
H5 O1 3.0555 1 0 0 0 2 2 1 1 W 2 6.29
H5 H15 3.3687 1 0 0 0 1 0 0 0 W 2 5.93
H5 C9 3.4036 1 0 0 0 2 2 1 1 W 2 3.06
H5 H14 3.4568 1 0 0 0 1 0 0 0 W 2 5.77
H5 C10 3.5267 1 0 0 0 2 2 1 1 W 2 3.67
H6 C3 0.9699 1 0 0 0 1 0 -1 0 V 2 28.45
```

H6 O3 2.7491 1 0 0 0 1 0 0 0 W 2 7.27
H6 C6 2.8441 1 0 0 0 1 0 0 0 W 2 5.67
H6 N7 3.0044 1 0 0 0 1 0 0 0 W 2 8.92
H6 N5 3.1977 1 0 0 0 2 1 0 1 W 2 3.75
H6 C11 3.2046 1 0 0 0 2 1 0 1 W 2 5.61
H6 C13 3.4230 1 0 0 0 2 1 0 1 W 2 5.05
H6 N6 3.8222 1 0 0 0 1 0 0 0 W 2 2.84
H6 C13 3.9880 1 0 0 0 1 0 0 0 W 2 1.87
H7 O2 0.8672 1 0 0 0 1 0 0 0 V 2 32.70
H7 N5 2.6441 1 0 0 0 2 1 0 1 W 2 9.23
H7 O3 2.9799 1 0 0 0 1 0 0 0 W 2 5.50
H7 N7 3.3074 1 0 0 0 1 0 0 0 W 2 5.56
H7 N8 4.0433 1 0 0 0 1 0 0 0 W 2 2.37
H7 N6 2.0047 1 0 0 0 1 0 0 0 H 2 25.03
H8 O2 0.8681 1 0 0 0 1 0 0 1 V 2 32.38
H8 N5 2.6613 1 0 0 0 1 0 0 0 W 2 8.65
H8 H17 3.0613 1 0 0 0 1 0 0 0 W 2 7.95
H8 O3 3.1468 1 0 0 0 1 0 0 1 W 2 2.50
H8 N1 2.0151 1 0 0 0 1 0 0 0 H 2 24.17
H9 O3 1.1436 1 0 0 0 1 0 0 0 V 2 27.75
H9 C1 1.6323 1 0 0 0 1 0 0 0 W 2 5.21
H9 N7 2.3446 1 0 0 0 1 0 0 0 W 2 14.90
H9 H10 1.4806 1 0 0 0 1 0 0 -1 W 2 23.04
H10 O4 1.1436 1 0 0 0 1 0 0 0 V 2 27.75
H10 H17 1.5382 1 0 0 0 1 0 0 0 W 2 17.67
H10 C20 1.6323 1 0 0 0 1 0 0 0 W 2 5.21
H10 N2 2.3446 1 0 0 0 1 0 0 0 W 2 14.90
H11 O5 0.8681 1 0 0 0 1 0 0 -1 V 2 32.38
H11 N4 2.6613 1 0 0 0 1 -1 0 0 W 2 8.65
H11 H15 2.7920 1 0 0 0 2 1 1 1 W 2 6.39
H11 O4 3.1468 1 0 0 0 1 -1 0 -1 W 2 2.50
H11 N8 2.0151 1 0 0 0 1 0 0 0 H 2 24.17
H12 O5 0.8672 1 0 0 0 1 0 0 0 V 2 32.70
H12 N4 2.6441 1 0 0 0 2 1 1 1 W 2 9.23
H12 O4 2.9799 1 0 0 0 1 -1 0 0 W 2 5.50
H12 N2 3.3074 1 0 0 0 1 -1 0 0 W 2 5.56
H12 N1 4.0433 1 0 0 0 1 0 0 0 W 2 2.37
H12 N3 2.0047 1 0 0 0 1 0 0 0 H 2 25.03
H13 C18 0.9699 1 0 0 0 1 0 0 0 V 2 28.45
H13 O4 2.7491 1 0 0 0 1 0 0 0 W 2 7.27
H13 C15 2.8441 1 0 0 0 1 0 0 0 W 2 5.67
H13 N2 3.0044 1 0 0 0 1 0 0 0 W 2 8.92
H13 N4 3.1977 1 0 0 0 2 2 1 1 W 2 3.75
H13 C10 3.2046 1 0 0 0 2 2 1 1 W 2 5.61
H13 C8 3.4230 1 0 0 0 2 1 1 1 W 2 5.05
H13 N3 3.8222 1 0 0 0 1 1 0 0 W 2 2.84

H13 C8 3.9880 1 0 0 0 1 1 0 0 W 2 1.87
H14 C18 0.9698 1 0 0 0 1 0 0 0 V 2 28.24
H14 C16 2.5071 1 0 0 0 1 0 0 0 W 2 10.40
H14 O6 3.0555 1 0 0 0 2 1 1 1 W 2 6.29
H14 C12 3.4036 1 0 0 0 2 1 1 1 W 2 3.06
H14 C11 3.5267 1 0 0 0 2 1 1 1 W 2 3.67
