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C1CE06011B_ccdc_838535_838540_cif.txt

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_cell_length_b
_cell_length_c
_cell_angle_alpha
cell_angle_beta 8.2563(8) 8.7222(9) 9.3840(9) 90.353(8) _cell_angle_beta 100.282(8) _cell_angle_gamma 96.189(8) Page 1

C1CE06011B_ccdc_838535_838540_cif.txt _cell_volume _cell_formula_units_z _cell_measurement_temperature 660.82(11)293(2) _cell_measurement_reflns_used 7965 _cell_measurement_theta_min 2.21 _cell_measurement_theta_max 27.00 block _exptl_crystal_description _exptl_crystal_colour blue _expt]_crysta]_size_max 0.13 _exptl_crystal_size_mid _exptl_crystal_size_min 0.09 0.07 _exptl_crystal_density_meas 1.538 _exptl_crystal_density_diffrn _exptl_crystal_density_method
_exptl_crystal_F_000 'not measured' 320 _exptl_absorpt_coefficient_mu 1.766 _exptl_absorpt_correction_type numerical 0.823 _expt]_absorpt_correction_T_min _exptl_absorpt_correction_T_max
_exptl_absorpt_process_details 0.879 'X-Shape and X-Red32 (STOE, 2008)' _exptl_special_details ? 293(2) 0.71073 _diffrn_ambient_temperature _diffrn_radiation_wavelength мок∖а _diffrn_radiation_type _diffrn_radiation_source 'fine-focus sealed tube' graphite _diffrn_radiation_monochromator _diffrn_measurement_device_type _diffrn_measurement_method ? _diffrn_detector_area_resol_mean _diffrn_standards_number _diffrn_standards_interval_count _diffrn_standards_interval_time ? _diffrn_standards_decay_% 7965 _diffrn_reflns_number _diffrn_reflns_av_R_equivalents 0.0559 _diffrn_reflns_av_sigmaI/netI _diffrn_reflns_limit_h_min 0.0425 -10 _diffrn_reflns_limit_h_max 10 _diffrn_reflns_limit_k_min _diffrn_reflns_limit_k_max _diffrn_reflns_limit_l_min _diffrn_reflns_limit_l_max -11 11 -11 11 2.21 _diffrn_reflns_theta_min _diffrn_reflns_theta_max 27.00 _reflns_number_total 2878 _reflns_number_gt _reflns_threshold_expression 2519 >2sigma(I) _computing_data_collection
_computing_cell_refinement ? ? _computing_data_reduction SHELXS-97 (Sheldrick, 1990) _computing_structure_solution _computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)' _computing_molecular_graphics ? _computing_publication_material

_refine_special_details

Refinement of F^2A against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2A, conventional R-factors R are based on F, with F set to zero for negative F^2A. The threshold expression of $F^2A > 2sigma(F^2A)$ is used only for calculating R-factors(gt) etc. and is

 $C1CE06011B_ccdc_838535_838540_cif.txt \\ not relevant to the choice of reflections for refinement. R-factors based \\ on F^{2^} are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger. ; \\$

_refine_ls_structure_factor_coef Fsqd _refine_ls_matrix_type full _refine_ls_weighting_scheme calc _refine_ls_weighting_details calc w=1/[\s^2^(Fo^2^)+(0.0512P)^2^+2.1941P] where P=(Fo^2^+2Fc^2^)/3' _atom_sites_solution_primary _atom_sites_solution_secondary direct difmap _atom_sites_solution_hydrogens geom _refine_ls_hydrogen_treatment constr _refine_ls_extinction_method
_refine_ls_extinction_coef none _refine_ls_number_reflns 2878 _refine_ls_number_parameters 145 _refine_ls_number_restraints
_refine_ls_R_factor_all
_refine_ls_R_factor_gt 0 0.0778 0.0686 _refine_ls_wR_factor_ref 0.1838 _refine_ls_wR_factor_gt _refine_ls_goodness_of_fit_ _refine_ls_restrained_S_all 0.1792 _ref 1.195 1.195 _refine_ls_shift/su_max 0.000 _refine_ls_shift/su_mean 0.000 loop_ _atom_site_label _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y
_atom_site_fract_z atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_symmetry_multiplicity _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly _atom_site_disorder_group Nil Ni 0.10031(10) 0.26414(8) 0.83401(8) 0.0447(2) Uani 1 1 d . s1 s 0.3929(3) -0.1875(2) 0.8553(3) 0.0760(6) Uani 1 1 d . c1 c 0.2863(8) -0.0414(6) 0.8517(6) 0.0485(13) Uani 1 1 d . N1 N 0.2124(7) 0.0622(6) 0.8485(6) 0.0599(13) Uani 1 1 d . . . S2 S 0.1828(3) 0.2907(2) 1.11887(19) 0.0675(5) Uani 1 1 d . . . C2 C 0.0787(8) 0.4339(7) 1.1534(6) 0.0519(14) Uani 1 1 d . . . N2 N 0.0097(7) 0.5348(6) 1.1780(6) 0.0576(13) Uani 1 1 d N11 N -0.1209(7) 0.1436(7) 0.8629(7) 0.0676(15) Uani 1 1 d . H17A H -0.1018 0.0445 0.8751 0.081 Uiso 1 1 calc R . . H17B H -0.1420 0.1779 0.9476 0.081 Uiso 1 1 calc R C11 C -0.2696(11) 0.1426(13) 0.7610(13) 0.102(3) Uani 1 1 d . . . H11A H -0.3082 0.2438 0.7606 0.123 Uiso 1 1 calc R . . H11B H -0.3538 0.0689 0.7895 0.123 Uiso 1 1 calc R . . C12 C -0.2461(13) 0.1014(13) 0.6128(14) 0.110(4) Uani 1 1 d . . . H12A H -0.3541 0.0903 0.5504 0.132 Uiso 1 1 calc R H12B H -0.2054 0.0011 0.6162 0.132 Uiso 1 1 calc R C13 C -0.1315(12) 0.2102(10) 0.5414(9) 0.083(3) Uani 1 1 d . . . H13A H -0.1414 0.1766 0.4412 0.099 Uiso 1 1 calc R . . H13B H -0.1679 0.3122 0.5415 0.099 Uiso 1 1 calc R N12 N 0.0439(8) 0.2214(8) 0.6101(6) 0.0689(16) Uani 1 1 d . . H18 H 0.0690 0.1232 0.6013 0.083 uiso 1 1 calc R . . C14 C 0.1496(15) 0.3075(11) 0.5237(9) 0.096(3) Uani 1 1 d . . . H14A H 0.1175 0.4113 0.5144 0.116 Uiso 1 1 calc R . H14B H 0.1276 0.2604 0.4273 0.116 Uiso 1 1 calc R c15 c 0.3271(13) 0.3191(12) 0.5768(10) 0.095(3) Uani 1 1 d . . . H15A H 0.3834 0.3482 0.4971 0.113 Uiso 1 1 calc R . .

C1CE06011B_ccdc_838535_838540_cif.txt H15B H 0.3559 0.2178 0.6067 0.113 Uiso 1 1 calc R . . C16 C 0.3905(13) 0.4284(10) 0.6974(13) 0.099(3) Uani 1 1 d . . . H16A H 0.3567 0.5288 0.6699 0.119 Uiso 1 1 calc R . H16B H 0.5106 0.4378 0.7141 0.119 Uiso 1 1 calc R N13 N 0.3342(7) 0.3859(7) 0.8354(7) 0.0667(15) Uani 1 1 d . . . H19A H 0.3386 0.4739 0.8872 0.080 Uiso 1 1 calc R . . H19B H 0.4097 0.3298 0.8850 0.080 Uiso 1 1 calc R . . loop_ _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom_site_aniso_U_33 _atom_site_aniso_U_23 _atom_site_aniso_U_13 _atom_site_aniso_U_12 Nil 0.0526(4) 0.0353(4) 0.0470(4) 0.0011(3) 0.0081(3) 0.0095(3) s1 0.0750(12) 0.0512(10) 0.0995(15) -0.0100(9) -0.0008(10) 0.0246(9)c1 0.053(3) 0.038(3) 0.053(3) 0.000(2) 0.006(3) 0.007(2)N1 0.070(4) 0.049(3) 0.064(3) -0.002(2) 0.012(3) 0.017(3)s2 0.0983(14) 0.0559(9) 0.0531(9) 0.0014(7) 0.0086(9) 0.0391(9) c2 0.069(4) 0.044(3) 0.041(3) 0.004(2) 0.005(3) 0.008(3) N2 0.072(4) 0.044(3) 0.058(3) 0.002(2) 0.006(3) 0.018(3) N11 0.064(4) 0.058(3) 0.083(4) 0.011(3) 0.019(3) 0.010(3) C11 0.059(5) 0.098(7) 0.135(9) 0.036(6) -0.007(5) -0.015(5) c12 0.076(6) 0.095(7) 0.139(10) -0.029(7) -0.024(6) 0.002(5) c13 0.107(7) 0.066(5) 0.064(4) -0.008(4) -0.017(4) 0.015(5) N12 0.082(4) 0.083(4) 0.044(3) -0.001(3) 0.006(3) 0.029(3) C14 0.152(10) 0.079(6) 0.060(5) 0.008(4) 0.023(5) 0.014(6) c15 0.113(8) 0.105(7) 0.087(6) 0.019(5) 0.058(6) 0.042(6) C16 0.099(7) 0.068(5) 0.145(9) -0.005(6) 0.068(7) -0.002(5) N13 0.062(3) 0.055(3) 0.081(4) -0.002(3) 0.009(3) 0.000(3) _geom_special_details All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. 100p_ _geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_2 _geom_bond_publ_flag Ni1 N2 2.055(5) 2_567 ? Ni1 N11 2.069(6) . ? . ? Ni1 N1 2.070(5) Ni1 N12 2.092(5) . ? Ni1 N13 2.099(6) . ? Ni1 S2 2.6404(19) . s1 c1 1.622(6) . C1 N1 1.142(8) . S2 C2 1.653(7) . ? C2 N2 1.142(8) . ? N2 Ni1 2.055(5) 2_567 ? N11 C11 1.414(11) C11 C12 1.485(15) ???? c12 c13 1.511(14) C13 N12 1.468(11). N12 C14 1.450(11) C14 C15 1.453(14) . c15 c16 1.459(14) ?

?

C16 N13 1.488(11)

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loop_ _geom_ang]e_atom_site_label_1 _geom_angle_atom_site_label_2 _geom_angle_atom_site_label_3 _geom_angle _geom_angle_site_symmetry_1 _geom_angle_site_symmetry_3 _geom_angle_publ_flag N2 Ni1 N11 89.6(2) 2_567 . N2 Ni1 N1 179.4(2) 2_567 . ? ? N11 Ni1 N1 90.5(2) . . ? N2 Ni1 N12 93.6(2) 2_567 ? . N11 N11 N12 91.7(3) . . ? N1 Ni1 N12 87.0(2) . . ? N2 Ni1 N13 91.5(2) 2_567 N11 Ni1 N13 172.2(2) . . ? ? N1 Ni1 N13 88.3(2) . . ? N1 N11 N13 95.9(3) . . ? N2 Ni1 S2 92.14(16) 2_567 N11 Ni1 S2 87.75(19) . . ? N1 Ni1 S2 87.24(16) . . ? ? N12 Ni1 S2 174.24(18) . . N13 Ni1 S2 84.51(18) . . N1 c1 S1 179.3(6) . . ? ? . ? C1 N1 N11 173.5(6) . . ? C2 S2 Ni1 101.2(2) . . ? N2 C2 S2 178.6(7) . . ? C2 N2 Ni1 163.7(5) . 2_567 ? C11 N11 Ni1 123.0(5) . . 7 ? N11 C11 C12 111.6(9) • . c11 c12 c13 118.0(8) ? . . N12 C13 C12 114.9(7) C14 N12 C13 111.9(7) C14 N12 Ni1 116.6(6) . . ? C13 N12 Ni1 117.2(5) . . N12 C14 C15 117.0(7) ? . . ? C14 C15 C16 115.8(8). . C15 C16 N13 114.6(7) ? • • ? C16 N13 Ni1 120.8(6) . _diffrn_measured_fraction_theta_max 0.996 27.00 _diffrn_reflns_theta_full _diffrn_measured_fraction_theta_full 0.996 _refine_diff_density_max _refine_diff_density_min _refine_diff_density_rms 0.893 -0.6530.096 # Attachment '- TA153.CIF' data_ta153 _database_code_depnum_ccdc_archive 'CCDC 838536' #TrackingRef '- TA153.CIF _audit_creation_method SHELXL-97 _chemical_name_systematic ? _chemical_name_common ? _chemical_melting_point 'C14 H34 N8 Ni S2' _chemical_formula_moiety 'C14 H34 N8 Ni S2' _chemical_formula_sum _chemical_formula_weight 437.32 loop_ _atom_type_symbol _atom_type_description

C1CE06011B_ccdc_838535_838540_cif.txt _atom_type_scat_dispersion_real _atom_type_scat_dispersion_imag _atom_type_scat_source C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' Н Н 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' Ni Ni 0.3393 1.1124 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' _symmetry_cell_setting monoclinic _symmetry_space_group_name_H-M 'P 21/c '-P 2ybc' _symmetry_space_group_name_Hall 100p_ _symmetry_equiv_pos_as_xyz 'x, y, z '-x, y+1/2, -z+1/2' '-x, -y, -z' 'x, -y-1/2, z-1/2' _cell_length_a _cell_length_b 9.4274(6) 18.1438(10)12.2373(7) _cell_length_c _cell_angle_alpha _cell_angle_beta 90.00 96.345(7)_cell_angle_gamma 90.00 _cell_volume 2080.4(2) _cell_formula_units_z _cell_measurement_temperature 170(2)_cell_measurement_reflns_used 12789 _cell_measurement_theta_min 2.83 28.04 _cell_measurement_theta_max block _exptl_crystal_description _exptl_crystal_colour blue _exptl_crystal_size_max 0.85 0.62 _exptl_crystal_size_mid _exptl_crystal_size_min _exptl_crystal_density_meas 0.45 1.396 _exptl_crystal_density_diffrn 'not measured' _exptl_crystal_density_method _exptl_crystal_F_000 _exptl_absorpt_coefficient_mu 936 1.148 _exptl_absorpt_correction_type numerical _exptl_absorpt_correction_T_min 0.425 _expt]_absorpt_correction_T_max 0.591 'X-Shape and X-Red32 (STOE, 2008)' _exptl_absorpt_process_details _exptl_special_details ; ? ; 170(2) _diffrn_ambient_temperature 0.71073 _diffrn_radiation_wavelength _diffrn_radiation_type мок∖а diffrn_radiation_source 'fine-focus sealed tube' graphite _diffrn_radiation_monochromator _diffrn_measurement_device_type _diffrn_measurement_method _diffrn_detector_area_resol_mean 7 _diffrn_standards_number ? _diffrn_standards_interval_count _diffrn_standards_interval_time _diffrn_standards_decay_% _diffrn_reflns_number 12789 _diffrn_reflns_av_R_equivalents 0.0833 _diffrn_reflns_av_sigmaI/netI 0.0639 Page 6

C1CE06011B_ccdc_838535_838540_cif.txt _diffrn_reflns_limit_h_min _diffrn_reflns_limit_h_max _diffrn_reflns_limit_k_min -12 9 -23 _diffrn_reflns_limit_k_max 23 _diffrn_ref]ns_limit_l_min -16 _diffrn_reflns_limit_l_max _diffrn_reflns_theta_min 16 2.83 _diffrn_reflns_theta_max 28.04 _reflns_number_total 4928 _reflns_number_gt 3937 _reflns_threshold_expression >2sigma(I) _computing_data_collection ? ? _computing_cell_refinement _computing_data_reduction 'SHELXS-97 (Sheldrick, 1990)' _computing_structure_solution _computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)' ? _computing_molecular_graphics ? _computing_publication_material _refine_special_details Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based on F, with F set to zero for negative F^2^. The threshold expression of $F^{2^{\prime}} > 2sigma(F^{2^{\prime}})$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and Rfactors based on ALL data will be even larger. _refine_ls_structure_factor_coef Fsqd _refine_ls_matrix_type _refine_ls_weighting_scheme full calc refine_ls_weighting_details 'calc w=1/[\s^2^(Fo^2^)+(0.0789P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3' direct _atom_sites_solution_primary _atom_sites_solution_secondary difmap _atom_sites_solution_hydrogens geom _refine_ls_hydrogen_treatment constr _refine_ls_extinction_method SHELXL _refine_ls_extinction_coef 0.0147(17)
_refine_ls_extinction_expression Fc^*^=kFc[1+0.001xFc^2^\]^3/sin(2\q)]^-1/4^ _refine_ls_number_reflns 4928 _refine_ls_number_parameters _refine_ls_number_restraints _refine_ls_R_factor_all _refine_ls_R_factor_gt 227 0 0.0630 0.0473 _refine_ls_wR_factor_ref 0.1285 _refine_ls_wR_factor_gt 0.1197 _refine_ls_goodness_of_fit_ref _refine_ls_restrained_s_all 1.030 1.030 _refine_ls_shift/su_max 0.001 _refine_ls_shift/su_mean 0.000 100p_ _atom_site_label _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y _atom_site_fract_z _atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_symmetry_multiplicity _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly

_atom_site_disorder_group Nil Ni 0, 72387(3) 0, 423133(16) 0.27838(2) 0.01148(12) Uani 1 1 d S1 s 1.13954(9) 0.28241(5) 0.4478(2) 0.0281(6) Uani 1 1 d NI N 1.2569(4) 0.42426(16) 0.4474(2) 0.0247(6) Uani 1 1 d NI N 1.2569(4) 0.474262(16) 0.4474(2) 0.0470(8) Uani 1 1 d N2 N 0.6698(5) 0.02053(15) 0.3590(3) 0.0680(14) Uani 1 1 d N2 N 0.6698(5) 0.02053(15) 0.3590(3) 0.0680(14) Uani 1 1 d N1 N 0.6119(2) 0.52349(11) 0.31584(17) 0.0180(4) Uani 1 1 d H1LA H 0.5164 0.5144 0.2967 0.022 Uiso 1 1 calc R H1LB H 0.5241 0.5228 0.3911 0.022 Uiso 1 1 calc R N12 N 0.8908(3) 0.48407(12) 0.20783(17) 0.0208(5) Uani 1 1 d H1A H 0.5806 0.2858 0.2613 0.022 Uiso 1 1 calc R H13A H 0.8986 0.3178 0.3227 0.022 Uiso 1 1 calc R H13A H 0.8986 0.3178 0.3227 0.022 Uiso 1 1 calc R H13A H 0.8986 0.3178 0.3227 0.022 Uiso 1 1 calc R H13A H 0.8530 0.6090 0.1996 0.035 Uiso 1 1 calc R H12A H 0.9610 0.6039 0.1996 0.035 Uiso 1 1 calc R H12A H 0.8510 0.6039 0.1996 0.035 Uiso 1 1 calc R H12A H 0.8513 0.6010 0.2243 0.039 Uiso 1 1 calc R H12A H 0.8513 0.6010 0.3243 0.039 Uiso 1 1 calc R H12A H 0.8513 0.6010 0.3248 0.039 Uiso 1 1 calc R H12A H 0.8513 0.6010 0.3248 0.039 Uiso 1 1 calc R H12A H 0.8513 0.60510 0.3248 0.01205(2) 0.0236(7) Uani 1 1 d H13C H 0.708 0.5543 0.1051 0.036 Uiso 1 1 calc R H13D H 0.9303 0.5830 0.1374 0.036 Uiso 1 1 calc R H13C H 0.708 0.5543 0.1051 0.036 Uiso 1 1 calc R H13C H 0.708 0.5543 0.1051 0.036 Uiso 1 1 calc R H13A H 1.0380 0.4775 0.0983 0.032 Uiso 1 1 calc R H15A H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R H15A H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R H15A H 1.0877 0.3550 0.0996 0.031 Uiso 1 1 calc R H15A H 1.0842 0.4275 0.0350 Uiso 1 1 calc R H15A H 0.9443 0.4282 0.4275 0.023 Uiso 1 1 calc R H22A H 0.4843 0.4851 0.4574 0.022 Uiso 1 1 calc R H23A H 0.5623 0.4263 0.1728 0.0227 (0.02278(6) Uani 1 1 d H15B H 0.8643 0.4285 0.4357 0.030 Uiso 1 1 calc R H23A H 0.5623 0.4357	C1CE06011B_ccdc_838535_838540_cif.txt
<pre>N11 N1 0.72387(3) 0.423133(16) 0.27838(2) 0.01148(12) Uani 1 1 d C1 C 1.2083(4) 0.36538(17) 0.44891(7) 0.0384(2) Uani 1 1 d S1 S 1.13954(9) 0.28241(5) 0.4447(2) 0.0470(8) Uani 1 1 d S2 S 0.80309(11) 0.15317(5) 0.34935(7) 0.04419(2) Uani 1 1 d S2 C 0.7178(4) 0.0773(2) 0.3556(3) 0.0350(7) Uani 1 1 d N1 N 0.6698(5) 0.02053(15) 0.3596(3) 0.0680(14) Uani 1 1 d N1 N 0.6119(2) 0.52349(11) 0.31584(17) 0.0180(4) Uani 1 1 d H11 H 0.5164 0.5144 0.2967 0.022 Uiso 1 1 calc R . N12 N 0.8098(3) 0.48407(12) 0.20783(17) 0.0208(5) Uani 1 1 d H12 H 0.9624 0.4916 0.2654 0.025 Uiso 1 1 calc R . N13 N 0.8350(2) 0.22334(12) 0.220783(17) 0.0282(4) Uani 1 1 d H13 H 0.68386 0.3178 0.3227 0.022 Uiso 1 1 calc R . H13 H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R . H13 H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R . H14 H 0.9624 0.4916 0.2554 0.025 Uiso 1 1 calc R . H12 H 0.9624 0.4916 0.2574(23) 0.032 Uiso 1 1 calc R . H12 H 0.6404(4) 0.59748(16) 0.2709(3) 0.0293(6) Uani 1 1 d H13 H 0.7969 0.2858 0.2613 0.022 Uiso 1 1 calc R . H12 H 0.6513 0.6001 0.3248 0.039 Uiso 1 1 calc R . H12 H 0.8553 0.6001 0.3248 0.039 Uiso 1 1 calc R . H12 H 0.9690 0.8530 0.1374 0.032 Uiso 1 1 calc R . H12 H 0.9708 0.55830 0.1374 0.036 Uiso 1 1 calc R . H13 C H 0.7708 0.55597(16) 0.1666(2) 0.0303(7) Uani 1 1 d H13 C H 0.7708 0.5597(16) 0.1666(2) 0.0203(7) Uani 1 1 d H13 C H 0.7870 0.5597(16) 0.1666(2) 0.0203(7) Uani 1 1 d H13 C H 0.4870 0.3580 0.032 Uiso 1 1 calc R . H13 C H 0.4810 0.3088 0.0340 Uiso 1 1 calc R . L14 C940(3) 0.37054(18) 0.1205(2) 0.0265(6) Uani 1 1 d H13 H H 0.8380 0.4475 0.0983 0.032 Uiso 1 1 calc R . L14 C9432(2) 0.4455(18) 0.1545(2) 0.0278(6) Uani 1 1 d H14 H 1.0840 0.4750 0.0359 Uiso 1 1 calc R . L14 L4414 1.0380 0.4775 0.0283 Uiso 1 1 calc R . L14 L4414 1.0346(2) 0.3263(17) 0.1645(2) 0.0278(6) Uani 1 1 d H14 H 1.08430 0.3560 0.0350 Uiso 1 1 calc R . L24 C 0.48410 0.3065 0.0560 0.031 Uiso 1 1 calc R . L24 C 0.48410 0.3065 0.3550 0</pre>	_atom_site_disorder_group
S1 S 1.13954(9) 0.28241(5) 0.4473(2) 0.0281(6) uani 1 1 d NI N 1.2569(4) 0.42426(16) 0.4447(2) 0.0281(6) uani 1 1 d NI N 1.2569(4) 0.472426(16) 0.4477(2) 0.0470(8) uani 1 1 d S2 S 0.80309(11) 0.15317(5) 0.34935(7) 0.0419(2) uani 1 1 d N2 N 0.6698(5) 0.02053(15) 0.3590(3) 0.0680(14) uani 1 1 d N11 N 0.6119(2) 0.52349(11) 0.31584(17) 0.0180(4) uani 1 1 d H11A H 0.5140 0.5144 0.2967 0.022 Uiso 1 1 calc R . H11B H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R . H11B H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R . H11B H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R . H11B H 0.6241 0.528 0.22334(12) 0.2068(17) 0.028(5) Uani 1 1 d H13A H 0.8986 0.3178 0.3227 0.022 Uiso 1 1 calc R . H13B H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R . H13B H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R . H11D H 0.5110 0.6039 0.1996 0.035 Uiso 1 1 calc R . H12A H 0.8910 0.6039 0.1996 0.035 Uiso 1 1 calc R . H12A H 0.8510 0.6039 0.1996 0.035 Uiso 1 1 calc R . H12A H 0.8510 0.6030 0.1936 0.039 Uiso 1 1 calc R . H12A H 0.8510 0.6010 0.3248 0.039 Uiso 1 1 calc R . H12A H 0.8553 0.6010 0.3248 0.039 Uiso 1 1 calc R . H12A H 0.8553 0.6010 0.3248 0.039 Uiso 1 1 calc R . H12A H 0.8553 0.6010 0.3248 0.039 Uiso 1 1 calc R . H12A H 0.8570 0.6030 0.1966 Uiso 1 1 calc R . H12A H 0.8570 0.6030 0.1974 0.036 Uiso 1 1 calc R . H12A H 0.898 0.4375 0.02257 0.033 Uiso 1 1 calc R . H14B H 0.898 0.4375 0.02257 0.033 Uiso 1 1 calc R . H15A H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R . H15A H 1.0877 0.3550 0.0993 0.032 Uiso 1 1 calc R . H15A H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R . H15A H 1.0877 0.3550 0.0996 0.031 Uiso 1 1 calc R . H15A H 0.8481 0.3088 0.0966 0.031 Uiso 1 1 calc R . H15A H 0.8481 0.3088 0.0966 0.031 Uiso 1 1 calc R . H12A H 0.8481 0.3088 0.0966 0.031 Uiso 1 1 calc R . H22A H 0.8492 0.4475 0.0220 Uiso 1 1 calc R . H22A H 0.8492 0.4451 0.4574 0.020 Uiso 1 1 calc R . H22A H 0.8491 0.3452 0.4775 0.023 Uiso 1 1 calc R . H22A H 0.8581 0.3436 0.3324 0.030 Uiso 1 1 calc R . H	Nil Ni 0.72387(3) 0.423133(16) 0.27838(2) 0.01148(12) Uani 1 1 d
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N1 N 1.2503(4) 0.3246(16) 0.34435(7) 0.0440(6) 20 Uani 1 1 d C2 C 0.7178(4) 0.0773(2) 0.3566(3) 0.0350(7) Uani 1 1 d N1 N 0.6119(2) 0.52349(11) 0.31584(17) 0.0180(4) Uani 1 1 d N11 N 0.5164 0.5144 0.2967 0.022 Uiso 1 1 calc R . H11B H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R . H11B H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R . H11B H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R . H13B H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R . H13B H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R . H13B H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R . H13B H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R . H12C N 0.8986(3) 0.48407(12) 0.20783(17) 0.0208(5) Uani 1 1 d . H12C N 0.6404(4) 0.59748(16) 0.2709(3) 0.0293(6) Uani 1 1 d . H12C H 0.6116 0.6356 0.3219 0.035 Uiso 1 1 calc R . H12C H 0.6116 0.6356 0.3219 0.035 Uiso 1 1 calc R . H12C H 0.6116 0.6356 0.3219 0.035 Uiso 1 1 calc R . H12C H 0.6116 0.6356 0.3219 0.035 Uiso 1 1 calc R . H12A H 0.8530 0.6001 0.3248 0.039 Uiso 1 1 calc R . H12A H 0.8530 0.6001 0.3248 0.039 Uiso 1 1 calc R . H12A H 0.8530 0.55927(16) 0.1666(2) 0.0303(7) Uani 1 1 d . H13C H 0.7708 0.5543 0.1051 0.036 Uiso 1 1 calc R . H13D H 0.9030 0.5543 0.1051 0.036 Uiso 1 1 calc R . H13D H 0.9030 0.5543 0.032 Uiso 1 1 calc R . H14B H 0.8898 0.4391 0.0553 0.032 Uiso 1 1 calc R . H15A H 1.0877 0.3550 0.0932 Uiso 1 1 calc R . H15A H 1.0877 0.3550 0.0932 Uiso 1 1 calc R . H15A H 1.0877 0.3550 0.0932 Uiso 1 1 calc R . H15A H 1.0877 0.3550 0.0232 Uiso 1 1 calc R . H15A H 1.0877 0.3550 0.0232 Uiso 1 1 calc R . H15A H 0.8482 0.3758 0.02257 0.033 Uiso 1 1 calc R . H15A H 0.8482 0.3758 0.02257 0.023 Uiso 1 1 calc R . H15A H 0.8482 0.3758 0.02257 0.023 Uiso 1 1 calc R . H15A H 0.8482 0.3758 0.02257 0.023 Uiso 1 1 calc R . H15A H 0.8482 0.34758 0.02257 0.023 Uiso 1 1 calc R . H15A H 0.8481 0.3088 0.0966 0.031 Uiso 1 1 calc R . H15A H 0.8481 0.3088 0.0966 0.031 Uiso 1 1 calc R . H22A H 0.4831 0.3965 0.3559 0.020 Uiso 1 1 calc R . H23A H 0.5620 0.4369 0.0704 0.023 Uiso 1 1 calc R	$(1 \ (1.2083(4) \ 0.30538(17) \ 0.4473(2) \ 0.0281(6) \ 0.011 \ 1 \ 1 \ 0 \ . \ .$
31: 30.00330(1) 0.0773(2) 0.0350(7) Uani 1 1 d N2 N 0.6698(5) 0.02033(15) 0.3590(3) 0.0680(14) Uani 1 1 d N11 N 0.6119(2) 0.52349(11) 0.031834(17) 0.0180(4) Uani 1 1 d H1LA H 0.5164 0.52349(11) 0.022 Uiso 1 1 calc R . H12 H 0.6241 0.52282 0.3311 0.022 Uiso 1 1 calc R . N12 N 0.8908(0.3) 0.48407(12) 0.20783(17) 0.0182(4) Uani 1 1 d H13A H 0.7896 0.32178 0.3227 0.022 Uiso 1 1 calc R . H13A H 0.7896 0.32178 0.3227 0.022 Uiso 1 1 calc R . H12 H 0.6404(4) 0.59748(16) 0.2709(3) 0.0293(6) Uani 1 1 d . H12 H 0.7956(1) 0.6350 Uiso 1 1 calc R . . . H12 H 0.8533 0.6001 0.333 Uiso 1 1 calc R . . H12 H 0.8096 0.6610 0.2333 0.302 Uiso 1 1 calc R . . H12 H 0.9303 0.533 0.302 Uiso 1 1 calc R . . . H12 H 0.9699(3) 0.4452(18	NIN 1.2509(4) $0.42420(10) 0.4447(2) 0.0470(0) 0.011 I I 0$
<pre>C2 C 0.1268(5) 0.02053(15) 0.3590(2) 0.0680(14) Uani 1 1 d N11 N 0.6119(2) 0.52349(11) 0.31584(17) 0.0180(4) Uani 1 1 d H11 H 0 0.6119(2) 0.52349(11) 0.221 Uiso 1 1 calc R H11 H 0 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R H11 H 0 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R H12 N 0.8908(3) 0.48407(12) 0.20783(17) 0.0208(5) Uani 1 1 d H13 H 0.8350(2) 0.32334(12) 0.2002 Uiso 1 1 calc R H13 H 0.8386 0.3178 0.3227 0.022 Uiso 1 1 calc R H13 H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R H13 H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R H12 H 0.9624 0.59748(16) 0.2709(3) 0.0293(6) Uani 1 1 d H12 H 0.5810 0.6039 0.1990 0.035 Uiso 1 1 calc R H11 D H 0.6116 0.6356 0.3219 0.035 Uiso 1 1 calc R H12 H 0.8533 0.6001 0.3248 0.039 Uiso 1 1 calc R H12 H 0.8533 0.6001 0.3248 0.039 Uiso 1 1 calc R H12 H 0.8533 0.6001 0.3248 0.039 Uiso 1 1 calc R H12 H 0.8533 0.6001 0.3248 0.039 Uiso 1 1 calc R H12 H 0.8533 0.6001 0.3248 0.039 Uiso 1 1 calc R H12 H 0.8533 0.6001 0.3248 0.039 Uiso 1 1 calc R H13 C H 0.7708 0.5543 0.1051 0.036 Uiso 1 1 calc R H13 C H 0.7708 0.44562(18) 0.1205(2) 0.0265(6) Uani 1 1 d H14 H 1.0380 0.4775 0.0983 0.032 Uiso 1 1 calc R H15 H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R H15 H 1.0877 0.3550 0.0992 0.033 Uiso 1 1 calc R H15 H 1.0874 0.3550 0.0996 0.031 Uiso 1 1 calc R H15 H 1.0874 0.3550 0.0277 0.033 Uiso 1 1 calc R H15 H 1.0842 0.3758 0.2257 0.033 Uiso 1 1 calc R H15 H 1.0843 0.3758 0.2257 0.033 Uiso 1 1 calc R H15 H 1.0843 0.3758 0.2257 0.033 Uiso 1 1 calc R H15 H 1.0843 0.3758 0.2257 0.033 Uiso 1 1 calc R H15 H 1.0843 0.3758 0.2257 0.033 Uiso 1 1 calc R H15 H 1.0843 0.3458 0.0475 0.023 Uiso 1 1 calc R H15 H 1.0843 0.3458 0.0306(1) 0.310 Uiso 1 1 calc R H15 H 1.0843 0.3451 0.4574 0.023 Uiso 1 1 calc R H15 H 1.0843 0.3451 0.4574 0.023 Uiso 1 1 calc R H22 H 0.4843 0.3368 0.3945 0.305 Uiso 1 1 calc R H23 H 0.6630 0.330 0.5344 0.035 Uiso 1 1 calc R H23 H</pre>	$c_{2} = 0.0000000000000000000000000000000000$
<pre>Ni1 N 0.06119(2) 0.52349(21) 0.31584(17) 0.0180(4) uani 1 1 d H11A H 0.5164 0.5144 0.2967 0.022 uiso 1 1 calc R H11B H 0.6241 0.5282 0.3911 0.022 uiso 1 1 calc R N12 N 0.8908(3) 0.48407(12) 0.20783(17) 0.0208(5) uani 1 1 d H12 H 0.9624 0.4916 0.2654 0.025 uiso 1 1 calc R N13 N 0.8350(2) 0.32334(12) 0.26061(17) 0.0182(4) uani 1 1 d H13A H 0.8966 0.3178 0.3227 0.022 uiso 1 1 calc R H13B H 0.7696 0.2858 0.2613 0.022 uiso 1 1 calc R C11 C 0.6404(4) 0.59748(16) 0.2709(3) 0.0293(6) uani 1 1 d H1D H 0.6116 0.6356 0.3219 0.035 uiso 1 1 calc R C11 C 0.6404(4) 0.59748(16) 0.2709(3) 0.0293(6) uani 1 1 d H1D H 0.5810 0.6039 0.1996 0.035 uiso 1 1 calc R C12 c 0.7959(4) 0.60901(16) 0.2542(3) 0.0325(7) uani 1 1 d H12A H 0.8966 0.6610 0.2333 0.039 uiso 1 1 calc R H12B H 0.8096 0.6610 0.2333 0.039 uiso 1 1 calc R H12B H 0.8096 0.6610 0.2333 0.039 uiso 1 1 calc R H12B H 0.8096 0.6610 0.2333 0.032 uiso 1 1 calc R H13D H 0.7708 0.5543 0.1051 0.036 uiso 1 1 calc R H14A H 1.0877 0.3550 0.0993 0.032 uiso 1 1 calc R H14A H 1.08877 0.3754 0.0125(2) 0.0265(6) uani 1 1 d H14A H 1.0877 0.3550 0.032 uiso 1 1 calc R C15 c 1.0240(3) 0.3754(18) 0.1542(2) 0.0278(6) uani 1 1 d H15A H 1.0877 0.3550 0.033 uiso 1 1 calc R L15B H 1.0834 0.3758 0.2257 0.033 uiso 1 1 calc R H15B H 1.0842(2) 0.43630(12) 0.43824(17) 0.0190(4) uani 1 1 d H166 H 0.8481 0.3068 0.0966 0.031 uiso 1 1 calc R L21A H 0.9449 0.2263 0.1722 0.032 uiso 1 1 calc R L21A H 0.9449 0.2425 0.4275 0.023 uiso 1 1 calc R L21A H 0.9430 0.4382 0.0474 0.023 uiso 1 1 calc R L21A H 0.8431 0.3965 0.3559 0.020 uiso 1 1 calc R L22 H 0.48431 0.3965 0.3559 0.020 uiso 1 1 calc R L22 H 0.48431 0.3967(40 0.023 uiso 1 1 calc R L22 H 0.48431 0.3480 0.3324 0.033 uiso 1 1 calc R L22 H 0.48431 0.3426 0.3410 0.035 uiso 1 1 calc R L22 H 0.48643 0.4179 0.6630 0.035 uiso 1 1 calc R L22 H 0.48643 0.4179 0.6630 0.035 uiso 1 1 calc R L22 H 0.48643 0.</pre>	$N_2 = 0.7170(4) = 0.0775(2) = 0.0500(3) = 0.0550(7) = 0.011 = 1 = 0 = 1$