H15 C19 0.9705 1 0 0 0 1 0 0 0 V 2 27.91
H15 N8 2.8281 1 0 0 0 2 1 1 1 W 2 11.21
H15 O5 2.9139 1 0 0 0 2 1 1 2 W 2 3.27
H15 N4 2.9482 1 0 0 0 2 2 1 1 W 2 7.18
H16 C19 0.9701 1 0 0 0 1 0 0 0 V 2 27.85
H16 C17 2.7246 1 0 0 0 2 1 1 1 W 2 7.29
H16 C15 2.8906 1 0 0 0 2 1 1 1 W 2 5.38
H16 C16 3.0188 1 0 0 0 2 1 1 1 W 2 7.28
H16 C12 3.0405 1 0 0 0 2 1 1 1 W 2 2.89
H16 C13 3.1408 1 0 0 0 2 1 1 1 W 2 6.15
H17 C20 0.9701 1 0 0 0 1 0 0 0 V 2 26.55
H17 O6 2.5848 1 0 0 0 1 0 0 0 W 2 10.05
H17 N5 3.1370 1 0 0 0 1 0 0 0 W 2 5.29
H17 N1 3.2737 1 0 0 0 1 0 0 0 W 2 5.63
H17 C11 3.2783 1 0 0 0 1 0 0 0 W 2 2.20
H18 C20 0.9693 1 0 0 0 1 0 0 0 V 2 27.83
H18 N7 2.7523 1 0 0 0 1 0 0 1 W 2 10.57
H18 O5 2.8560 1 0 0 0 2 1 1 2 W 2 10.38
H18 C16 3.8823 1 0 0 0 1 0 0 1 W 2 3.45
C1 O3 1.4340 1 0 0 0 1 0 0 0 V 2 17.86
C1 C2 1.5104 1 0 0 0 1 0 -1 0 V 2 17.84
C2 C3 1.5076 1 0 0 0 1 0 0 0 V 2 17.83
C3 O1 1.4553 1 0 0 0 1 0 1 0 V 2 20.79
C4 O1 1.3380 1 0 0 0 1 0 0 0 V 2 27.70
C4 C6 1.4013 1 0 0 0 1 0 0 0 V 2 27.38
C4 C9 1.4063 1 0 0 0 1 0 0 0 V 2 27.20
C4 N7 3.2613 1 0 0 0 1 0 0 0 W 2 4.21
C5 N8 1.1474 1 0 0 0 2 1 1 1 V 2 34.63
C5 C6 1.4174 1 0 0 0 1 0 1 0 V 2 27.98
C5 N6 3.4301 1 0 0 0 2 1 1 1 W 2 5.81
C6 C7 1.4142 1 0 0 0 1 0 0 0 V 2 29.34
C7 N2 1.1496 1 0 0 0 1 0 0 0 V 2 34.56
C7 C8 2.8380 1 0 0 0 1 1 0 0 W 2 7.39
C7 C14 3.9616 1 0 0 0 1 0 0 0 W 2 2.44
C7 N6 4.0089 1 0 0 0 2 1 0 1 W 2 2.05
C8 N3 1.1483 1 0 0 0 1 0 0 0 V 2 34.87
C8 C9 1.4212 1 0 0 0 1 -1 0 0 V 2 28.91
C8 N3 3.3801 1 0 0 0 2 0 1 1 W 2 6.32
C9 C10 1.4107 1 0 0 0 1 0 0 0 V 2 28.57
C9 N7 3.3524 1 0 0 0 1 0 0 0 W 2 1.79

C10 N4 1.1421 1 0 0 0 1 0 0 0 V 2 34.12
C10 O1 2.6698 1 0 0 0 1 0 0 0 W 2 6.88
C10 N7 3.2274 1 0 0 0 1 0 0 0 W 2 6.00
C10 N3 3.3606 1 0 0 0 2 1 1 1 W 2 5.27
C11 N5 1.1421 1 0 0 0 1 0 0 0 V 2 34.12
C11 C12 1.4107 1 0 0 0 1 0 0 0 V 2 28.57
C11 O6 2.6698 1 0 0 0 1 0 0 0 W 2 6.88
C11 N2 3.2274 1 0 0 0 1 0 0 0 W 2 6.00
C11 N6 3.3606 1 0 0 0 2 1 0 1 W 2 5.27
C12 C17 1.4063 1 0 0 0 1 0 0 0 V 2 27.20
C12 C13 1.4212 1 0 0 0 1 0 0 0 V 2 28.91
C12 N2 3.3524 1 0 0 0 1 0 0 0 W 2 1.79
C13 N6 1.1483 1 0 0 0 1 0 0 0 V 2 34.87
C13 C14 2.8380 1 0 0 0 1 0 0 0 W 2 7.39
C13 N6 3.3801 1 0 0 0 2 1 0 1 W 2 6.32
C14 N7 1.1496 1 0 0 0 1 0 0 0 V 2 34.56
C14 C15 1.4142 1 0 0 0 1 0 0 0 V 2 29.34
C14 N3 4.0089 1 0 0 0 2 1 1 1 W 2 2.05
C15 C17 1.4013 1 0 0 0 1 0 0 0 V 2 27.38
C15 C16 1.4174 1 0 0 0 1 0 0 0 V 2 27.98
C16 N1 1.1474 1 0 0 0 2 1 1 1 V 2 34.63
C16 N3 3.4301 1 0 0 0 2 1 1 1 W 2 5.81
C17 O6 1.3380 1 0 0 0 1 0 0 0 V 2 27.70
C17 N2 3.2613 1 0 0 0 1 0 0 0 W 2 4.21
C18 O6 1.4553 1 0 0 0 1 0 0 0 V 2 20.79
C18 C19 1.5076 1 0 0 0 1 0 0 0 V 2 17.83
C19 C20 1.5104 1 0 0 0 1 0 0 0 V 2 17.84
C20 O4 1.4340 1 0 0 0 1 0 0 0 V 2 17.86
N1 Ni1 4.1849 1 0 0 0 1 0 0 1 V 2 0.00
N1 N3 3.5481 1 0 0 0 1 0 0 0 W 2 4.63
N1 Ni2 6.0434 1 0 0 0 1 0 0 1 N 2 0.00
N2 Ni2 4.4666 1 0 0 0 1 1 0 1 V 2 0.00
N2 N3 3.3167 1 0 0 0 1 1 0 0 W 2 2.85
N2 O6 3.3480 1 0 0 0 1 0 0 0 W 2 1.94
N2 Ni1 4.6211 1 0 0 0 1 0 0 1 N 2 0.00
N3 Ni2 4.1737 1 0 0 0 1 0 0 1 N 2 0.00
N3 Ni2 6.1161 1 0 0 0 1 0 0 0 N 2 0.00
N3 Ni1 6.9115 1 0 0 0 1 0 0 1 N 2 0.00
N4 Ni2 1.9902 1 0 0 0 1 1 0 0 V 2 17.27
N4 O5 2.7615 1 0 0 0 2 1 1 1 W 2 1.78
N4 O4 3.0136 1 0 0 0 2 2 1 1 W 2 3.44
N4 Ni1 6.7929 1 0 0 0 1 0 0 0 N 2 0.00
N5 Ni1 1.9902 1 0 0 0 1 0 0 1 V 2 17.27
N5 O2 2.7615 1 0 0 0 2 1 0 1 W 2 1.78
N5 O3 3.0136 1 0 0 0 2 1 0 1 W 2 3.44
N5 Ni2 6.7929 1 0 0 0 1 1 0 1 N 2 0.00

N6 N7 3.3167 1 0 0 0 1 0 0 0 W 2 2.85
N6 N8 3.5481 1 0 0 0 1 0 0 0 W 2 4.63
N6 Ni1 4.1737 1 0 0 0 1 0 0 0 N 2 0.00
N6 Ni1 6.1161 1 0 0 0 1 0 0 1 N 2 0.00
N6 Ni2 6.9115 1 0 0 0 1 0 0 0 N 2 0.00
N7 O1 3.3480 1 0 0 0 1 0 0 0 W 2 1.94
N7 Ni2 4.6211 1 0 0 0 1 1 0 0 N 2 0.00
N7 Ni1 4.4666 1 0 0 0 1 0 0 0 N 2 0.00
N8 Ni2 4.1849 1 0 0 0 1 0 0 0 N 2 0.00
N8 Ni1 6.0434 1 0 0 0 1 0 0 0 N 2 0.00
O1 O1 2.9555 1 0 0 0 2 2 0 1 W 1 6.36
O2 Ni1 1.9721 1 0 0 0 1 0 0 0 S 2 15.96
O2 O3 3.0016 1 0 0 0 2 1 0 0 W 2 2.10
O3 Ni1 2.2903 1 0 0 0 1 0 0 0 V 2 13.76
O3 Ni2 5.1537 1 0 0 0 1 1 0 0 N 2 0.00
O4 Ni2 2.2903 1 0 0 0 1 1 0 1 V 2 13.76
O4 O5 3.0016 1 0 0 0 2 1 1 2 W 2 2.10
O4 Ni1 5.1537 1 0 0 0 1 0 0 1 N 2 0.00
O5 Ni2 1.9721 1 0 0 0 1 0 0 1 S 2 15.96
O6 O6 2.9555 1 0 0 0 2 1 1 1 W 1 6.36
#End of data_1-TOPOS_f31_start/P-1->P-1(2b,-a-b,c;1/2,0,0)[Ind=2];Bondsets:1,4,8,10,19,21

data_1-TOPOS_f32_start/P-1->P-1(a+c,b-c,2c;1/2,0,0)[Ind=2];Bondsets:1,3,14,20,23,25
_audit_creation_date 2020-04-09
_audit_creation_method ToposPro
_chemical_formula_structural 'f32_start/P -1->P -1 (a+c,b-c,2c; 1/2,0,0)[Ind=2];Bond sets:
1,3,14,20,23,25'
_chemical_name_systematic
;
?.