HILA H 0.5164 0.5144 0.2967 0.022 Uiso 1 1 calc R . HIB H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R . HIE H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R . HIZ N 0.8908(3) 0.48407(12) 0.2006(117) 0.0182(4) Uani 1 1 d HIZ N 0.8908(3) 0.32334(12) 0.2606(117) 0.0182(4) Uani 1 1 d HISA H 0.8986 0.3178 0.3227 0.022 Uiso 1 1 calc R . HISA H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R . HIL H 0.6116 0.6356 0.3213 0.022 Uiso 1 1 calc R . HIL H 0.5810 0.6039 0.1996 0.035 Uiso 1 1 calc R . HIL H 0.5810 0.6039 0.1996 0.035 Uiso 1 1 calc R . HIL H 0.5810 0.6039 0.1996 0.035 Uiso 1 1 calc R . HIZA H 0.8553 0.6010 0.3248 0.039 Uiso 1 1 calc R . HIZA H 0.8553 0.6010 0.3248 0.039 Uiso 1 1 calc R . HIZA H 0.8553 0.6010 0.3248 0.039 Uiso 1 1 calc R . HIZA H 0.8553 0.6010 0.3248 0.039 Uiso 1 1 calc R . HIZA H 0.8553 0.6510 0.1514 0.036 Uiso 1 1 calc R . HIZA H 0.8096 0.5543 0.1051 0.036 Uiso 1 1 calc R . HIZA H 0.8898 0.44562(18) 0.1205(2) 0.0265(6) Uani 1 1 d HIA H 1.0380 0.4775 0.0983 0.032 Uiso 1 1 calc R . HIA H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R . HISA H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R . HISA H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R . HISA H 1.0877 0.3550 0.02277 0.033 Uiso 1 1 calc R . HISA H 1.0877 0.3550 0.023 Uiso 1 1 calc R . HISA H 0.8492 (0.31052(7) 0.1645(2) 0.0278(6) Uani 1 1 d HISA H 0.8492 (0.3451 0.4574 0.023 Uiso 1 1 calc R . HISA H 0.8492 (0.3451 0.4574 0.023 Uiso 1 1 calc R . HISA H 0.8492 (0.4363 0.1728 0.031 Uiso 1 1 calc R . HISA H 0.8492 (0.36145(11) 0.34657(17) 0.0190(4) Uani 1 1 d HIZA H 0.8492 (0.3451 0.4574 0.023 Uiso 1 1 calc R . HIZA H 0.8493 0.3485 0.3537 (2) 0.0288(6) Uani 1 1 d HIZA H 0.4841 0.3088 0.5324 0.032 Uiso 1 1 calc R . HIZA H 0.6523 0.2857 (112) 0.34267(12) 0.0288(6) Uani 1 1 d HIZA H 0.6561 0.3627 0.6168 0.032 Uiso 1 1 calc R . HIZA H 0.6561 0.3627 0.6168 0.032 Uiso 1 1 calc R . HIZA H 0.6561 0.3627 0.6168 0.032 Uiso 1 1 calc R . HIZA H 0.65610 0.3627 0.6161 0.028 Uiso 1 1 calc R . HIZA H 0.5461 0.3627	N11 N $0.6119(2)$ $0.52349(11)$ $0.31584(17)$ $0.0180(4)$ Uani 1 1 d
<pre>H11E H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R N12 N 0.8908(3) 0.48407(12) 0.20783(17) 0.0208(5) Uani 1 1 d N13 N 0.8350(2) 0.32334(12) 0.26061(17) 0.0182(4) Uani 1 1 d H13A H 0.8986 0.3178 0.3227 0.022 Uiso 1 1 calc R H13B H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R H13B H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R H11C H 0.6116 0.6356 0.3219 0.035 Uiso 1 1 calc R H11C H 0.6116 0.6396 0.3219 0.035 Uiso 1 1 calc R H11D H 0.5810 0.6039 0.1996 0.035 Uiso 1 1 calc R H11D H 0.5810 0.6091 0.13248 0.039 Uiso 1 1 calc R H12A H 0.8553 0.6001 0.3248 0.039 Uiso 1 1 calc R H12A H 0.8553 0.6001 0.3248 0.039 Uiso 1 1 calc R H12A H 0.8553 0.6001 0.3248 0.039 Uiso 1 1 calc R H13C H 0.7708 0.5543 0.1051 0.036 Uiso 1 1 calc R H13C H 0.7708 0.5543 0.1051 0.036 Uiso 1 1 calc R H13C H 0.7708 0.5543 0.1051 0.036 Uiso 1 1 calc R H13C H 0.9703 0.5830 0.1374 0.036 Uiso 1 1 calc R H14A H 1.0380 0.4775 0.0993 0.032 Uiso 1 1 calc R H14A H 1.0380 0.4775 0.0993 0.032 Uiso 1 1 calc R H14A H 1.0877 0.3550 0.0993 0.031 Uiso 1 1 calc R H15E H 1.0877 0.3550 0.0993 0.031 Uiso 1 1 calc R H15E H 1.0877 0.3550 0.0227 0.033 Uiso 1 1 calc R H15E H 1.0884 0.3758 0.2257 0.033 Uiso 1 1 calc R H15E H 1.0884 0.3768 0.2257 0.033 Uiso 1 1 calc R H15E H 1.0884 0.3768 0.0267 0.031 Uiso 1 1 calc R H15E H 0.8492(2) 0.43630(12) 0.43824(17) 0.0190(4) Uani 1 1 d H15A H 0.8492 0.4574 0.1220 Uiso 1 1 calc R N21 N 0.8492(2) 0.43630(12) 0.43827(17) 0.019(4) Uani 1 1 d H21A H 0.8493 0.3965 0.3559 0.020 Uiso 1 1 calc R N21 N 0.5359 0.4574 0.1223 Uiso 1 1 calc R N23 N 0.6019(2) 0.41988(12) 0.12223(17) 0.0288(6) Uani 1 1 d H23A H 0.6623 0.4309 0.0704 0.023 Uiso 1 1 calc R N23 N 0.6019(2) 0.41988(12) 0.12223(17) 0.0288(6) Uani 1 1 d H23A H 0.6523 0.4374 0.1204 0.023 Uiso 1 1 calc R M23A H 0.6523 0.4374 0.1204 0.023 Uiso 1 1 calc R M23A H 0.6523 0.4374 0.1204 0.023 Uiso 1 1 calc R H23A H 0.6523 0.4374 0.0324 Uis</pre>	H11A H 0.5164 0.5144 0.2967 0.022 Uiso 1 1 calc R
<pre>N12 N 0.8908(3) 0.48407(12) 0.20783(17) 0.0208(5) uani 1 1 d H12 H 0.9624 0.4916 0.2654 0.025 Uiso 1 1 calc R H13A H 0.8986 0.3178 0.3227 0.022 Uiso 1 1 calc R C11 C 0.6404(4) 0.59748(16) 0.2709(3) 0.0293(6) uani 1 1 d H13B H 0.6116 0.6356 0.3219 0.035 Uiso 1 1 calc R C11 C 0.6404(4) 0.59748(16) 0.2709(3) 0.0293(6) uani 1 1 d H11C H 0.5810 0.6039 0.1996 0.035 Uiso 1 1 calc R C12 C 0.7959(4) 0.60901(16) 0.2542(3) 0.0325(7) uani 1 1 d H12A H 0.8553 0.6010 0.3248 0.039 Uiso 1 1 calc R C13 C 0.8478(4) 0.5927(6) 0.1666(2) 0.0303(7) uani 1 1 d H12A H 0.8553 0.6010 0.3248 0.039 Uiso 1 1 calc R C13 C 0.8478(4) 0.55927(6) 0.1666(2) 0.0303(7) uani 1 1 d H13C H 0.7708 0.5543 0.1051 0.036 Uiso 1 1 calc R H13D H 0.9303 0.5830 0.1374 0.036 Uiso 1 1 calc R H14A H 1.0380 0.44752 0.0983 0.032 Uiso 1 1 calc R H14A H 1.0380 0.44755 0.0983 0.032 Uiso 1 1 calc R H15A H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R H15A H 1.0877 0.3550 0.0993 0.033 Uiso 1 1 calc R H15A H 1.0877 0.3550 0.0993 0.031 Uiso 1 1 calc R H15A H 1.0874 0.3758 0.2277 0.033 Uiso 1 1 calc R H15A H 1.0840 0.3788 0.2277 0.033 Uiso 1 1 calc R H15A H 0.9449 0.2623 0.1728 0.031 Uiso 1 1 calc R H15A H 0.9430 0.4262 0.4275 0.023 Uiso 1 1 calc R H15A H 0.9430 0.4262 0.4275 0.023 Uiso 1 1 calc R H15A H 0.9430 0.4262 0.4275 0.023 Uiso 1 1 calc R H15A H 0.9430 0.4262 0.4275 0.023 Uiso 1 1 calc R H21A H 0.9430 0.4262 0.4275 0.023 Uiso 1 1 calc R H21A H 0.9430 0.4262 0.4275 0.023 Uiso 1 1 calc R H21A H 0.9430 0.4282 0.4275 0.023 Uiso 1 1 calc R H21A H 0.9430 0.4282 0.4276 0.023 Uiso 1 1 calc R H22A H 0.6621 0.3496 0.3559 0.020 Uiso 1 1 calc R H23A H 0.5359 0.4574 0.1204 0.023 Uiso 1 1 calc R H23A H 0.5359 0.4574 0.1204 0.023 Uiso 1 1 calc R H23A H 0.5359 0.4574 0.1204 0.023 Uiso 1 1 calc R H23A H 0.5329 0.3742 (0.303 Uiso 1 1 calc R H23A H 0.5329 0.3742 (0.303 Uiso 1 1 calc R H23A H 0.5329 0.3742 (0.303 Uiso 1 1 calc R</pre>	H11B H 0.6241 0.5282 0.3911 0.022 Uiso 1 1 calc R
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N13 N 0.8350(2) 0.32334(12) 0.26061(17) 0.0182(4) Uani 1 1 d H13A H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R H13B H 0.7696 0.2858 0.2613 0.022 Uiso 1 1 calc R H11C H 0.6116 0.6356 0.3219 0.035 Uiso 1 1 calc R H11C H 0.6116 0.6636 0.3219 0.035 Uiso 1 1 calc R H11D H 0.5810 0.6039 0.1996 0.035 Uiso 1 1 calc R H12A H 0.8553 0.6001 0.3248 0.039 Uiso 1 1 calc R H12B H 0.8096 0.6610 0.2333 0.039 Uiso 1 1 calc R H12B H 0.8096 0.6610 0.2333 0.039 Uiso 1 1 calc R H12B H 0.8096 0.6610 0.2333 0.039 Uiso 1 1 calc R H13C H 0.7708 0.5543 0.1051 0.036 Uiso 1 1 calc R H13C H 0.7708 0.5543 0.1051 0.036 Uiso 1 1 calc R H14B H 0.8808 0.4775 0.0983 0.032 Uiso 1 1 calc R C14 C 0.9609(3) 0.44562(18) 0.1205(2) 0.0265(6) Uani 1 1 d H14A H 1.0380 0.4775 0.0983 0.032 Uiso 1 1 calc R C14 C 0.9609(3) 0.44562(18) 0.1542(2) 0.0278(6) Uani 1 1 d H15A H 1.0874 0.3550 0.0993 0.033 Uiso 1 1 calc R C15 C 1.0240(3) 0.37054(18) 0.1542(2) 0.0278(6) Uani 1 1 d H15A H 1.0874 0.3758 0.2257 0.033 Uiso 1 1 calc R H15A H 1.0843 0.3788 0.2257 0.033 Uiso 1 1 calc R H15A H 0.8481 0.3088 0.0966 0.031 Uiso 1 1 calc R H15A H 0.9649 0.2623 0.1728 0.031 Uiso 1 1 calc R H15A H 0.9449 0.2623 0.1728 0.031 Uiso 1 1 calc R H15A H 0.9443 0.3425 0.4275 0.023 Uiso 1 1 calc R H15A H 0.9443 0.4282 0.4275 0.023 Uiso 1 1 calc R H15A H 0.9443 0.4351 0.4574 0.023 Uiso 1 1 calc R H21A H 0.9430 0.4282 0.4275 0.023 Uiso 1 1 calc R H23A H 0.5359 0.4574 0.023 Uiso 1 1 calc R H23A H 0.5359 0.4574 0.023 Uiso 1 1 calc R H23A H 0.5359 0.4574 0.023 Uiso 1 1 calc R H23A H 0.5423 0.4352 0.3559 0.020 Uiso 1 1 calc R H23A H 0.5623 0.4309 0.0704 0.023 Uiso 1 1 calc R H23A H 0.5623 0.4309 0.0704 0.023 Uiso 1 1 calc R H23A H 0.5623 0.4309 0.5341 0.032 Uiso 1 1 calc R H23A H 0.5623 0.4329 0.5357(2) 0.0248(6) Uani 1 1 d H23A H 0.5623 0.3257 0.4540 0.032 Uiso 1 1 calc R H23A H 0.5623 0.32657 0.4507 0.030 Uiso 1 1 calc R H23A H 0.5623 0.	H12 H 0.9624 0.4916 0.2654 0.025 Uiso 1 1 calc R
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H22B H 0.6501 0.3627 0.6168 0.032 Uiso 1 1 calc R . C23 C 0.5893(3) 0.32874(16) 0.4575(2) 0.0247(6) Uani 1 1 d H23C H 0.6523 0.2857 0.4507 0.030 Uiso 1 1 calc R . H23D H 0.5005 0.3105 0.4845 0.030 Uiso 1 1 calc R . C24 C 0.4779(3) 0.30363(15) 0.2754(2) 0.0234(6) Uani 1 1 d H24A H 0.4003 0.2826 0.3140 0.028 Uiso 1 1 calc R . H24B H 0.5462 0.2635 0.2651 0.028 Uiso 1 1 calc R . H24B H 0.5462 0.2635 0.2651 0.028 Uiso 1 1 calc R . H25A H 0.3539 0.3742 0.1733 0.032 Uiso 1 1 calc R . H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R . H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R . H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R . H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R .	$H_{22} = 0.0030(3) 0.30140(17) 0.3420(2) 0.0203(0) 0.0011 1 1 0 1 1 0 1 1 0 1 1 0 1 1 0 1 1 0 1 1 0 1 1 0 1 1 0 1 0 1 0$
C23 C 0.5893(3) 0.32874(16) 0.4575(2) 0.0247(6) Uani 1 1 d H23C H 0.6523 0.2857 0.4507 0.030 Uiso 1 1 calc R H23D H 0.5005 0.3105 0.4845 0.030 Uiso 1 1 calc R C24 C 0.4779(3) 0.30363(15) 0.2754(2) 0.0234(6) Uani 1 1 d H24A H 0.4003 0.2826 0.3140 0.028 Uiso 1 1 calc R H24B H 0.5462 0.2635 0.2651 0.028 Uiso 1 1 calc R C25 C 0.4146(3) 0.33067(16) 0.1631(2) 0.0264(6) Uani 1 1 d H25A H 0.3539 0.3742 0.1733 0.032 Uiso 1 1 calc R H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R C26 C 0.5240(3) 0.35161(16) 0.0860(2) 0.0249(6) Uani 1 1 d H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	H22B H 0.6501 0.3627 0.6168 0.032 Uiso 1 1 calc R
H23C H 0.6523 0.2857 0.4507 0.030 Uiso 1 1 calc R H23D H 0.5005 0.3105 0.4845 0.030 Uiso 1 1 calc R C24 C 0.4779(3) 0.30363(15) 0.2754(2) 0.0234(6) Uani 1 1 d H24A H 0.4003 0.2826 0.3140 0.028 Uiso 1 1 calc R H24B H 0.5462 0.2635 0.2651 0.028 Uiso 1 1 calc R C25 C 0.4146(3) 0.33067(16) 0.1631(2) 0.0264(6) Uani 1 1 d H25A H 0.3539 0.3742 0.1733 0.032 Uiso 1 1 calc R H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R C26 C 0.5240(3) 0.35161(16) 0.0860(2) 0.0249(6) Uani 1 1 d H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	C23 C 0.5893(3) 0.32874(16) 0.4575(2) 0.0247(6) Uani 1 1 d
H23D H 0.5005 0.3105 0.4845 0.030 Uiso 1 1 calc R C24 C 0.4779(3) 0.30363(15) 0.2754(2) 0.0234(6) Uani 1 1 d H24A H 0.4003 0.2826 0.3140 0.028 Uiso 1 1 calc R H24B H 0.5462 0.2635 0.2651 0.028 Uiso 1 1 calc R C25 C 0.4146(3) 0.33067(16) 0.1631(2) 0.0264(6) Uani 1 1 d H25A H 0.3539 0.3742 0.1733 0.032 Uiso 1 1 calc R H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R C26 C 0.5240(3) 0.35161(16) 0.0860(2) 0.0249(6) Uani 1 1 d H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	H23C H 0.6523 0.2857 0.4507 0.030 Ùiso 1 1 càlc R
C24 C 0.4779(3) 0.30363(15) 0.2754(2) 0.0234(6) Uani 1 1 d H24A H 0.4003 0.2826 0.3140 0.028 Uiso 1 1 calc R H24B H 0.5462 0.2635 0.2651 0.028 Uiso 1 1 calc R C25 C 0.4146(3) 0.33067(16) 0.1631(2) 0.0264(6) Uani 1 1 d H25A H 0.3539 0.3742 0.1733 0.032 Uiso 1 1 calc R H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R C26 C 0.5240(3) 0.35161(16) 0.0860(2) 0.0249(6) Uani 1 1 d H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	H23D H 0.5005 0.3105 0.4845 0.030 Uiso 1 1 calc R
H24A H 0.4003 0.2826 0.3140 0.028 Uiso 1 1 calc R H24B H 0.5462 0.2635 0.2651 0.028 Uiso 1 1 calc R C25 C 0.4146(3) 0.33067(16) 0.1631(2) 0.0264(6) Uani 1 1 d H25A H 0.3539 0.3742 0.1733 0.032 Uiso 1 1 calc R H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R C26 C 0.5240(3) 0.35161(16) 0.0860(2) 0.0249(6) Uani 1 1 d H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	C24 C 0.4779(3) 0.30363(15) 0.2754(2) 0.0234(6) Uani 1 1 d
H24B H 0.5462 0.2635 0.2651 0.028 Uiso 1 1 calc R C25 C 0.4146(3) 0.33067(16) 0.1631(2) 0.0264(6) Uani 1 1 d H25A H 0.3539 0.3742 0.1733 0.032 Uiso 1 1 calc R H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R C26 C 0.5240(3) 0.35161(16) 0.0860(2) 0.0249(6) Uani 1 1 d H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	H24A H 0.4003 0.2826 0.3140 0.028 Uiso 1 1 calc R
<pre>C25 C 0.4146(3) 0.33067(16) 0.1631(2) 0.0264(6) Uan1 1 1 d H25A H 0.3539 0.3742 0.1733 0.032 Uiso 1 1 calc R H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R C26 C 0.5240(3) 0.35161(16) 0.0860(2) 0.0249(6) Uani 1 1 d H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R</pre>	H24B H 0.5462 0.2635 0.2651 0.028 Uiso 1 1 calc R
H25A H 0.3539 0.3742 0.1733 0.032 0150 1 1 Calc R H25B H 0.3521 0.2916 0.1278 0.032 Uiso 1 1 calc R C26 C 0.5240(3) 0.35161(16) 0.0860(2) 0.0249(6) Uani 1 1 d H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	$(25 \ C \ U.414b(3) \ U.33Ub/(1b) \ U.1b31(2) \ U.02b4(b) \ Uan1 \ I \ I \ d \ . \ .$
C26 C 0.5240(3) 0.35161(16) 0.0860(2) 0.0249(6) Uani 1 1 d H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	HZDA H U.3039 U.3/42 U.1/33 U.U32 UISO I I Calc K μ 250 μ 0 2521 0 2016 0 1278 0 022 μ ico 1 1 colc p
H26A H 0.5931 0.3108 0.0831 0.030 Uiso 1 1 calc R H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	$C_{20} = 0.3321 0.2310 0.1270 0.032 0150 1 1 call K C_{26} C = 0.5240(3) 0.35161(16) 0.0860(2) 0.0240(6) uppi 1 1 d$
H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R	$H_{20} = 0.3240(3) 0.33101(10) 0.0000(2) 0.0249(0) 0.011 1 1 0 H_{20} H_{0} 5931 0 3108 0 0.831 0 0.30 Hiso 1 1 calc R$
	H26B H 0.4750 0.3589 0.0110 0.030 Uiso 1 1 calc R

•

loop_ _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom_site_aniso_U_33 _atom_site_aniso_U_23 _atom_site_aniso_U_13

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_atom_site_aniso_U_12
Ni1 0.00968(17) 0.01485(17) 0.01032(17) -0.00047(10) 0.00288(11) -0.00136(11)
s1 0.0264(4) 0.0417(4) 0.0345(4) 0.0076(3) 0.0013(3) -0.0004(3)
$(1 \ 0.0315(16) \ 0.0359(16) \ 0.0161(11) \ -0.0051(11) \ -0.0009(11) \ 0.0129(13))$
N1 $0.070(2)$ $0.0345(16)$ $0.0360(15)$ $-0.0117(12)$ $0.0019(16)$ $0.0033(15)$
$s_{2} 0.0481(6) 0.0344(4) 0.0412(4) 0.0077(3) -0.0051(4) -0.0039(4)$
C2 0.0234(15) 0.055(2) 0.0256(14) -0.0016(13) -0.0036(13) 0.0106(14)
N2 $0.079(3)$ $0.0174(13)$ $0.092(3)$ $0.0099(14)$ $-0.060(2)$ $-0.0125(14)$
N11 $0.0193(11)$ $0.0155(9)$ $0.0195(10)$ $-0.0026(8)$ $0.0031(9)$ $0.0015(8)$
N12 $0.0183(11)$ $0.0297(12)$ $0.0149(9)$ $-0.0007(8)$ $0.0036(9)$ $-0.0089(9)$
N13 $0.0137(10)$ $0.0210(10)$ $0.0209(10)$ $-0.0028(8)$ $0.0066(9)$ $0.0021(8)$
$c11 \ 0.0349(17) \ 0.0195(12) \ 0.0327(14) \ 0.0047(11) \ 0.0003(13) \ -0.0005(12)$
$c12 \ 0.0400(19) \ 0.0231(14) \ 0.0346(15) \ 0.0001(12) \ 0.0051(14) \ -0.0117(12)$
$c13 \ 0.0412(18) \ 0.0258(14) \ 0.0254(13) \ 0.0055(11) \ 0.0106(13) \ -0.0132(13)$
$C14 \ 0.0193(13) \ 0.0456(16) \ 0.0158(11) \ 0.0007(11) \ 0.0079(10) \ -0.0077(12)$
$c15 \ 0.0135(12) \ 0.0524(18) \ 0.0192(12) \ -0.0036(12) \ 0.0096(11) \ 0.0024(12)$
$C16 \ 0.0224(14) \ 0.0360(15) \ 0.0200(12) \ -0.0077(11) \ 0.0075(11) \ 0.0053(11)$
N21 $0.0142(10)$ $0.0288(11)$ $0.0136(9)$ $-0.0015(8)$ $0.0000(8)$ $0.0014(9)$
N22 $0.0154(10)$ $0.0164(9)$ $0.0194(9)$ $0.0003(8)$ $0.0106(8)$ $-0.0017(8)$
N23 $0.0165(11) 0.0265(11) 0.0135(9) -0.0007(8) -0.0014(8) -0.0042(8)$
$ C21 \ 0.0250(15) \ 0.0428(17) \ 0.0180(11) \ 0.0074(11) \ 0.0008(11) \ 0.0059(12) $
$ C22 \ 0.0262(15) \ 0.0404(16) \ 0.0159(11) \ 0.0043(11) \ 0.0100(11) \ 0.0016(12) $
$ C23 \ 0.0265(14) \ 0.0268(13) \ 0.0235(12) \ 0.0072(11) \ 0.0150(11) \ 0.0002(11) $
$C24 \ 0.0168(13) \ 0.0210(12) \ 0.0338(14) \ -0.0027(11) \ 0.0089(11) \ -0.0065(10)$
$ c25 \ 0.0149(13) \ 0.0289(14) \ 0.0348(14) \ -0.0086(12) \ 0.0004(12) \ -0.0054(10) $
$C26 \ 0.0232(14) \ 0.0295(14) \ 0.0209(12) \ -0.0114(10) \ -0.0025(11) \ -0.0030(11)$

_geom_special_details

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

loop_

_geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_2 _geom_bond_publ_flag Ni1 N13 2.115(2) . ? Ni1 N13 2.115(2) . Ni1 N23 2.119(2) . Ni1 N12 2.178(2) . Ni1 N12 2.178(2) . Ni1 N11 2.179(2) . Ni1 N21 2.184(2) . ?? ?? Ni1 N22 2.202(2) ? s1 c1 1.640(3). ? C1 N1 1.164(5) ? . s2 c2 1.602(4) ? . C2 N2 1.126(5) ? N11 C11 1.486(3) ???? . N12 C14 1.491(4)• N12 C13 1.495(4). N13 C16 1.487(3) . ? ? ? C11 C12 1.517(5)1.523(5) C12 C13 . C14 C15 1.525(4). C15 C16 1.508(4) ? ? . N21 C21 1.480(3) • N22 C23 1.486(3) ???? N22 C24 1.491(3). N23 C26 1.483(3). C21 C22 1.519(4) • ? C22 C23 1.525(4) • C24 C25 1.517(4) ? .

C25 C26 1.521(4) . ? 100p_ _geom_angle_atom_site_label_1 _geom_angle_atom_site_label_2 _geom_angle_atom_site_label_3 _geom_angle _geom_angle_site_symmetry_1 _geom_angle_site_symmetry_3 _geom_angle_publ_flag N13 Ni1 N23 96.26(9) ? . N13 Ni1 N12 90.34(9) ? . . ? N23 Ni1 N12 90.04(9) . . ? N12 Ni1 N11 92.70(9) . . N13 Ni1 N21 87.75(8) ? • N23 Ni1 N21 175.31(9) . . ? N12 Ni1 N21 87.51(8) ? . . N11 Ni1 N21 86.94(8) . . ? N13 Ni1 N22 89.75(8) . . ? N23 Ni1 N22 88.87(8) N23 N11 N22 00.0. N12 N11 N22 178.91(8) . . ? N11 Ni1 N22 87.31(8) . . N21 N11 N22 93.58(8) ? N1 C1 S1 179.2(3) . . N2 C2 S2 173.1(4) ? C11 N11 Ni1 124.45(19) . ? ? C14 N12 C13 108.1(2). ? C14 N12 Ni1 116.32(17) • ? C13 N12 Ni1 114.56(19) . • C16 N13 Ni1 121.15(17) ? ? 113.0(2) . N11 C11 C12 . ? 113.8(3) C11 C12 C13 . . ? N12 C13 C12 113.6(2) . • ? N12 C14 C15 114.5(2) . c16 c15 c14 114.8(2) ? . . ? N13 C16 C15 111.3(2). C21 N21 Ni1 122.48(18) ? . ? C23 N22 C24 107.4(2) . C23 N22 Ni1 116.34(17) ? • ? C24 N22 Ni1 117.11(16). . C26 N23 Ni1 119.62(17) ? • ? N21 C21 C22 112.2(2) . . ? c21 c22 c23 114.9(2) . N22 C23 C22 114.5(2) ? . . N22 C24 C25 ?? 114.5(2)• . c24 c25 c26 114.6(2) . . ? N23 C26 C25 111.8(2) . _diffrn_measured_fraction_theta_max 0.977 _diffrn_reflns_theta_full 28.04 _diffrn_measured_fraction_theta_full 0.977 _refine_diff_density_max _refine_diff_density_min _refine_diff_density_rms 0.840 -1.1680.100 # Attachment '- TA176TT.CIF' data_ta176tt _database_code_depnum_ccdc_archive 'CCDC 838537' #TrackingRef '- TA176TT.CIF _audit_creation_method SHELXL-97 _chemical_name_systematic ? ;

C1CE06011B_ccdc_838535_838540_cif.txt

C1CE06011B_ccdc_838535_838540_cif.txt _chemical_name_common _chemical_melting_point _chemical_formula_moiety 'C22 H53 N13 Ni2 O S4' _chemical_formula_sum 'C22 H53 N13 Ni2 O S4' _chemical_formula_weight 761.43 loop_ _atom_type_symbol _atom_type_description _atom_type_scat_dispersion_real _atom_type_scat_dispersion_imag _atom_type_scat_source C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' O 0 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' Ni Ni 0.3393 1.1124 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' _symmetry_cell_setting monoclinic C C' _symmetry_space_group_name_H-M -2yc' _symmetry_space_group_name_Hall 1000 _symmetry_equiv_pos_as_xyz 'x, y, z' 'x, -y, z+1/2' 'x+1/2, y+1/2, z' 'x+1/2, -y+1/2, z+1/2' _cell_length_a 9.1530(6) _cell_length_b _cell_length_c _cell_angle_alpha 29.835(2) 12.9934(7)90.00 _cell_angle_beta 97.272(7) _cell_angle_gamma 90.00 _cell_volume _cell_formula_units_z 3519.7(4) _cell_measurement_temperature 200(2) _cell_measurement_reflns_used 8474 2.34 _cell_measurement_theta_min _cell_measurement_theta_max 25.00 _expt]_crystal_description block _exptl_crystal_colour blue _exptl_crystal_size_max _exptl_crystal_size_mid _exptl_crystal_size_min 0.35 0.28 0.25 _exptl_crystal_density_meas _exptl_crystal_density_diffrn 1.437 _exptl_crystal_density_method
_exptl_crystal_F_000 'not measured' 1616 _exptl_absorpt_coefficient_mu 1.346 _exptl_absorpt_correction_type numerical _exptl_absorpt_correction_T_min _exptl_absorpt_correction_T_max 0.638 0.709 _exptl_absorpt_process_details 'X-Shape and X-Red32 (STOE, 2008)' _exptl_special_details ; ? _diffrn_ambient_temperature 200(2) 0.71073 _diffrn_radiation_wavelength _diffrn_radiation_type мок∖а 'fine-focus sealed tube' _diffrn_radiation_source _diffrn_radiation_monochromator graphite Page 11

C1CE06011B_ccdc_838535_838540_cif.txt _diffrn_measurement_device_type _diffrn_measurement_method 7 _diffrn_detector_area_resol_mean _diffrn_standards_number _diffrn_standards_interval_count _diffrn_standards_interval_time _diffrn_standards_decay_% ? _diffrn_reflns_number 8474 _diffrn_reflns_av_R_equivalents 0.1100 _diffrn_reflns_av_sigmaI/netI _diffrn_reflns_limit_h_min _diffrn_reflns_limit_h_max 0.1335 -1010 _diffrn_reflns_limit_k_min -35 _diffrn_reflns_limit_k_max 35 _diffrn_reflns_limit_l_min _diffrn_reflns_limit_l_max -11 15 _diffrn_reflns_theta_min 2.34 _diffrn_reflns_theta_max 25.00 _reflns_number_total _reflns_number_gt 5459 3631 _reflns_threshold_expression >2sigma(I) _computing_data_collection 7 _computing_cell_refinement 7 _computing_data_reduction _computing_structure_solution 'SHELXS-97 (Sheldrick, 1990)' 'SHELXL-97 (Sheldrick, 1997)' _computing_structure_refinement _computing_molecular_graphics ? _computing_publication_material _refine_special_details Refinement of $F^{2^{1}}$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^{2^{1}}$, conventional R-factors R are based on F, with F set to zero for negative $F^{2^{-1}}$. The threshold expression of $F^2^{\prime} > 2sigma(F^2^{\prime})$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and Rfactors based on ALL data will be even larger. _refine_ls_structure_factor_coef Fsqd _refine_ls_matrix_type full _refine_ls_weighting_scheme calc _refine_ls_weighting_details 'calc w=1/[\s^2^(Fo^2^)+(0.0503P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3' _atom_sites_solution_primary direct _atom_sites_solution_secondary difmap _atom_sites_solution_hydrogens geom _refine_ls_hydrogen_treatment constr _refine_ls_extinction_method
_refine_ls_extinction_coef none _refine_ls_abs_structure_details 'Flack H D (1983), Acta Cryst. A39, 876-881' 0.01(3) _refine_ls_abs_structure_Flack _refine_ls_number_reflns _refine_ls_number_parameters _refine_ls_number_restraints 5459 379 _refine_ls_R_factor_all _refine_ls_R_factor_gt 0.1115 0.0657 _refine_ls_wR_factor_ref _refine_ls_wR_factor_gt _refine_ls_goodness_of_fit_ref 0.1366 0.1200 0.979 _refine_ls_restrained_s_all 0.979 0.001 _refine_ls_shift/su_max _refine_ls_shift/su_mean 0.000 100p_