;
_chemical_formula_sum 'C20 Co1 H18 N8 O6'
_citation_special_details
;
Temperature: 296(2). Experiment details: ?. Experiment details: ?. Fi
le: f32_start.cif.
CENTAT: Co1 Co2
LIGAND: C10H7N4O2[T3] C10H7N4O2
[T3] H2O[0D] H2O[0D]
ATOMLIG: H1#1 H2#1 O5#1 H10#2 H11#2 O2#2 H3#3 H
4#3 H5#3 H6#3 H7#3 H8#4 H9#4 H12#4 H13#4 H14#4 H15#4 H16#4 H17#3 H18#
3 C1#4 C2#4 C3#4 C4#4 C5#4 C6#3 C7#4 C8#4 C9#3 C10#3 C11#3 C12#3 C13#
3 C14#3 C15#3 C16#4 C17#3 C18#3 C19#4 C20#4 N1#4 N2#4 N3#4 N4#4 N5#3
N6#3 N7#3 N8#3 O1#4 O3#3 O4#3 O6#4
SIMPPAR: METH=Stand; INTRA=V
;

```
_cell_length_a                  11.2012
_cell_length_b                  8.679428
_cell_length_c                  13.51053
_cell_angle_alpha                104.743
_cell_angle_beta                 70.44721
_cell_angle_gamma                104.1514
_cell_volume                    1178.566
_cell_formula_units_Z            2
_symmetry_space_group_name_H-M     'P -1'
_symmetry_Int_Tables_number       2
_refine_ls_R_factor_all           0.0391
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 2 0.97380 0.29510 0.33800 1.0000
H2 H 2 0.91660 0.41880 0.34090 1.0000
H3 H 2 0.24085 0.50945 0.67675 1.0000
H4 H 2 0.85315 0.25975 0.87355 1.0000
H5 H 2 0.92330 0.34030 0.77220 1.0000
H6 H 2 0.04240 0.31480 0.92040 1.0000
H7 H 2 0.06790 0.21750 0.80280 1.0000
H8 H 2 0.74030 0.92700 0.31100 1.0000
H9 H 2 0.64765 0.05475 0.35965 1.0000
H10 H 2 0.47380 0.79510 0.83800 1.0000
H11 H 2 0.41660 0.91880 0.84090 1.0000
H12 H 2 0.74085 0.00945 0.17675 1.0000
H13 H 2 0.35315 0.75975 0.37355 1.0000
H14 H 2 0.42330 0.84030 0.27220 1.0000
H15 H 2 0.54240 0.81480 0.42040 1.0000
H16 H 2 0.56790 0.71750 0.30280 1.0000
H17 H 2 0.24030 0.42700 0.81100 1.0000
H18 H 2 0.14765 0.55475 0.85965 1.0000
C1 C 2 0.19445 0.98679 0.38510 1.0000
C2 C 2 0.34757 0.24314 0.41129 1.0000
C3 C 2 0.12103 0.04606 0.34076 1.0000
C4 C 2 0.25488 0.34131 0.43560 1.0000
```

C5 C 2 0.31267 0.07491 0.40075 1.0000
C6 C 2 0.92132 0.34415 0.84509 1.0000
C7 C 2 0.13944 0.83877 0.41909 1.0000
C8 C 2 0.47725 0.31763 0.39965 1.0000
C9 C 2 0.04930 0.32039 0.84785 1.0000
C10 C 2 0.16062 0.45253 0.81109 1.0000
C11 C 2 0.69445 0.48679 0.88510 1.0000
C12 C 2 0.84757 0.74314 0.91129 1.0000
C13 C 2 0.62103 0.54606 0.84076 1.0000