_atom_site_label

C1CE06011B_ccdc_838535_838540_cif.txt _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y _atom_site_fract_z _atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_symmetry_multiplicity _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly _atom_site_disorder_group Nil Ni 0.28905(11) 0.83345(4) 0.16584(9) 0.0271(3) Uani 1 1 d . . . Ni2 Ni 0.75020(13) 0.94177(4) 0.58497(11) 0.0323(3) Uani 1 1 d . . . N1 N 0.428(2) 0.8402(4) -0.2767(10) 0.091(4) Uani 1 1 d . . . C1 C 0.3180(13) 0.8350(4) -0.2628(9) 0.040(3) Uani 1 1 d . . s1 s 0.1497(5) 0.82838(14) -0.2354(3) 0.0749(11) Uani 1 1 d . . N2 N 0.5630(10) 0.9570(3) 0.4797(8) 0.048(2) Uani 1 1 d . . . C2 C 0.4735(11) 0.9679(3) 0.4159(10) 0.041(3) Uani 1 1 d . . . S2 S 0.3449(3) 0.98411(10) 0.3229(2) 0.0469(8) Uani 1 1 d . . . N3 N 0.7375(10) 0.8723(3) 0.5441(8) 0.049(2) Uani 1 1 d . . . C3 C 0.7306(11) 0.8412(4) 0.4873(9) 0.039(3) Uani 1 1 d . . . S3 S 0.7229(3) 0.79827(9) 0.4097(2) 0.0395(7) Uani 1 1 d . . . N4 N 0.7739(9) 1.0097(3) 0.6223(7) 0.040(2) Uani 1 1 d . . . C4 C 0.7734(11) 1.0451(3) 0.6584(9) 0.034(2) Uani 1 1 d . . . s4 s 0.7733(3) 1.09600(9) 0.7060(3) 0.0455(7) Uani 1 1 d . . N11 N 0.4315(9) 0.7758(3) 0.1776(8) 0.040(2) Uani 1 1 d . . . H11C H 0.4972 0.7793 0.2368 0.048 Uiso 1 1 calc R H11D H 0.3742 0.7513 0.1883 0.048 Uiso 1 1 calc R N12 N 0.4341(9) 0.8688(3) 0.0694(7) 0.033(2) Uani 1 1 d . . . H12 H 0.5055 0.8823 0.1167 0.040 Uiso 1 1 calc R . N13 N 0.1504(8) 0.8908(3) 0.1705(6) 0.0313(19) Uani 1 1 d . . . H13A H 0.0591 0.8809 0.1830 0.038 Uiso 1 1 calc R . H13B H 0.1879 0.9079 0.2266 0.038 Uiso 1 1 calc R . c11 c 0.5196(12) 0.7639(4) 0.0913(9) 0.043(3) Uani 1 1 d . . . H11A H 0.4526 0.7534 0.0303 0.051 Uiso 1 1 calc R . H11B H 0.5889 0.7393 0.1140 0.051 Uiso 1 1 calc R . . C12 C 0.6054(12) 0.8047(3) 0.0614(10) 0.044(3) Uani 1 1 d . . . H12A H 0.6589 0.8177 0.1255 0.053 Uiso 1 1 calc R . . H12B H 0.6800 0.7945 0.0178 0.053 Uiso 1 1 calc R C13 C 0.5171(13) 0.8408(4) 0.0050(9) 0.047(3) Uani 1 1 d . . . H13C H 0.5841 0.8602 -0.0292 0.057 Uiso 1 1 calc R H13D H 0.4470 0.8269 -0.0502 0.057 Uiso 1 1 calc R . . c14 c 0.3683(13) 0.9062(4) 0.0036(10) 0.050(3) Uani 1 1 d . . . H14A H 0.3072 0.8931 -0.0573 0.060 Uiso 1 1 calc R . H14B H 0.4493 0.9230 -0.0225 0.060 Uiso 1 1 calc R . c15 c 0.2750(12) 0.9391(4) 0.0539(9) 0.046(3) Uani 1 1 d . . . H15A H 0.2542 0.9651 0.0070 0.055 Uiso 1 1 calc R . H15B H 0.3320 0.9501 0.1188 0.055 Uiso 1 1 calc R C16 C 0.1297(11) 0.9201(3) 0.0793(9) 0.040(3) Uani 1 1 d . . . H16A H 0.0632 0.9450 0.0923 0.049 Uiso 1 1 calc R . . H16B H 0.0822 0.9029 0.0190 0.049 Uiso 1 1 calc R N21 N 0.4185(8) 0.8603(3) 0.3017(6) 0.0330(19) Uani 1 1 d . . . H1A H 0.5041 0.8438 0.3122 0.040 Uiso 1 1 calc R . . H1B H 0.4448 0.8890 0.2858 0.040 Uiso 1 1 calc R . . N22 N 0.1481(8) 0.7952(2) 0.2579(6) 0.0303(18) Uani 1 1 d . . H2 H 0.1922 0.7671 0.2652 0.036 Uiso 1 1 calc R . . N23 N 0.1705(8) 0.8074(3) 0.0286(7) 0.036(2) Uani 1 1 d . . . H3A H 0.1859 0.8267 -0.0244 0.044 Uiso 1 1 calc R . H3B H 0.2140 0.7807 0.0151 0.044 Uiso 1 1 calc R C21 C 0.3588(11) 0.8625(4) 0.4033(8) 0.040(2) Uani 1 1 d . H1C H 0.2837 0.8865 0.4009 0.048 Uiso 1 1 calc R . H1D H 0.4392 0.8699 0.4590 0.048 Uiso 1 1 calc R C22 C 0.2908(12) 0.8185(4) 0.4272(8) 0.044(3) Uani 1 1 d . . . H2A H 0.2815 0.8175 0.5022 0.053 Uiso 1 1 calc R . H2B H 0.3579 0.7940 0.4122 0.053 Uiso 1 1 calc R . C23 C 0.1392(12) 0.8101(4) 0.3660(8) 0.043(3) Uani 1 1 d . . . H3C H 0.0873 0.7869 0.4021 0.052 Uiso 1 1 calc R . . Page 13

C1CE06011B_ccdc_838535_838540_cif.txt H3D H 0.0805 0.8380 0.3644 0.052 Uiso 1 1 calc R . . C24 C -0.0068(10) 0.7857(3) 0.2115(9) 0.036(3) Uani 1 1 d . . . H4A H -0.0637 0.8140 0.2083 0.043 Uiso 1 1 calc R . H4B H -0.0521 0.7648 0.2576 0.043 Uiso 1 1 calc R . C25 C -0.0185(12) 0.7657(4) 0.1043(10) 0.046(3) Uani 1 1 d . . . H5A H -0.1188 0.7533 0.0862 0.056 Uiso 1 1 calc R . . H5B H 0.0522 0.7406 0.1049 0.056 Uiso 1 1 calc R C26 C 0.0121(11) 0.7993(4) 0.0199(9) 0.041(3) Uani 1 1 d . . H6A H -0.0236 0.7871 -0.0495 0.050 Uiso 1 1 calc R H6B H -0.0405 0.8278 0.0289 0.050 Uiso 1 1 calc R . . N31 N 0.8642(10) 0.9505(3) 0.4567(8) 0.048(2) Uani 1 1 d . . . H21C H 0.8391 0.9265 0.4137 0.058 Uiso 1 1 calc R H21D H 0.8237 0.9754 0.4224 0.058 Uiso 1 1 calc R N32 N 0.9433(8) 0.9272(3) 0.6890(6) 0.0292(19) Uani 1 1 d . . . H22 H 0.9506 0.8961 0.6884 0.035 Uiso 1 1 calc R . . N33 N 0.6116(9) 0.9324(3) 0.6972(7) 0.040(2) Uani 1 1 d . . . H23A H 0.5284 0.9493 0.6785 0.048 Uiso 1 1 calc R . H23B H 0.5828 0.9028 0.6945 0.048 Uiso 1 1 calc R C31 C 1.0209(13) 0.9554(5) 0.4611(11) 0.063(4) uani 1 1 d . . . H21A H 1.0468 0.9876 0.4688 0.075 Uiso 1 1 calc R . . H21B H 1.0520 0.9448 0.3950 0.075 Uiso 1 1 calc R . . c32 c 1.1035(12) 0.9296(4) 0.5499(9) 0.048(3) Uani 1 1 d . . . H22A H 1.0752 0.8976 0.5414 0.058 Uiso 1 1 calc R . H22B H 1.2099 0.9316 0.5435 0.058 Uiso 1 1 calc R . . C33 C 1.0826(10) 0.9431(4) 0.6549(9) 0.041(2) Uani 1 1 d . . H23C H 1.0852 0.9763 0.6588 0.050 Uiso 1 1 calc R . H23D H 1.1660 0.9316 0.7036 0.050 Uiso 1 1 calc R C34 C 0.9407(11) 0.9386(4) 0.7970(8) 0.043(3) Uani 1 1 d . . . H24A H 0.9430 0.9717 0.8038 0.051 Uiso 1 1 calc R . . H24B H 1.0311 0.9267 0.8377 0.051 Uiso 1 1 calc R C35 C 0.8050(12) 0.9205(4) 0.8448(9) 0.050(3) Uani 1 1 d . . . H25A H 0.7947 0.8881 0.8297 0.059 Uiso 1 1 calc R . . H25B H 0.8235 0.9240 0.9211 0.059 Uiso 1 1 calc R . . C36 C 0.6652(13) 0.9430(5) 0.8067(9) 0.055(3) Uani 1 1 d . . . H26A H 0.6788 0.9758 0.8139 0.066 Uiso 1 1 calc R . H26B H 0.5894 0.9339 0.8506 0.066 Uiso 1 1 calc R Olw O 0.2407(12) 0.6940(3) 0.2439(10) 0.094(4) Uani 1 1 d . . . H1O H 0.1637 0.6789 0.2282 0.142 Uiso 1 1 d R . . H2O H 0.3073 0.6766 0.2701 0.142 Uiso 1 1 d R . . loop_ _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom_site_aniso_U_33 _atom_site_aniso_U_23 _atom_site_aniso_U_13 _atom_site_aniso_U_12 Ni1 0.0289(6) 0.0282(6) 0.0245(7) 0.0016(6) 0.0049(5) 0.0002(6) Ni2 0.0333(6) 0.0307(7) 0.0316(8) -0.0027(6) -0.0007(5) -0.0035(6) N1 0.166(14) 0.064(8) 0.045(8) -0.013(6) 0.026(9) -0.009(10)C1 0.052(6) 0.026(5) 0.041(7) -0.008(5) -0.001(5) -0.006(5)S1 0.093(3) 0.073(2) 0.056(2) 0.005(2) -0.002(2) 0.004(2) N2 0.045(5) 0.052(6) 0.044(7) 0.005(5) -0.010(5) 0.001(5) C2 0.029(5) 0.039(6) 0.055(8) -0.002(5) 0.004(5) -0.004(5) S2 0.0467(16) 0.0478(17) 0.0424(19) -0.0013(14) -0.0091(13) 0.0002(13) N3 0.053(6) 0.037(5) 0.055(7) -0.009(5) 0.001(5) -0.011(4) C3 0.036(5) 0.040(6) 0.041(7) 0.003(5) 0.002(5) -0.001(5)s3 0.0441(15) 0.0353(14) 0.0385(17) -0.0025(13) 0.0027(13) 0.0062(12) N4 0.040(5) 0.034(5) 0.047(6) 0.002(4) 0.003(4) -0.003(4)c4 0.028(5) 0.038(6) 0.037(6) 0.011(5) 0.007(4) 0.008(5) s4 0.0427(14) 0.0341(14) 0.058(2) -0.0025(13) 0.0018(13) 0.0034(12) N11 0.039(5) 0.028(5) 0.055(7) 0.007(4) 0.010(4) 0.001(4) N12 0.038(4) 0.037(5) 0.026(5) -0.005(4) 0.010(4) -0.009(4) N13 0.032(4) 0.036(5) 0.025(5) 0.006(4) -0.004(3) 0.002(3) C11 0.038(6) 0.050(7) 0.044(7) -0.011(6) 0.021(5) 0.011(5) $c12 \ 0.038(6) \ 0.035(6) \ 0.064(9) \ -0.007(6) \ 0.023(6) \ -0.010(5)$ c13 0.052(6) 0.061(7) 0.034(6) 0.005(6) 0.023(5) 0.021(6)

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C14	0.060(7)	0.046(7)	0.045(8)	0.018(6)	0.014(6)	0.006(6)
C15	0.056(7)	0.041(6)	0.041(7)	0.008(6)	0.008(5)	0.006(5)
C16	0.054(6)	0.037(6)	0.031(6)	0.017(5)	0.008(5)	0.013(5)
N21	0.035(4)	0.034(4)	0.031(5)	-0.006(4)	0.006(4)	-0.005(4)
N22	0.034(4)	0.029(4)	0.030(5)	0.008(4)	0.011(4)	-0.002(3)
N23	0.032(4)	0.041(5)	0.036(5)	0.000(4)	-0.001(4)	0.004(4)
C21	0.043(6)	0.046(6)	0.031(6)	0.001(5)	0.003(5)	-0.007(5)
C22	0.049(6)	0.063(7)	0.018(6)	0.008(5)	-0.004(5)	0.002(6)
C23	0.056(7)	0.053(7)	0.023(6)	0.005(5)	0.016(5)	-0.007(5)
C24	0.029(5)	0.032(5)	0.051(7)	0.000(5)	0.019(5)	-0.006(4)
C25	0.041(6)	0.049(7)	0.049(8)	0.000(6)	0.005(5)	-0.008(5)
C26	0.041(6)	0.046(6)	0.036(7)	-0.006(5)	0.001(5)	-0.015(5)
N31	0.057(6)	0.051(6)	0.033(6)	0.001(5)	-0.004(4)	-0.001(5)
N32	0.033(4)	0.027(4)	0.028(5)	-0.005(4)	0.003(4)	-0.003(3)
N33	0.035(5)	0.040(5)	0.049(6)	0.012(4)	0.017(4)	-0.003(4)
C31	0.061(8)	0.083(10)) 0.051(8)) -0.001(7) 0.035(7) -0.012(7)
C32	0.044(6)	0.056(7)	0.047(8)	0.005(6)	0.016(6)	-0.003(5)
C33	0.025(5)	0.051(6)	0.049(7)	-0.003(6)	0.007(4)	-0.007(5)
C34	0.052(6)	0.050(6)	0.024(6)	-0.002(5)	-0.004(5) -0.003(5)
C35	0.063(7)	0.061(7)	0.028(6)	0.003(6)	0.017(5)	0.001(6)
C36	0.056(7)	0.073(8)	0.041(7)	-0.008(7)	0.022(6)	-0.014(7)
01W	0.099(8)	0.057(6)	0.129(11)) 0.014(6)	0.020(8)	-0.002(6)

_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.

100p_ _geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_2 _geom_bond_publ_flag Ni1 N23 2.114(8) . ? Ni1 N23 2.114(8) Ni1 N13 2.135(8) Ni1 N11 2.152(8) Ni1 N21 2.152(8) ? ? . ? . Ni1 N22 2.189(7) Ni1 N12 2.207(8) Ni2 N33 2.070(8) ? . ? . ? . Ni2 N4 2.089(9) .? Ni2 N31 2.092(10) . ? ? Ni2 N2 2.103(10) . Ni2 N32 2.130(8) ? . ? Ni2 N3 2.140(9) . ?? N1 C1 1.052(16) c1 s1 1.636(14) . N2 C2 1.137(13) C2 S2 1.649(12) N3 C3 1.182(13) ???? . C3 S3 1.626(11) . · ? ? N4 C4 1.156(13) C4 S4 1.640(11) N11 C11 1.504(13) . N12 C13 1.461(13) ???????? . N12 C14 1.486(13) . N13 C16 1.466(12) 1.525(14)1.482(16)C11 C12 . C12 C13 . c14 c15 1.503(15) . c15 c16 1.520(15) ? N21 C21 1.493(13)

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N22 N23 C21 C22 C24 C25 N31 N32 N32 N33 C31 C32 C34 C35	C23 C24 C26 C22 C23 C25 C26 C31 C34 C33 C36 C32 C33 C35 C36	1.4 1.4 1.5 1.5 1.5 1.4 1.4 1.4 1.4 1.4 1.5 1.4	85() 96() 00() 31() 37() 37() 37() 37() 37() 37() 37() 37	13) 12) 12) 14) 15) 16) 15) 12) 12) 15) 15) 15) 15) 17)		???????????????????	
loop gee stattt stattt stattt stattt stattt stattt stattt stattt stattt stattt stattt stattt stattt stattt statttt statttt statttt statttt stattttt statttttttttt	p	19 12 <td< td=""><td>$\begin{array}{c} \text{att}\\ \text{att}\\$</td><td>opon tttb47</td><td>sill sill sill</td><td>te_ te_ te_ nmee ag ag b ag b ag b b c <</td><td>label_2 label_2 try_1 .????????????????????????????????????</td></td<>	$\begin{array}{c} \text{att}\\ \text{att}\\$	opon tttb47	sill sill	te_ te_ te_ nmee ag ag b ag b ag b b c <	label_2 label_2 try_1 .????????????????????????????????????