C14 C 2 0.75488 0.84131 0.93560 1.0000
C15 C 2 0.81267 0.57491 0.90075 1.0000
C16 C 2 0.42131 0.84416 0.34508 1.0000
C17 C 2 0.63943 0.33877 0.91909 1.0000
C18 C 2 0.97725 0.81763 0.89965 1.0000
C19 C 2 0.54931 0.82038 0.34785 1.0000
C20 C 2 0.66062 0.95253 0.31109 1.0000
N1 N 2 0.17472 0.41623 0.45752 1.0000
N2 N 2 0.09121 0.71789 0.44773 1.0000
N3 N 2 0.05999 0.08931 0.30246 1.0000
N4 N 2 0.58360 0.37804 0.38901 1.0000
N5 N 2 0.67472 0.91623 0.95753 1.0000
N6 N 2 0.59121 0.21789 0.94773 1.0000
N7 N 2 0.55999 0.58931 0.80246 1.0000
N8 N 2 0.08360 0.87805 0.88902 1.0000
O1 O 2 0.39925 0.00207 0.41039 1.0000
O2 O 2 0.48562 0.90020 0.84851 1.0000
O3 O 2 0.16825 0.46528 0.70576 1.0000
O4 O 2 0.89925 0.50207 0.91039 1.0000
O5 O 2 0.98562 0.40020 0.34851 1.0000
O6 O 2 0.66825 0.96528 0.20576 1.0000
Co1 Co 1 0.00000 0.50000 0.50000 1.0000
Co2 Co 1 0.50000 0.00000 0.00000 1.0000
loop_
_topol_link.node_label_1
_topol_link.node_label_2
_topol_link.distance
_topol_link.site_symmetry_symop_1
_topol_link.site_symmetry_translation_1_x
_topol_link.site_symmetry_translation_1_y
_topol_link.site_symmetry_translation_1_z
_topol_link.site_symmetry_symop_2
_topol_link.site_symmetry_translation_2_x
_topol_link.site_symmetry_translation_2_y
_topol_link.site_symmetry_translation_2_z
_topol_link.type
_topol_link.multiplicity

_topol_link.voronoi_solidangle
H1 O5 0.8703 1 0 0 0 1 0 0 0 V 2 31.98
H1 N2 2.7638 1 0 0 0 2 1 1 1 W 2 9.90
H1 C18 3.0087 1 0 0 0 2 2 1 1 W 2 5.42
H1 N1 3.0314 1 0 0 0 1 1 0 0 W 2 3.51
H1 C12 3.2714 1 0 0 0 2 2 1 1 W 2 2.86
H1 H8 3.6250 1 0 0 0 1 0 -1 0 W 2 3.62
H1 H9 3.6949 1 0 0 0 1 0 0 0 W 2 3.43
H1 N3 2.1093 1 0 0 0 1 1 0 0 H 2 21.41
H2 O5 0.8701 1 0 0 0 1 0 0 0 V 2 31.54
H2 N1 2.7166 1 0 0 0 2 1 1 1 W 2 9.48
H2 H5 2.8073 1 0 0 0 2 2 1 1 W 2 4.98
H2 N8 3.4951 1 0 0 0 2 1 1 1 W 2 2.05
H2 H9 3.7902 1 0 0 0 1 0 0 0 W 2 3.00
H2 O3 1.8720 1 0 0 0 2 1 1 1 H 2 17.16
H3 O3 0.8201 1 0 0 0 1 0 0 0 V 2 34.60
H3 N1 3.1515 1 0 0 0 1 0 0 0 W 2 2.77
H3 C4 3.1811 1 0 0 0 1 0 0 0 W 2 5.02
H3 N4 1.9857 1 0 0 0 2 1 1 1 H 2 24.28
H4 C6 0.9700 1 0 0 0 1 0 0 0 V 2 28.27
H4 C17 2.4863 1 0 0 0 1 0 0 0 W 2 10.60
H4 N6 2.7278 1 0 0 0 1 0 0 0 W 2 8.38
H4 C3 3.3788 1 0 0 0 2 1 0 1 W 2 4.22
H4 N5 3.3855 1 0 0 0 1 0 -1 0 W 2 7.56