N12 C13 C12 115.0(10) ?? N12 C14 C15 116.8(10) C14 C15 C16 114.3(10) . . ? . . ? N13 C16 C15 111.8(9) . . C21 N21 Ni1 121.1(6) . . C23 N22 C24 105.9(7) ? . . ? C23 N22 Ni1 117.8(6) . . ?? C24 N22 Ni1 118.2(6) • C26 N23 Ni1 121.6(7) . ? N21 C21 C22 110.6(9) • ? C21 C22 C23 114.2(9). . ?? N22 C23 C22 112.7(8). . N22 C24 C25 113.6(8) . . ?? C24 C25 C26 113.7(9) . N23 C26 C25 108.8(9) . . ?? C31 N31 Ni2 125.3(8). • C34 N32 C33 109.7(8) . . ? C34 N32 Ni2 117.0(6) . . C33 N32 Ni2 114.9(6) • C36 N33 Ni2 119.4(6)• • N31 C31 C32 112.3(10) . . ? c33 c32 c31 117.5(10) . . ? C32 C33 N32 114.3(9) . . N32 C34 C35 114.8(8) . . ? C36 C35 C34 114.3(10) . . ? C35 C36 N33 113.3(10) . . ? _diffrn_measured_fraction_theta_max 0.998 _diffrn_reflns_theta_full 25.00 _diffrn_measured_fraction_theta_full 0.998 _refine_diff_density_max 0.417 _refine_diff_density_min _refine_diff_density_rms -0.403 0.092 # Attachment '- TA181.CIF' data_ta181 _database_code_depnum_ccdc_archive 'CCDC 838538' #TrackingRef '- TA181.CIF' _audit_creation_method SHELXL-97 _chemical_name_systematic ? _chemical_name_common _chemical_melting_point _chemical_formula_moiety 'C13 H22 N6 Ni S2' 'C13 H22 N6 Ni S2' _chemical_formula_sum _chemical_formula_weight 385.20 loop_ _atom_type_symbol _atom_type_description _atom_type_scat_dispersion_real _atom_type_scat_dispersion_imag atom_type_scat_source C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' Ni Ni 0.3393 1.1124 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' _symmetry_cell_setting monoclinic _symmetry_space_group_name_H-M 'P 21/c' '-P 2ybc' _symmetry_space_group_name_Hall loop_

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C1CE06011B_ccdc_838535_838540_cif.txt _symmetry_equiv_pos_as_xyz 'x, y, z' '-x, y+1/2, '-x, -y, -z' -z+1/2' 'x, -y-1/2, z-1/2' _cell_length_a _cell_length_b _cell_length_c 13.0449(8)8.9722(8) 15.1744(9)90.00 _cell_angle_alpha _cell_angle_beta _cell_angle_gamma _cell_volume 98.385(7) 90.00 1757.0(2)_cell_formula_units_z _cell_measurement_temperature
_cell_measurement_reflns_used 170(2)16789 _cell_measurement_theta_min 2.64 _cell_measurement_theta_max 27.98 _exptl_crystal_description _exptl_crystal_colour block blue _exptl_crystal_size_max 0.17 0.14 _exptl_crystal_size_mid _exptl_crystal_size_min _exptl_crystal_density_meas _exptl_crystal_density_diffrn 0.11 1.456 'not measured' _exptl_crystal_density_method 808 _expt]_crystal_F_000 _exptl_absorpt_coefficient_mu 1.347 _exptl_absorpt_correction_type numerical _expt]_absorpt_correction_T_min 0.789 0.854 _exptl_absorpt_correction_T_max _exptl_absorpt_process_details 'X-Shape and X-Red32 (STOE, 2008)' _exptl_special_details ? ; _diffrn_ambient_temperature 170(2)0.71073 _diffrn_radiation_wavelength _diffrn_radiation_type мок∖а _diffrn_radiation_source fine-focus sealed tube' _diffrn_radiation_monochromator graphite _diffrn_measurement_device_type _diffrn_measurement_method ? _diffrn_detector_area_resol_mean _diffrn_standards_number _diffrn_standards_interval_count ? _diffrn_standards_interval_time 7 _diffrn_standards_decay_% 2 _diffrn_reflns_number 16789 _diffrn_reflns_av_R_equivalents 0.0399 _diffrn_reflns_av_sigmaI/netI _diffrn_reflns_limit_h_min _diffrn_reflns_limit_h_max _diffrn_reflns_limit_k_min 0.0286 -16 16 -11 _diffrn_reflns_limit_k_max _diffrn_reflns_limit_l_min _diffrn_reflns_limit_l_max 11 -19 20 _diffrn_reflns_theta_min 2.64 _diffrn_reflns_theta_max 27.98 4152 _reflns_number_total 3509 _reflns_number_gt _reflns_threshold_expression >2sigma(I) ? _computing_data_collection ? _computing_cell_refinement Page 18

C1CE06011B_ccdc_838535_838540_cif.txt _computing_data_reduction 'SHELXS-97 (Sheldrick, 1990)' 'SHELXL-97 (Sheldrick, 1997)' _computing_structure_solution _computing_structure_refinement ? _computing_molecular_graphics _computing_publication_material ? _refine_special_details Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of F^2 > 2sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and Rfactors based on ALL data will be even larger. _refine_ls_structure_factor_coef Fsqd _refine_ls_matrix_type full _refine_ls_weighting_scheme calc _refine_ls_weighting_details 'calc w=1/[\s^2^(Fo^2^)+(0.0439P)^2^+0.1732P] where P=(Fo^2^+2Fc^2^)/3' _atom_sites_solution_primary direct _atom_sites_solution_secondary _atom_sites_solution_hydrogens difmap geom _refine_ls_hydrogen_treatment constr _refine_ls_extinction_method SHELXL _refine_ls_extinction_coef 0.0115(9)_refine_ls_extinction_expression Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^ _refine_ls_number_reflns 4152 _refine_ls_number_parameters 200 _refine_ls_number_restraints 0 _refine_ls_R_factor_all _refine_ls_R_factor_gt 0.0371 0.0284 _refine_ls_wR_factor_ref _refine_ls_wR_factor_gt 0.0715 0.0689 _refine_ls_goodness_of_fit_ref 1.042 _refine_ls_restrained_s_all 1.042 _refine_ls_shift/su_max 0.001 _refine_ls_shift/su_mean 0.000 loop _atom_site_label _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y _atom_site_fract_z _atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_symmetry_multiplicity _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly _atom_site_disorder_group Nil Ni 0.748193(15) 0.69833(2) 0.624213(12) 0.01433(8) Uani 1 1 d . . . N1 N 0.89331(12) 0.74414(18) 0.59217(10) 0.0223(3) Uani 1 1 d . . . C1 C 0.97436(13) 0.74568(19) 0.56931(10) 0.0183(3) Uani 1 1 d . . . S1 S 1.08902(4) 0.74797(7) 0.53805(4) 0.03661(14) Uani 1 1 d . . . N2 N 0.60089(12) 0.65218(18) 0.65594(10) 0.0229(3) Uani 1 1 d . . . C2 C 0.51465(13) 0.62296(18) 0.65918(10) 0.0176(3) Uani 1 1 d . s2 s 0.39285(3) 0.58240(6) 0.66316(3) 0.02590(11) Uani 1 1 d N11 N 0.74403(12) 0.50005(17) 0.54898(9) 0.0212(3) Uani 1 1 d . . H11D H 0.6995 0.5135 0.4967 0.025 Uiso 1 1 calc R . H11C H 0.8090 0.4831 0.5343 0.025 Uiso 1 1 calc R N12 N 0.81645(11) 0.57610(16) 0.73973(9) 0.0193(3) Uani 1 1 d . . . H12C H 0.7624 0.5477 0.7699 0.023 Uiso 1 1 calc R N13 N 0.74674(12) 0.89741(17) 0.69815(9) 0.0210(3) Uani 1 1 d . . .

C1CE06011B_ccdc_838535_838540_cif.txt H13D H 0.7418 0.9755 0.6584 0.025 Uiso 1 1 calc R H13C H 0.6871 0.8977 0.7238 0.025 Uiso 1 1 calc R C11 C 0.71107(16) 0.3656(2) 0.59449(13) 0.0284(4) Uani 1 1 d . . . H11A H 0.6993 0.2828 0.5511 0.034 Uiso 1 1 calc R . H11B H 0.6446 0.3867 0.6163 0.034 Uiso 1 1 calc R c12 c 0.79160(17) 0.3171(2) 0.67321(14) 0.0321(4) Uani 1 1 d . . . H12A H 0.7542 0.2770 0.7203 0.039 Uiso 1 1 calc R H12B H 0.8327 0.2344 0.6530 0.039 Uiso 1 1 calc R c13 c 0.86646(15) 0.4365(2) 0.71459(12) 0.0267(4) Uani 1 1 d . . . H13A H 0.9085 0.3947 0.7685 0.032 Uiso 1 1 calc R H13B H 0.9143 0.4617 0.6718 0.032 Uiso 1 1 calc R c14 c 0.89165(16) 0.6598(2) 0.80451(12) 0.0280(4) Uani 1 1 d . . H14A H 0.9536 0.6830 0.7763 0.034 Uiso 1 1 calc R . H14B H 0.9142 0.5950 0.8566 0.034 Uiso 1 1 calc R C15 C 0.84880(17) 0.8047(2) 0.83714(12) 0.0309(4) Uani 1 1 d . . . H15A H 0.7811 0.7834 0.8567 0.037 Uiso 1 1 calc R H15B H 0.8964 0.8398 0.8899 0.037 Uiso 1 1 calc R c16 c 0.83413(15) 0.9295(2) 0.76906(11) 0.0247(4) Uani 1 1 d . . . H16A H 0.8207 1.0240 0.7991 0.030 Uiso 1 1 calc R H16B H 0.8984 0.9419 0.7423 0.030 Uiso 1 1 calc R N21 N 0.67586(11) 0.82235(15) 0.50925(9) 0.0183(3) Uani 1 1 d . . . C21 C 0.58133(14) 0.7884(2) 0.46604(11) 0.0238(4) Uani 1 1 d . . . H21 H 0.5476 0.7021 0.4840 0.029 Uiso 1 1 calc R C22 C 0.53064(15) 0.8729(2) 0.39662(12) 0.0290(4) Uani 1 1 d . . . H22 H 0.4643 0.8439 0.3673 0.035 Uiso 1 1 calc R . . C23 C 0.57808(15) 1.0005(2) 0.37058(11) 0.0254(4) Uani 1 1 d . . H23 H 0.5446 1.0614 0.3238 0.031 Uiso 1 1 calc R C24 C 0.67553(15) 1.0371(2) 0.41430(11) 0.0228(4) Uani 1 1 d . . . H24 H 0.7100 1.1241 0.3983 0.027 Uiso 1 1 calc R . . C25 C 0.72220(14) 0.94459(19) 0.48203(11) 0.0201(3) Uani 1 1 d . . . H25 H 0.7899 0.9688 0.5104 0.024 Uiso 1 1 calc R . . 1000 _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom_site_aniso_U_33 _atom_site_aniso_U_23 _atom_site_aniso_U_13 _atom_site_aniso_U_12 Ni1 0.00985(12) 0.01849(12) 0.01493(11) 0.00123(7) 0.00277(7) -0.00034(8)N1 0.0158(8) 0.0284(8) 0.0237(7) 0.0020(6) 0.0061(6) -0.0014(6)C1 0.0170(9) 0.0204(8) 0.0171(7) -0.0007(6) 0.0011(6) -0.0014(6)S1 0.01/2(3) 0.0483(3) 0.0479(3) -0.0090(2) 0.0168(2) -0.0052(2)N2 0.0151(8) 0.0289(8) 0.0258(7) 0.0037(6) 0.0062(5) -0.0014(6)C2 0.0191(9) 0.0188(8) 0.0150(7) 0.0022(6) 0.0032(6) 0.0012(6)S2 0.0145(2) 0.0371(3) 0.0259(2) 0.00492(18) 0.00231(16) -0.00726(18)N11 0.0199(8) 0.0230(8) 0.0204(6) -0.0033(6) 0.0025(5) 0.0004(6)N12 0.0163(7) 0.0237(7) 0.0178(6) 0.0050(5) 0.0019(5) 0.0013(6)N13 0.0190(8) 0.0221(7) 0.0217(7) -0.0028(5) 0.0022(5) 0.0035(6)C11 0.0276(11) 0.0187(9) 0.0397(10) -0.0043(7) 0.0071(8) -0.0044(7)C12 0.0428(13) 0.0202(9) 0.0349(10) 0.0045(7) 0.0111(8) -0.0002(8)C13 0.0274(10) 0.0252(9) 0.0272(9) 0.0061(7) 0.0028(7) 0.0095(8)C14 0.0274(11) 0.0304(10) 0.0231(8) 0.0028(7) -0.0069(7) 0.0012(8)s1 0.0172(3) 0.0483(3) 0.0479(3) -0.0090(2) 0.0168(2) -0.0052(2) C14 0.0274(11) 0.0304(10) 0.0231(8) 0.0028(7) -0.0069(7) 0.0012(8) C15 0.0387(12) 0.0336(11) 0.0182(8) -0.0027(7) -0.0028(7) 0.0000(9) C16 0.0239(10) 0.0248(9) 0.0246(8) -0.0044(7) 0.0007(7) -0.0020(7) N21 0.0179(7) 0.0196(7) 0.0171(6) 0.0016(5) 0.0014(5) -0.0006(5) $(25 \ 0.0196(9) \ 0.0208(8) \ 0.0197(7) \ -0.0002(6) \ 0.0019(6) \ -0.0027(6)$

_geom_special_details

Áll 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

C1CE06011B_ccdc_838535_838540_cif.txt and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. loop_ _geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_2 _geom_bond_publ_flag Ni1 N1 2.0634(15) . ? Ni1 N2 2.0894(15) . ? 7 Ni1 N11 2.1102(14) . Ni1 N13 2.1108(14) . ? 7 Ni1 N12 2.1478(14) Ni1 N21 2.1660(14) ? N1 C1 1.160(2) C1 S1 1.6340(18) . N2 C2 1.163(2) . ? ? C2 S2 1.6396(17) 7 . Ż N11 C11 1.484(2) . ?? N12 C14 1.487(2) N12 C13 1.487(2). ? N13 C16 1.477(2) . ? c11 c12 1.534(3) • ? c12 c13 1.522(3) C14 C15 1.526(3) ? • ? C15 C16 1.517(3). N21 C21 ? 1.345(2). ? N21 C25 1.346(2) . C21 C22 1.385(3) ? C22 C23 C23 C24 1.386(3) 1.385(3) ? . ? . ? C24 C25 1.390(2) loop_ _geom_ang]e_atom_site_label_1 _geom_angle_atom_site_label_ 2 _geom_angle_atom_site_label_3 _geom_angle _geom_angle_site_symmetry_1 _geom_angle_site_symmetry_3 _geom_angle_publ_flag NI NiI NZ 179.69(6) ? N1 Ni1 N11 89.58(6) N2 Ni1 N11 90.32(6) ? . . ?? . . N1 Ni1 N13 92.08(6) . • ? N2 Ni1 N13 88.02(6) • N11 Ni1 N13 178.01(6) ? • ? N1 N11 N12 90.49(6) . • N2 Ni1 N12 89.80(6) . ? N11 N11 N12 89.19(6) ? . . ? N13 Ni1 N12 91.90(6) ? N1 Ni1 N21 90.85(6). • N2 Ni1 N21 88.86(6) . ? ? N11 Ni1 N21 91.35(5) . • N13 Ni1 N21 87.52(5) ? . ? N12 Ni1 N21 178.56(5) ? C1 N1 Ni1 168.66(15) . . N1 C1 S1 179.48(16) . ? ? C2 N2 Ni1 169.14(14) . ? N2 C2 S2 179.63(17) C11 N11 Ni1 114.82(11) . . ?? C14 N12 C13 108.84(14)

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C14 N12 Ni1 115.90(11)

C13 N12 Ni1 111.46(10)

C16 N13 Ni1 119.09(11)

C1CE06011B_ccdc_838535_838540_cif.txt N11 C11 C12 112.40(16) C13 C12 C11 116.51(15) . ? . N12 C13 C12 114.81(16) ? . ? N12 C14 C15 114.02(16) . ?? c16 c15 c14 115.08(15) N13 C16 C15 111.08(15) . . ? C21 N21 C25 117.14(15). C21 N21 Ni1 122.49(11) ?? . C25 N21 Ni1 120.22(12) . N21 C21 C22 123.28(17) C21 C22 C23 119.05(18) ?? . . C24 C23 C22 118.43(16) ? . . ? c23 c24 c25 119.02(16) . . ? N21 C25 C24 123.04(17) _diffrn_measured_fraction_theta_max 0.981 _diffrn_reflns_theta_full 27.98 _diffrn_measured_fraction_theta_full 0.981 _refine_diff_density_max _refine_diff_density_min _refine_diff_density_rms 0.323 -0.389 0.064 # Attachment '- TA219.CIF' data_ta219 _database_code_depnum_ccdc_archive 'CCDC 838539' #TrackingRef '- TA219.CIF' _audit_creation_method SHELXL-97 _chemical_name_systematic ? _chemical_name_common ? _chemical_melting_point 'C32 H80 N20 Ni4 O6 S8' _chemical_formula_moiety _chemical_formula_sum _chemical_formula_weight 'C32 H80 N20 Ni4 O6 S8' 1332.48 100p_ _atom_type_symbol _atom_type_description _atom_type_scat_dispersion_real _atom_type_scat_dispersion_imag _atom_type_scat_source C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' Ni Ni 0.3393 1.1124 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' 0 0 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' _symmetry_cell_setting triclinic 'P -1' '-P 1' _symmetry_space_group_name_H-M _symmetry_space_group_name_Hall loop_ _symmetry_equiv_pos_as_xyz 'x, y, z' '-x, -y, -z' _cell_length_a 7.9392(6) _cell_length_b _cell_length_c _cell_angle_alpha _cell_angle_beta 13.2900(10) 14.4127(11) 82.925(9) 87.647(10) 89.775(9) _cell_angle_gamma _cell_volume 1507.9(2)Page 22

C1CE06011B_ccdc_838535_838540_cif.txt _cell_formula_units_z 1 _cell_measurement_temperature _cell_measurement_reflns_used 170(2) 17362 _cell_measurement_theta_min 2.57 _cell_measurement_theta_max 27.00 _exptl_crystal_description block _exptl_crystal_colour blue _exptl_crystal_size_max 0.30 _exptl_crystal_size_mid 0.16 _exptl_crystal_size_min _exptl_crystal_density_meas 0.12 _exptl_crystal_density_diffrn 1.467 _exptl_crystal_density_method 'not measured' _exptl_crystal_F_000 _exptl_absorpt_coefficient_mu 700 1.561 _exptl_absorpt_correction_type numerical _exptl_absorpt_correction_T_min 0.735 _expt]_absorpt_correction_T_max 0.818 _exptl_absorpt_process_details X-Shape and X-Red32 (STOE, 2008)' _exptl_special_details ? ; _diffrn_ambient_temperature 170(2) _diffrn_radiation_wavelength 0.71073 _diffrn_radiation_type мок∖а _diffrn_radiation_source 'fine-focus sealed tube' _diffrn_radiation_monochromator graphite _diffrn_measurement_device_type _diffrn_measurement_method _diffrn_detector_area_resol_mean ? diffrn_standards_number ? _diffrn_standards_interval_count _diffrn_standards_interval_time _diffrn_standards_decay_% _diffrn_reflns_number 17362 _diffrn_reflns_av_R_equivalents 0.0677 _diffrn_reflns_av_sigmaI/netI _diffrn_reflns_limit_h_min _diffrn_reflns_limit_h_max 0.0600 -10 10 _diffrn_reflns_limit_k_min -16 _diffrn_reflns_limit_k_max _diffrn_reflns_limit_l_min _diffrn_reflns_limit_l_max _diffrn_reflns_theta_min 16 -18 18 2.57 _diffrn_reflns_theta_max 27.00 _reflns_number_total 6273 _reflns_number_gt 4539 _reflns_threshold_expression >2sigma(I) _computing_data_collection
_computing_cell_refinement
_computing_data_reduction ? 'SHELXS-97 (Sheldrick, 1990)' _computing_structure_solution 'SHELXL-97 (Sheldrick, 1997)' _computing_structure_refinement _computing_molecular_graphics _computing_publication_material ?

_refine_special_details

Refinement of F^2A against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2A, conventional R-factors R are based on F, with F set to zero for negative F^2A. The threshold expression of F^2A > 2sigma(F^2A) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based

C1CE06011B_ccdc_838535_838540_cif.txt on F^2^ are statistically about twice as large as those based on F, and Rfactors based on ALL data will be even larger. _refine_ls_structure_factor_coef Fsqd _refine_ls_matrix_type full _refine_ls_weighting_scheme calc refine_ls_weighting_details 'calc w=1/[\s^2^(Fo^2^)+(0.0508P)^2^+0.7492P] where P=(Fo^2^+2Fc^2^)/3' _atom_sites_solution_primary direct _atom_sites_solution_secondary _atom_sites_solution_hydrogens difmap geom _refine_ls_hydrogen_treatment constr _refine_ls_extinction_method SHELXL _refine_ls_extinction_coef
_refine_ls_extinction_expression 0.0052(10)Fc^*^=kFc[1+0.001xFc^2^\1^3^/sin(2\q)]^-1/4^ _refine_ls_number_reflns 6273 _refine_ls_number_parameters 326 _refine_ls_number_restraints
_refine_ls_R_factor_all
_refine_ls_R_factor_gt 0 0.0710 0.0440 _refine_ls_wR_factor_ref 0.1093 _refine_ls_wR_factor_gt 0.0980 _refine_ls_goodness_of_fit_ _refine_ls_restrained_S_all _ref 1.015 1.015 _refine_ls_shift/su_max 0.000 _refine_ls_shift/su_mean 0.000 loop_ _atom_site_label _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y
_atom_site_fract_z atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_symmetry_multiplicity _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly _atom_site_disorder_group Nil Ni 0.68158(5) 0.69451(3) -0.02000(3) 0.02025(12) Uani 1 1 d . . Ni2 Ni 0.78131(7) 0.70916(4) 0.41196(3) 0.03697(15) Uani 1 1 d . . . s1 s 0.66965(11) 0.55673(7) 0.13565(6) 0.0305(2) Uani 1 1 d . . . C1 C 0.5346(4) 0.4713(2) 0.1094(2) 0.0223(6) Uani 1 1 d . . . N1 N 0.4420(4) 0.4106(2) 0.0909(2) 0.0264(6) Uani 1 1 d . . . s2 s 0.98899(13) 0.92786(7) 0.13985(7) 0.0378(2) Uani 1 1 d . . . C2 C 0.8792(4) 0.8469(2) 0.0909(2) 0.0239(7) Uani 1 1 d . . . N2 N 0.7990(4) 0.7903(2) 0.0564(2) 0.0314(7) Uani 1 1 d . . . s3 s 0.42440(15) 0.77484(13) 0.67638(9) 0.0646(4) Uani 1 1 d . A . C3 C 0.5502(6) 0.7610(3) 0.5860(3) 0.0390(9) Uani 1 1 d . . N3 N 0.6378(6) 0.7500(3) 0.5236(3) 0.0597(12) Uani 1 1 d . Α. S4 S 1.14787(11) 0.59295(7) 0.16663(7) 0.0349(2) Uani 1 1 d . A . C4 C 1.0178(4) 0.6342(3) 0.2451(3) 0.0282(7) Uani 1 1 d . . . N4 N 0.9289(4) 0.6627(3) 0.3015(2) 0.0376(8) Uani 1 1 d . A . N11 N 0.9116(3) 0.6273(2) -0.0491(2) 0.0287(6) Uani 1 1 d . H11A H 0.9608 0.6081 0.0070 0.034 Uiso 1 1 calc R H11B H 0.8894 0.5689 -0.0747 0.034 Uiso 1 1 calc R N12 N 0.6853(3) 0.8005(2) -0.1411(2) 0.0240(6) Uani 1 1 d . . . H12 H 0.6235 0.7706 -0.1839 0.029 Uiso 1 1 calc R N13 N 0.4438(4) 0.7402(2) 0.0247(2) 0.0312(6) Uani 1 1 d . . . H13A H 0.3654 0.7044 -0.0032 0.037 Uiso 1 1 calc R . H13B H 0.4323 0.7203 0.0881 0.037 Uiso 1 1 calc R C11 C 1.0378(4) 0.6856(3) -0.1114(3) 0.0403(9) Uani 1 1 d . . H11C H 1.1310 0.6401 -0.1270 0.048 Uiso 1 1 calc R . . H11D H 1.0853 0.7395 -0.0786 0.048 Uiso 1 1 calc R c12 c 0.9612(5) 0.7329(3) -0.2004(3) 0.0421(10) Uani 1 1 d . . . Page 24

C1CE06011B_ccdc_838535_838540_cif.txt H12A H 0.8922 0.6811 -0.2251 0.051 Uiso 1 1 calc R . . H12B H 1.0533 0.7531 -0.2473 0.051 Uiso 1 1 calc R . . C13 C 0.8524(5) 0.8243(3) -0.1890(3) 0.0377(9) Uani 1 1 d . . H13C H 0.9140 0.8701 -0.1531 0.045 Uiso 1 1 calc R . H13D H 0.8344 0.8613 -0.2517 0.045 Uiso 1 1 calc R C14 C 0.5996(5) 0.8982(3) -0.1313(3) 0.0338(8) Uani 1 1 d . . . H14A H 0.6020 0.9398 -0.1933 0.041 Uiso 1 1 calc R . . H14B H 0.6639 0.9351 -0.0887 0.041 Uiso 1 1 calc R c15 c 0.4185(5) 0.8879(3) -0.0942(3) 0.0364(9) Uani 1 1 d . . . H15A H 0.3637 0.9551 -0.1048 0.044 Uiso 1 1 calc R . H15B H 0.3588 0.8417 -0.1307 0.044 Uiso 1 1 calc R . C16 C 0.3975(5) 0.8484(3) 0.0081(3) 0.0370(9) Uani 1 1 d . . H16A H 0.4698 0.8880 0.0447 0.044 Uiso 1 1 calc R . H16B H 0.2789 0.8570 0.0296 0.044 Uiso 1 1 calc R N21 N 1.0096(6) 0.7282(3) 0.4798(3) 0.0635(12) Uani 1 1 d . A . H21A H 1.0022 0.6887 0.5369 0.076 Uiso 1 1 calc R . . H21B H 1.0950 0.7018 0.4452 0.076 Uiso 1 1 calc R N22 N 0.7759(4) 0.8583(2) 0.3455(2) 0.0301(6) Uani 1 1 d . A . H22 H 0.8305 0.8557 0.2875 0.036 Uiso 1 1 calc R . . N23 N 0.5700(5) 0.6664(3) 0.3466(3) 0.0531(10) Uani 1 1 d . A . H23A H 0.6062 0.6441 0.2912 0.064 Uiso 1 1 calc R . H23B H 0.5226 0.6116 0.3836 0.064 Uiso 1 1 calc R C21 C 1.0625(7) 0.8294(4) 0.4965(4) 0.0669(16) Uani 1 1 d . . . H21C H 1.1806 0.8267 0.5162 0.080 Uiso 1 1 calc R A . H21D H 0.9911 0.8519 0.5480 0.080 Uiso 1 1 calc R . C22 C 1.0491(6) 0.9045(4) 0.4104(4) 0.0586(13) Uani 1 1 d . A . H22A H 1.1013 0.8750 0.3563 0.070 Uiso 1 1 calc R . H22B H 1.1139 0.9661 0.4186 0.070 Uiso 1 1 calc R . . C23 C 0.8696(6) 0.9349(3) 0.3885(3) 0.0447(10) Uani 1 1 d . . . H23C H 0.8087 0.9478 0.4472 0.054 Uiso 1 1 calc R A H23D H 0.8718 0.9991 0.3456 0.054 Uiso 1 1 calc R C24 C 0.6071(5) 0.9011(3) 0.3238(3) 0.0408(9) Uani 1 1 d . . . H24A H 0.6218 0.9689 0.2873 0.049 Uiso 1 1 calc R A . H24B H 0.5452 0.9103 0.3832 0.049 Uiso 1 1 calc R . . C25 C 0.5020(6) 0.8366(4) 0.2694(3) 0.0527(12) Uani 1 1 d . A . H25A H 0.4066 0.8777 0.2438 0.063 Uiso 1 1 calc R . H25B H 0.5717 0.8174 0.2158 0.063 Uiso 1 1 calc R . . C26 C 0.4332(5) 0.7420(4) 0.3249(4) 0.0559(13) Uani 1 1 d . . . H26A H 0.3785 0.7589 0.3840 0.067 Uiso 1 1 calc R A H26B H 0.3467 0.7121 0.2889 0.067 Uiso 1 1 calc R O1W O 0.8181(8) 0.5598(5) 0.4811(5) 0.0529(15) Uani 0.70 1 d P A 1 H101 H 0.7548 0.5358 0.5265 0.079 Uiso 1 1 d R . H201 H 0.7843 0.5105 0.4557 0.079 Uiso 1 1 d R . . 01W' 0 0.722(2) 0.5503(11) 0.4751(11) 0.061(4) Uani 0.30 1 d P A 2 O2W O 0.8197(7) 0.4190(3) 0.3537(3) 0.0914(15) Uani 1 1 d . . . H1O2 H 0.7152 0.4236 0.3475 0.137 Uiso 1 1 d R . . H2O2 H 0.8907 0.4319 0.3090 0.137 Uiso 1 1 d R . . O3W O 0.6633(6) 0.5288(3) 0.6564(3) 0.0851(14) Uani 1 1 d . . . H103 H 0.5879 0.5655 0.6772 0.128 Uiso 1 1 d R . . H2O3 H 0.7253 0.5162 0.7023 0.128 Uiso 1 1 d R . loop_ _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom_site_aniso_U_33 _atom_site_aniso_U_23 _atom_site_aniso_U_13 _atom_site_aniso_U_12 Ni1 0.0186(2) 0.01780(19) 0.0252(2) -0.00542(16) -0.00252(16) -0.00276(14) Ni2 0.0517(3) 0.0343(3) 0.0254(3) -0.0080(2) 0.0044(2) 0.0103(2) s1 0.0326(4) 0.0285(4) 0.0315(5) -0.0044(4) -0.0099(4) -0.0115(3)C1 0.0250(15) 0.0211(14) 0.0212(16) -0.0023(12) -0.0039(13) -0.0010(12) N1 0.0283(14) 0.0219(13) 0.0292(15) -0.0030(12) -0.0033(12) -0.0048(11) $\begin{array}{c} \text{S2} & 0.0384(5) & 0.0381(5) & 0.0400(5) & -0.0180(4) & 0.0027(4) & -0.0174(4) \\ \text{C2} & 0.0245(15) & 0.0223(15) & 0.0260(17) & -0.0074(13) & 0.0000(13) & -0.0021(12) \\ \text{N2} & 0.0313(15) & 0.0275(15) & 0.0372(17) & -0.0101(13) & -0.0052(13) & -0.0029(12) \\ \end{array}$ s3 0.0368(6) 0.1249(12) 0.0393(6) -0.0393(7) -0.0003(5) 0.0075(7) Page 25

C1CE06011B_ccdc_838535_838540_cif.txt C3 0.054(2) 0.038(2) 0.0252(19) -0.0049(16) -0.0015(18) 0.0116(18)N3 0.092(3) 0.049(2) 0.037(2) -0.0074(18) 0.026(2) 0.009(2)S4 0.0258(4) 0.0426(5) 0.0393(5) -0.0181(4) 0.0031(4) 0.0008(4)C4 0.0297(17) 0.0249(16) 0.0318(18) -0.0088(14) -0.0064(15) 0.0013(13) N4 0.0359(17) 0.0441(18) 0.0354(17) -0.0160(15) 0.0004(14) 0.0094(14) N11 0.0225(13) 0.0258(14) 0.0394(17) -0.0090(13) -0.0043(13) 0.0033(11)N12 0.0254(13) 0.0198(12) 0.0273(14) -0.0043(11) -0.0015(12) -0.0007(10)N13 0.0236(14) 0.0357(16) 0.0345(16) -0.0067(13) 0.0035(12) 0.0015(12)C11 0.0176(16) 0.042(2) 0.061(3) -0.0067(13) 0.0035(12) 0.0015(12) C11 0.0176(16) 0.042(2) 0.061(3) -0.011(2) 0.0077(17) 0.0018(15) C12 0.037(2) 0.041(2) 0.046(2) -0.0061(19) 0.0198(19) 0.0019(17) C13 0.0318(19) 0.0293(18) 0.049(2) 0.0038(17) 0.0116(18) -0.0058(15) C14 0.039(2) 0.0210(16) 0.040(2) 0.0030(15) -0.0030(17) 0.0063(14) C15 0.0319(18) 0.0369(19) 0.040(2) -0.0039(17) -0.0032(16) 0.0158(16) C14 0.0347(10) 0.0447(10c16 0.0347(19) 0.041(2) 0.037(2) -0.0127(17) 0.0008(17) 0.0142(16) N21 0.074(3) 0.070(3) 0.053(2) -0.024(2) -0.030(2) 0.034(2) N22 0.0302(15) 0.0334(15) 0.0278(15) -0.0085(13) -0.0025(13) 0.0044(12) N23 0.047(2) 0.050(2) 0.066(3) -0.027(2) 0.0136(19) -0.0071(17) C21 0.066(3) 0.078(4) 0.067(3) -0.037(3) -0.037(3) 0.023(3) C22 0.046(3) 0.076(3) 0.061(3) -0.035(3) -0.017(2) 0.005(2) C23 0.050(2) 0.039(2) 0.049(2) -0.0162(19) -0.012(2) 0.0043(18) olw 0.066(4) 0.040(3) 0.052(3) -0.001(2) 0.000(3) -0.002(3) olw' 0.097(12) 0.042(7) 0.041(7) 0.003(6) 0.011(9) 0.030(9) 02w 0.148(4) 0.057(2) 0.069(3) -0.013(2) 0.016(3) -0.009(3) 03W 0.097(3) 0.081(3) 0.067(3) 0.028(2) 0.012(2) 0.033(2) _geom_special_details All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. loop_ _geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_2 _geom_bond_publ_flag N11 N2 2.035(3) . ? Ni1 N11 2.080(3) . ? Ni1 N13 2.082(3) . ? Ni1 N1 2.098(3) 2_665 ? Ni1 N12 2.102(3) . Ni1 S1 2.7142(11) . Ni2 N3 2.060(4) . ? .? ? Ni2 N23 2.072(4) . ? Ni2 N4 2.091(3) . ? Ni2 N22 2.094(3) Ni2 N21 2.125(4) Ni2 Olw 2.133(7) Ni2 Olw' 2.238(16) ? ? S1 C1 1.653(3) . C1 N1 1.155(4) . N1 Ni1 2.098(3) 2_665 ? S2 C2 1.631(3) C2 N2 1.158(4) S3 C3 1.636(4) C3 N3 1.138(5) S4 C4 1.643(4) 7 . . C4 N4 1.153(5) N11 C11 1.473(5) . N12 C14 1.483(4) . ?

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N12 N13	C13	1.4	88	(5)		? 7	C.	LCE	060	11
C11 C12 C14	C12 C13 C15	1.5 1.5 1.5	07 10 14	(6) (5) (5)	•	????				
N21 N22 N22	C16 C21 C23 C24	1.3 1.4 1.4	61 74 84	(7) (5)	:	? ? ?				
N23 C21 C22	C26 C22 C23	1.4 1.5 1.5	93 01 14	(6) (8) (6)	:	? ? ?				
C24 C25	C25 C26	1.5 1.4	07 97	(6) (7)	:	? ?				
loop _geo	o_ om_ar om_ar	ngle	_at		_S ⁻	ite ite	_1	abe abe	e]_1 e]_2	
_geo _geo _geo	om_ar om_ar om_ar	ngle ngle ngle		ite	_s _s	ymm vmm	et let	ry_ rv	1 3	,
_geo N2 I N2 I	om_ar Nil N Nil N	ngle v11 v13	pi 90 92	ub1 .15 .19	_f (1) (1)	ĺag 2) 2)	•	,? .?		
N11 N2 I N11	Nil Nil N Nil	N13 N1 1 N1	17 76 89	70. 33 .97	49 (1) (1)	(12 3) 1))		? 65 65	????
N13 N2 I N11 N13	NIL Nil M Nil Nil	NI N12 N12 N12	87 93 96	.11 .27 5.2	(1) (1) 2() 5()	2) 2) 11) 12)		2_6 . ?	?	£
N1 I N2 I N11	vil N vil S vil S Nil	N12 51 8 51	90 7.6 84	.36 53(.66) (1 9) (9)	1)	2_ ·	665 ? ?		?
N13 N1 I N12	Nil Nil S Nil	\$1 51 8 51	86 8.7 178	.22 74(3.7	(9) 8) 4(8) . 2_ 8)	.66	? 5. .?	?	
N3 I N3 I N23	vi2 M vi2 M vi2	N23 N4 1 N4	92 77 88	.08 .92 .25	(1) (1) (1)	8) 5) 4)	•	· ? · ?)))	
N3 1 N23 N4 1	NIZ M NIZ NIZ M	NZZ N22 N22	90 93 91 92	.72 3.4 .31 11	(14) (1) (1)	4) 15) 3) 9)		· ? .?	?	
N23 N4 I N22	Ni2 Ni2 Ni2 Mi2	N21 N21 N21 N21	87 87	.11 70. .27 4.6	(1 83 (1 6()	(16 5) 15))	· · · · · ?	?	
N3 1 N23 N4 1	vi2 (Ni2 Ni2 (01W 01W 01W	92 92 86	.0(2.7 .0(2) (2) 2)).		? ? ?		
N22 N21 N3 I	Ni2 Ni2 Ni2 (01w 01w 1w20		73. 9.0 4.6	19 (2) (4)	(18) .) .)		?	
N23 N4 I N22 N21	NIZ Ni2 (Ni2 Ni2	010 1W' 01W 01W	93	74. 3.5 166 98	0() (4) .3 3()	5)). (4) 5)	· ·	· · ? ? · ?	?	
01W C1 9 N1 0	Ni2 S1 N ⁻ C1 S1	01w i1 1 1 17	03	20. .06 L(3	5(4 (1)	4) 2)	?	· ? . ?))	
C1 I N2 (C2 I	N1 N C2 S2 N2 N	i1 1 2 17 i1 1	62 8.9	.8(9(3 .9(3)) 3)	• • • •	2_ ?	665 ?	?	
N3 (C3 N4 (C3 S3 N3 N C4 S4	3 17 i2 1 4 17	9.(71 8.()(4 .7(5(3) 4))	· · ·	? ?	?		
C4 1	N4 IN	1 Z I	.13	(י כ	•	•	:		