H4 N3 3.4650 1 0 0 0 2 1 0 1 W 2 2.57
H4 H18 3.5521 1 0 0 0 2 1 1 2 W 2 3.93
H5 C6 0.9696 1 0 0 0 1 0 0 0 V 2 28.47
H5 O3 2.6272 1 0 0 0 1 1 0 0 W 2 8.19
H5 C7 2.8681 1 0 0 0 2 1 1 1 W 2 8.64
H5 O5 2.8993 1 0 0 0 2 2 1 1 W 2 5.58
H5 C11 2.9161 1 0 0 0 1 0 0 0 W 2 4.82
H5 N2 2.9377 1 0 0 0 2 1 1 1 W 2 7.10
H5 C3 3.3030 1 0 0 0 2 1 0 1 W 2 3.56
H6 C9 0.9700 1 0 0 0 1 0 0 0 V 2 27.92
H6 O4 2.6120 1 0 0 0 2 1 1 2 W 2 10.95
H6 C18 2.8672 1 0 0 0 2 1 1 2 W 2 7.66
H6 C12 3.1151 1 0 0 0 2 1 1 2 W 2 3.86
H6 H18 3.1426 1 0 0 0 2 0 1 2 W 2 5.31
H7 C9 0.9699 1 0 0 0 1 0 0 0 V 2 27.95
H7 H8 2.5841 1 0 0 0 2 1 1 1 W 2 14.85
H7 N3 2.9558 1 0 0 0 2 0 0 1 W 2 11.19
H7 N8 3.4936 1 0 0 0 1 0 -1 0 W 2 4.17
H8 C20 0.9703 1 0 0 0 1 0 0 0 V 2 27.86
H8 H17 3.1167 1 0 0 0 2 1 1 1 W 2 3.54
H8 N3 3.4872 1 0 0 0 1 1 1 0 W 2 5.63
H8 C5 3.7416 1 0 0 0 2 1 1 1 W 2 3.38

H8 C7 4.1738 1 0 0 0 2 1 2 1 W 2 1.95
H9 C20 0.9703 1 0 0 0 1 0 -1 0 V 2 28.20
H9 O1 2.5848 1 0 0 0 1 0 0 0 W 2 9.15
H9 N4 2.9620 1 0 0 0 1 0 0 0 W 2 9.91
H9 O1 3.1197 1 0 0 0 2 1 0 1 W 2 5.41
H9 H15 3.1426 1 0 0 0 2 1 1 1 W 2 5.31
H9 C8 3.1548 1 0 0 0 1 0 0 0 W 2 2.41
H9 H13 3.5521 1 0 0 0 2 1 1 1 W 2 3.93
H10 O2 0.8703 1 0 0 0 1 0 0 0 V 2 31.98
H10 N6 2.7638 1 0 0 0 2 1 1 2 W 2 9.90
H10 C8 3.0087 1 0 0 0 2 1 1 1 W 2 5.42
H10 N5 3.0314 1 0 0 0 1 0 0 0 W 2 3.51
H10 C2 3.2714 1 0 0 0 2 1 1 1 W 2 2.86
H10 H17 3.6250 1 0 0 0 1 0 0 0 W 2 3.62
H10 H18 3.6949 1 0 0 0 1 0 0 0 W 2 3.43
H10 N7 2.1093 1 0 0 0 1 0 0 0 H 2 21.41
H11 O2 0.8701 1 0 0 0 1 0 0 0 V 2 31.54
H11 N5 2.7166 1 0 0 0 2 1 2 2 W 2 9.48
H11 H14 2.8073 1 0 0 0 2 1 2 1 W 2 4.98
H11 N4 3.4951 1 0 0 0 2 1 1 1 W 2 2.05
H11 H18 3.7902 1 0 0 0 1 0 0 0 W 2 3.00
H11 O6 1.8720 1 0 0 0 2 1 2 1 H 2 17.16
H12 O6 0.8201 1 0 0 0 1 0 -1 0 V 2 34.60
H12 N5 3.1515 1 0 0 0 1 0 -1 -1 W 2 2.77
H12 C14 3.1811 1 0 0 0 1 0 -1 -1 W 2 5.02
H12 N8 1.9857 1 0 0 0 2 1 1 1 H 2 24.28
H13 C16 0.9700 1 0 0 0 1 0 0 0 V 2 28.27
H13 C7 2.4863 1 0 0 0 1 0 0 0 W 2 10.60
H13 N2 2.7278 1 0 0 0 1 0 0 0 W 2 8.38
H13 C13 3.3788 1 0 0 0 2 1 1 1 W 2 4.22
H13 N1 3.3855 1 0 0 0 1 0 0 0 W 2 7.56
H13 N7 3.4650 1 0 0 0 2 1 1 1 W 2 2.57
H14 C16 0.9696 1 0 0 0 1 0 0 0 V 2 28.47
H14 O6 2.6272 1 0 0 0 1 0 0 0 W 2 8.19
H14 C17 2.8681 1 0 0 0 2 1 1 1 W 2 8.64
H14 O2 2.8993 1 0 0 0 2 1 2 1 W 2 5.58