C1CE06011B_ccdc_838535_838540_cif.txt C11 N11 Ni1 119.1(2) C14 N12 C13 107.4(3) C14 N12 N11 115.7(2) ? . . ?? . . C13 N12 Ni1 116.9(2) . . ?? C16 N13 Ni1 119.3(2) . N11 C11 C12 111.3(3). . ? C11 C12 C13 114.3(3). N12 C13 C12 114.6(3) ?? • N12 C14 C15 114.4(3) . ? c16 c15 c14 114.7(3) • ? N13 C16 C15 110.8(3). . ?? C21 N21 Ni2 120.0(3). . C23 N22 C24 107.5(3) . . C23 N22 Ni2 117.0(2) ?? . C24 N22 Ni2 116.5(2) . . ? C26 N23 Ni2 119.3(3). . N21 C21 C22 111.4(4) ? . ? C21 C22 C23 113.7(5) . N22 C23 C22 113.9(3) N22 C24 C25 114.0(3) ? . • • c26 c25 c24 114.7(4) ? • • N23 C26 C25 110.9(4) . _diffrn_measured_fraction_theta_max 0.954 27.00 _diffrn_reflns_theta_full _diffrn_measured_fraction_theta_full 0.954 _refine_diff_density_max _refine_diff_density_min _refine_diff_density_rms 0.950 -1.0700.085 # Attachment '- TA243.CIF' data_ta243 _database_code_depnum_ccdc_archive 'CCDC 838540' #TrackingRef '- TA243.CIF _audit_creation_method SHELXL-97 _chemical_name_systematic $\frac{2}{2}$? _chemical_name_common
_chemical_melting_point 7 _chemical_formula_moiety 'C13 H22 N6 Ni S2' 'C13 H22 N6 Ni S2' _chemical_formula_sum _chemical_formula_weight 385.20 loop_ _atom_type_symbol _atom_type_description _atom_type_scat_dispersion_real _atom_type_scat_dispersion_imag _atom_type_scat_source С С 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' Н Н 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' Ni Ni 0.3393 1.1124 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' _symmetry_cell_setting orthorhombic _symmetry_space_group_name_H-M 'Pbca' _symmetry_space_group_name_Hall '-P 2ac 2ab' loop _symmetry_equiv_pos_as_xyz 'x, y, z' '-x+1/2, -y, z+1/2' '-x, y+1/2, -z+1/2'

C1CE06011B_ccdc_838535_838540_cif.txt 'x+1/2, -y+1/2, -z' '-x, -y, -z' 'x-1/2, y, -z-1/2' 'x, -y-1/2, z-1/2' '-x-1/2, y-1/2, z' _cell_length_a _cell_length_b _cell_length_c 8.5835(3) 14.7666(4) 28.9345(7) _cell_angle_alpha 90.00 _cell_angle_beta _cell_angle_gamma _cell_volume 90.00 90.00 3667.42(18)_cell_formula_units_Z _cell_measurement_temperature
_cell_measurement_reflns_used 293(2) 25954 _cell_measurement_theta_min 2.76 _cell_measurement_theta_max 26.85 _exptl_crystal_description _exptl_crystal_colour hexagon blue _exptl_crystal_size_max 0.09 0.07 _exptl_crystal_size_mid _exptl_crystal_size_min _exptl_crystal_density_meas _exptl_crystal_density_diffrn 0.05 1.395 'not measured' _exptl_crystal_density_method _expt]_crystal_F_000 1616 _exptl_absorpt_coefficient_mu 1.290 _exptl_absorpt_correction_type numerical _exptl_absorpt_correction_T_min 0.889 0.931 _exptl_absorpt_correction_T_max _exptl_absorpt_process_details 'X-Shape and X-Red32 (STOE, 2008)' _exptl_special_details ? ; _diffrn_ambient_temperature 293(2) 0.71073 _diffrn_radiation_wavelength _diffrn_radiation_type мок∖а _diffrn_radiation_source fine-focus sealed tube' _diffrn_radiation_monochromator graphite _diffrn_measurement_device_type _diffrn_measurement_method ? _diffrn_detector_area_resol_mean _diffrn_standards_number _diffrn_standards_interval_count ? _diffrn_standards_interval_time 7 _diffrn_standards_decay_% 2 25954 _diffrn_reflns_number _diffrn_reflns_av_R_equivalents 0.0292 _diffrn_reflns_av_sigmaI/netI _diffrn_reflns_limit_h_min _diffrn_reflns_limit_h_max _diffrn_reflns_limit_k_min 0.0146 -10 10 -18 _diffrn_reflns_limit_k_max _diffrn_reflns_limit_l_min _diffrn_reflns_limit_l_max 18 -36 36 2.76 _diffrn_reflns_theta_min _diffrn_reflns_theta_max 26.85 3880 _reflns_number_total 3461 _reflns_number_gt _reflns_threshold_expression >2sigma(I) ? _computing_data_collection ? _computing_cell_refinement

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C1CE06011B_ccdc_838535_838540_cif.txt _computing_data_reduction 'SHELXS-97 (Sheldrick, 1990)' 'SHELXL-97 (Sheldrick, 1997)' _computing_structure_solution _computing_structure_refinement ? _computing_molecular_graphics _computing_publication_material ? _refine_special_details Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based on F, with F set to zero for negative F^{2A} . The threshold expression of $F^{2A} > 2 \text{sigma}(F^{2A})$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and Rfactors based on ALL data will be even larger. _refine_ls_structure_factor_coef Fsqd _refine_ls_matrix_type full _refine_ls_weighting_scheme calc _refine_ls_weighting_details 'calc w=1/[\s^2^(Fo^2^)+(0.0254P)^2^+2.1456P] where P=(Fo^2^+2Fc^2^)/3' _atom_sites_solution_primary direct _atom_sites_solution_secondary _atom_sites_solution_hydrogens difmap geom _refine_ls_hydrogen_treatment constr _refine_ls_extinction_method none _refine_ls_extinction_coef 3880 _refine_ls_number_reflns _refine_ls_number_parameters _refine_ls_number_restraints 199 0 0.0469 _refine_ls_R_factor_all _refine_ls_R_factor_gt _refine_ls_wR_factor_ref 0.0398 0.0809 ______refine_ls_wR_factor_gt 0.0781 _refine_ls_goodness_of_fit_ref 1.146 _refine_ls_restrained_s_all 1.146 _refine_ls_shift/su_max 0.001 _refine_ls_shift/su_mean 0.000 loop_ _atom_site_label _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y _atom_site_fract_z _atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_symmetry_multiplicity _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly _atom_site_disorder_group Nil Ni 0.54953(3) 0.654059(19) 0.376845(9) 0.04257(9) Uani 1 1 d . . . N1 N 0.7569(2) 0.67144(14) 0.33858(7) 0.0550(5) Uani 1 1 d . . . C1 C 0.8719(3) 0.69014(15) 0.32030(8) 0.0462(5) Uani 1 1 d . . . S1 S 1.03505(8) 0.71629(6) 0.29479(2) 0.06577(19) Uani 1 1 d . . N2 N 0.3460(2) 0.63942(14) 0.41461(7) 0.0521(5) Uani 1 1 d . . . C2 C 0.2352(3) 0.65319(15) 0.43588(8) 0.0454(5) Uani 11d. . s2 s 0.07959(8) 0.67080(6) 0.46669(3) 0.0708(2) Uani 1 1 d N11 N 0.4228(2) 0.64216(14) 0.31539(7) 0.0540(5) Uani 1 1 d . . . H11A H 0.3337 0.6733 0.3195 0.065 Uiso 1 1 calc R . . H11B H 0.4772 0.6718 0.2935 0.065 Uiso 1 1 calc R . . N12 N 0.6044(2) 0.51314(13) 0.38195(7) 0.0511(5) Uani 1 1 d . . . H12 H 0.7060 0.5096 0.3732 0.061 Uiso 1 1 calc Ŕ N13 N 0.6802(2) 0.67833(13) 0.43732(6) 0.0504(5) Uani 1 1 d . . . H13A H 0.7816 0.6796 0.4293 0.060 Uiso 1 1 calc R . .

C1CE06011B_ccdc_838535_838540_cif.txt H13B H 0.6555 0.7340 0.4476 0.060 Uiso 1 1 calc R . . C11 C 0.3793(4) 0.5541(2) 0.29549(10) 0.0696(8) Uani 1 1 d . . . H11C H 0.3578 0.5616 0.2628 0.084 Uiso 1 1 calc R . H11D H 0.2848 0.5327 0.3102 0.084 Uiso 1 1 calc R . C12 C 0.5061(4) 0.4844(2) 0.30159(10) 0.0741(8) Uani 1 1 d . . . H12A H 0.6045 0.5106 0.2919 0.089 Uiso 1 1 calc R . . H12B H 0.4845 0.4333 0.2815 0.089 Uiso 1 1 calc R . . C13 C 0.5226(4) 0.45029(19) 0.35057(10) 0.0713(8) Uani 1 1 d . H13C H 0.4195 0.4385 0.3629 0.086 Uiso 1 1 calc R . H13D H 0.5786 0.3933 0.3500 0.086 Uiso 1 1 calc R . . C14 C 0.6020(4) 0.47393(18) 0.42891(9) 0.0642(7) Uani 1 1 d . . . H14A H 0.6309 0.4106 0.4269 0.077 Uiso 1 1 calc R H14B H 0.4963 0.4768 0.4407 0.077 Uiso 1 1 calc R C16 C 0.6634(3) 0.61478(18) 0.47625(8) 0.0574(6) Uani 1 1 d . . . H16A H 0.5561 0.6151 0.4868 0.069 Uiso 1 1 calc R . . H16B H 0.7286 0.6347 0.5017 0.069 Uiso 1 1 calc R . . N21 N 0.5080(2) 0.79993(13) 0.37198(6) 0.0468(4) Uani 1 1 d . C21 C 0.5511(3) 0.84918(17) 0.33554(8) 0.0556(6) Uani 1 1 d . . . H21 H 0.5979 0.8199 0.3107 0.067 Uiso 1 1 calc R C22 C 0.5293(3) 0.94154(18) 0.33306(9) 0.0610(7) Uani 1 1 d . . . H22 H 0.5600 0.9733 0.3068 0.073 Uiso 1 1 calc R . . C23 C 0.4625(3) 0.98612(17) 0.36930(9) 0.0596(6) Uani 1 1 d . . . H23 H 0.4480 1.0485 0.3684 0.071 Uiso 1 1 calc R C24 C 0.4172(3) 0.93660(17) 0.40706(10) 0.0592(6) Uani 1 1 d . . . H24 H 0.3712 0.9649 0.4323 0.071 Uiso 1 1 calc R . . C25 C 0.4406(3) 0.84440(16) 0.40705(9) 0.0519(5) Uani 1 1 d . . . H25 H 0.4082 0.8113 0.4327 0.062 Uiso 1 1 calc R C15 C 0.7085(3) 0.51999(19) 0.46276(9) 0.0660(7) Uani 1 1 d . . . H15A H 0.8124 0.5217 0.4496 0.079 Uiso 1 1 calc R . . H15B H 0.7135 0.4834 0.4906 0.079 Uiso 1 1 calc R . loop _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom_site_aniso_U_33 _atom_site_aniso_U_23 _atom_site_aniso_U_13 _atom_site_aniso_U_12 Ni1 0.04309(15) 0.04508(16) 0.03952(15) 0.00016(12) 0.00431(12) 0.00061(12) N1 0.0515(11) 0.0604(12) 0.0529(11) 0.0018(10) 0.0114(10) 0.0016(10)C1 0.0515(13) 0.0436(11) 0.0434(12) -0.0010(9) 0.0007(10) 0.0054(10)S1 0.0533(4) 0.0805(5) 0.0635(4) 0.0022(3) 0.0121(3) -0.0088(3)S1 0.0535(4) 0.0605(5) 0.0635(4) 0.0022(5) 0.0121(5) -0.0086(5) N2 0.0474(10) 0.0549(12) 0.0540(11) 0.0013(9) 0.0071(9) -0.0021(9) C2 0.0452(11) 0.0426(11) 0.0483(12) -0.0026(10) -0.0017(10) -0.0042(10) S2 0.0502(3) 0.0863(5) 0.0758(5) -0.0235(4) 0.0144(3) -0.0014(3) N11 0.0534(11) 0.0616(12) 0.0469(11) -0.0039(9) -0.0017(9) 0.0016(10) N12 0.0560(11) 0.0474(10) 0.0501(11) -0.0011(9) 0.0068(9) 0.0030(9) N13 0.0505(11) 0.0544(11) 0.0462(11) 0.0014(9) -0.0014(9) 0.0003(9) $(11 \ 0.0776(19) \ 0.0740(19) \ 0.0574(16) \ -0.0077(14) \ -0.0078(14) \ -0.0138(16)$ c14 0.0840(19) 0.0483(14) 0.0602(16) 0.0108(12) 0.0028(14) 0.0038(13) C16 0.0611(15) 0.0677(16) 0.0434(13) 0.0040(11) -0.0038(11) 0.0038(13) N21 0.0515(10) 0.0460(10) 0.0430(10) 0.0006(8) 0.0023(8) 0.0007(8) C21 0.0678(15) 0.0543(14) 0.0446(12) 0.0028(11) 0.0041(11) 0.0012(13) $c22 \ 0.0753(17) \ 0.0561(15) \ 0.0516(14) \ 0.0126(12) \ -0.0027(13) \ -0.0041(13)$ $c23 \ 0.0672(16) \ 0.0451(13) \ 0.0664(16) \ 0.0045(12) \ -0.0040(13) \ 0.0015(12)$ c15 0.0758(18) 0.0646(16) 0.0577(15) 0.0095(13) -0.0066(14) 0.0123(14)

_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

N11 C11 C12 112.0(2) . .

C1CE06011B_ccdc_838535_838540_cif.txt used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. loop_ _geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symme _geom_bond_publ_flag Ni1 N2 2.072(2) . ? Ni1 N11 2.092(2) . ? Ni1 N13 2.1093(19) . Ni1 N1 2.112(2) . ? _geom_bond_site_symmetry_2 ? Ni1 N12 2.1386(19) . Ni1 N21 2.1879(19) . ? ? N1 C1 1.154(3) ? C1 S1 1.629(2) N2 C2 1.150(3) C2 S2 1.627(2) N11 C11 1.470(3) . ? N12 C13 1.476(3) • ?? N12 C14 1.477(3) N13 C16 1.473(3) . ? C11 C12 1.509(4). C12 C13 1.511(4) ? . ? c14 c15 1.503(4) c16 c15 1.504(4) ? . ? N21 C21 1.333(3). ? N21 C25 1.340(3) ? c21 c22 1.378(4) . C22 C23 1.365(4) ? C23 C24 1.371(4) C24 C25 1.376(3) ? • ? loop_ _geom_angle_atom_site_label_1 _geom_angle_atom_site_label_2 _geom_angle_atom_site_label_3 _geom_angle _geom_angle_site_symmetry_1 _geom_angle_site_symmetry_3 _geom_angle_publ_flag NŽ Nil NIL 90.06(8) . . ? N2 Ni1 N13 91.65(8) N11 Ni1 N13 174.89(8) . N2 Ni1 N1 179.00(8) . . · · . ? . ? ? N11 Ni1 N1 90.16(8) . . ? N13 Ni1 N1 88.05(8) • . N2 Ni1 N12 92.73(8) N11 Ni1 N12 95.24(8) . ? · · · ? • • N13 Ni1 N12 89.48(8) ? N1 Ni1 N12 88.22(8) . . ? N2 Ni1 N21 89.95(8) . . ? N11 Ni1 N21 86.74(8) • • N13 Ni1 N21 88.45(7) · · . ? ? N1 Ni1 N21 89.08(8) N1 N11 N21 05.00 N12 N11 N21 176.66(8) . . ? C1 N1 Ni1 172.2(2) . . . ? N1 C1 S1 179.6(2) C2 N2 Ni1 163.81(19) . ? N2 C2 S2 178.7(2) C11 N11 Ni1 122.64(17) . ? ? C13 N12 C14 108.2(2) . . C13 N12 Ni1 117.69(17) . ?? . C14 N12 Ni1 116.23(15) . • ? C16 N13 Ni1 118.28(16) .

C1CE06011B_ccdc_838535_838540_cif.txt

CTT	CTZ	CT3	TT 2	.9(3)			•				
N12	C13	C12	114	.3(2)			?				
N12	C14	C15	114	.4(2)			?				
N13	C16	C15	111	.7(2)			?				
C21	N21	C25	116	.8(2)			?				
C21	N21	Ni1	122	. 87	(16)	5)			?			
C25	N21	Ni1	120	.27	(15	j)			?			
N21	C21	C22	122	.9(2)			?				
C23	C22	C21	119	.6(2)			?				
C22	C23	C24	118	.3(2)			?				
C23	C24	C25	119	.1(2)			?				
N21	C25	C24	123	.2(2)			?				
C14	C15	C16	115	.7(2)			?				
dit	ffrn	_meas	sure	d_f	rac	ti	or	∟t	theta_r	nax O	.984	
dit	ffrn	_ref	lns_ [.]	the	ta_	fι	ררו			26.8	5	
di1	Ffrn	_meas	sure	d_f	rac	ti	or	ו_t	theta_	full	0.984	ŀ
ref	fine	dif	f dei	nsi	tv	ma	ιx			0.31	.3	

_retine_diff_density_max	0.313
refine diff density min	-0.305
_refine_diff_density_rms	0.038
-	