H14 C1 2.9161 1 0 0 0 1 0 0 0 W 2 4.82
H14 N6 2.9377 1 0 0 0 2 1 1 1 W 2 7.10
H14 C13 3.3030 1 0 0 0 2 1 1 1 W 2 3.56
H15 C19 0.9700 1 0 0 0 1 0 0 0 V 2 27.92
H15 O1 2.6120 1 0 0 0 2 1 1 1 W 2 10.95
H15 C8 2.8672 1 0 0 0 2 1 1 1 W 2 7.66
H15 C2 3.1151 1 0 0 0 2 1 1 1 W 2 3.86
H16 C19 0.9699 1 0 0 0 1 0 0 0 V 2 27.95
H16 H17 2.5841 1 0 0 0 2 1 1 1 W 2 14.85
H16 N7 2.9558 1 0 0 0 2 1 1 1 W 2 11.19

H16 N4 3.4936 1 0 0 0 1 0 0 0 W 2 4.17
H17 C10 0.9703 1 0 0 0 1 0 0 0 V 2 27.86
H17 N7 3.4872 1 0 0 0 1 0 0 0 W 2 5.63
H17 C15 3.7416 1 0 0 0 2 1 1 2 W 2 3.38
H17 C17 4.1738 1 0 0 0 2 1 1 2 W 2 1.95
H18 C10 0.9703 1 0 0 0 1 0 0 0 V 2 28.20
H18 O4 2.5848 1 0 0 0 1 -1 0 0 W 2 9.15
H18 N8 2.9620 1 0 0 0 1 0 0 0 W 2 9.91
H18 O4 3.1197 1 0 0 0 2 1 1 2 W 2 5.41
H18 C18 3.1548 1 0 0 0 1 -1 0 0 W 2 2.41
C1 C7 1.4017 1 0 0 0 1 0 0 0 V 2 28.89
C1 C3 1.4118 1 0 0 0 1 0 1 0 V 2 29.27
C1 C5 1.4118 1 0 0 0 1 0 1 0 V 2 28.63
C2 C5 1.3990 1 0 0 0 1 0 0 0 V 2 28.38
C2 C4 1.4049 1 0 0 0 1 0 0 0 V 2 29.20
C2 C8 1.4115 1 0 0 0 1 0 0 0 V 2 27.81
C2 N7 3.3055 1 0 0 0 2 1 1 1 W 2 2.87
C3 N3 1.1565 1 0 0 0 1 0 0 0 V 2 34.91
C3 C4 2.8621 1 0 0 0 1 0 0 0 W 2 7.59
C3 N2 3.5874 1 0 0 0 2 0 1 1 W 2 1.94
C3 C7 3.6711 1 0 0 0 2 0 1 1 W 2 3.54
C4 N1 1.1517 1 0 0 0 1 0 0 0 V 2 34.74
C4 N7 3.3043 1 0 0 0 2 1 1 1 W 2 6.93
C4 N4 3.5495 1 0 0 0 2 1 1 1 W 2 3.25
C5 O1 1.3354 1 0 0 0 1 0 0 0 V 2 28.04
C5 O2 3.3958 1 0 0 0 2 1 1 1 W 2 3.90
C6 O4 1.4568 1 0 0 0 1 0 0 0 V 2 20.88
C6 C9 1.5112 1 0 0 0 1 1 0 0 V 2 17.86
C7 N2 1.1541 1 0 0 0 1 0 0 0 V 2 33.72
C8 N4 1.1545 1 0 0 0 1 0 0 0 V 2 33.63
C8 O1 2.6895 1 0 0 0 1 0 0 0 W 2 5.21
C8 N7 3.2144 1 0 0 0 2 1 1 1 W 2 4.71
C8 N4 3.3664 1 0 0 0 2 1 1 1 W 2 5.84
C9 C10 1.5143 1 0 0 0 1 0 0 0 V 2 17.84
C10 O3 1.4279 1 0 0 0 1 0 0 0 V 2 20.05
C11 C17 1.4017 1 0 0 0 1 0 0 0 V 2 28.89
C11 C13 1.4118 1 0 0 0 1 0 0 0 V 2 29.27
C11 C15 1.4118 1 0 0 0 1 0 0 0 V 2 28.63
C12 C15 1.3990 1 0 0 0 1 0 0 0 V 2 28.38
C12 C14 1.4049 1 0 0 0 1 0 0 0 V 2 29.20
C12 C18 1.4115 1 0 0 0 1 0 0 0 V 2 27.81
C12 N3 3.3055 1 0 0 0 2 1 1 1 W 2 2.87
C13 N7 1.1565 1 0 0 0 1 0 0 0 V 2 34.91
C13 C14 2.8621 1 0 0 0 1 0 0 0 W 2 7.59
C13 N6 3.5874 1 0 0 0 2 1 1 2 W 2 1.94
C13 C17 3.6711 1 0 0 0 2 1 1 2 W 2 3.54

C14 N5 1.1517 1 0 0 0 1 0 0 0 V 2 34.74
C14 N3 3.3043 1 0 0 0 2 1 1 1 W 2 6.93
C14 N8 3.5495 1 0 0 0 2 1 2 2 W 2 3.25
C15 O4 1.3354 1 0 0 0 1 0 0 0 V 2 28.04
C15 O5 3.3958 1 0 0 0 2 2 1 1 W 2 3.90
C16 O1 1.4568 1 0 0 0 1 0 1 0 V 2 20.88
C16 C19 1.5112 1 0 0 0 1 0 0 0 V 2 17.86
C17 N6 1.1541 1 0 0 0 1 0 0 0 V 2 33.72
C18 N8 1.1545 1 0 0 0 1 1 0 0 V 2 33.63
C18 O4 2.6895 1 0 0 0 1 0 0 0 W 2 5.21
C18 N3 3.2144 1 0 0 0 2 1 1 1 W 2 4.71
C18 N8 3.3664 1 0 0 0 2 1 2 2 W 2 5.84
C19 C20 1.5143 1 0 0 0 1 0 0 0 V 2 17.84
C20 O6 1.4279 1 0 0 0 1 0 0 0 V 2 20.05
N1 Co1 2.1023 1 0 0 0 1 0 0 0 V 2 15.98
N1 N2 2.8943 1 0 0 0 2 0 1 1 W 2 7.04
N1 O5 2.9180 1 0 0 0 1 -1 0 0 W 2 4.55
N1 O3 3.2496 1 0 0 0 1 0 0 0 W 2 1.97
N1 N3 3.3295 1 0 0 0 1 0 0 0 W 2 2.21
N1 Co2 6.6732 1 0 0 0 1 0 0 0 N 2 0.00
N2 Co1 2.0907 1 0 0 0 1 0 0 0 V 2 16.26
N2 O5 2.8956 1 0 0 0 1 -1 0 0 W 2 4.91
N2 N3 3.4271 1 0 0 0 2 0 1 1 W 2 1.92
N2 Co1 6.9348 1 0 0 0 1 0 1 0 N 2 0.00
N2 Co2 6.8607 1 0 0 0 1 0 1 0 N 2 0.00
N3 Co1 3.9255 1 0 0 0 1 0 0 0 N 2 0.00
N3 Co2 5.3260 1 0 0 0 1 0 0 0 N 2 0.00
N3 Co1 6.1484 1 0 0 0 1 0 -1 0 N 2 0.00
N4 N4 3.4540 1 0 0 0 2 1 1 1 W 1 1.68
N4 Co1 5.1559 1 0 0 0 1 1 0 0 N 2 0.00
N4 Co2 5.6816 1 0 0 0 1 0 0 0 N 2 0.00
N4 Co1 6.4896 1 0 0 0 1 0 0 0 N 2 0.00
N5 N6 2.8943 1 0 0 0 2 1 1 2 W 2 7.04
N5 O2 2.9180 1 0 0 0 1 0 0 0 W 2 4.55
N5 O6 3.2496 1 0 0 0 1 0 0 1 W 2 1.97
N5 N7 3.3295 1 0 0 0 1 0 0 0 W 2 2.21
N5 Co2 2.1023 1 0 0 0 1 0 1 1 H 2 15.98
N5 Co1 6.6732 1 0 0 0 1 1 0 0 N 2 0.00
N6 Co2 2.0907 1 0 0 0 1 0 0 1 V 2 16.26
N6 O2 2.8956 1 0 0 0 1 0 -1 0 W 2 4.91
N6 N7 3.4271 1 0 0 0 2 1 1 2 W 2 1.92
N6 Co2 6.9348 1 0 0 0 1 0 1 1 N 2 0.00
N6 Co1 6.8607 1 0 0 0 1 1 0 0 N 2 0.00
N7 Co2 3.9255 1 0 0 0 1 0 1 1 N 2 0.00
N7 Co1 5.3260 1 0 0 0 1 1 0 0 N 2 0.00
N7 Co2 6.1484 1 0 0 0 1 0 0 1 N 2 0.00

N8 Co2 5.1559 1 0 0 0 1 0 1 1 V 2 0.00
N8 N8 3.4540 1 0 0 0 2 0 2 2 W 1 1.68
N8 Co1 5.6816 1 0 0 0 1 0 0 0 N 2 0.00
N8 Co2 6.4896 1 0 0 0 1 -1 1 1 N 2 0.00
O2 Co2 2.0531 1 0 0 0 1 0 1 1 S 2 15.07
O3 Co1 3.9473 1 0 0 0 1 0 0 0 V 2 0.00
O3 Co2 6.5739 1 0 0 0 1 0 1 1 N 2 0.00
O5 Co1 2.0531 1 0 0 0 1 1 0 0 S 2 15.07
O6 Co2 3.9473 1 0 0 0 1 0 1 0 V 2 0.00
O6 Co1 6.5739 1 0 0 0 1 1 1 0 N 2 0.00
#End of data_1-TOPOS_f32_start/P-1->P-1(a+c,b-c,2c;1/2,0,0)[Ind=2];Bondsets:1,3,14,20,23,25