

Electronic Supplementary Information (ESI): S1-S4, followed by

CIF of 1

**Carboxylate-bridged Ni^{II}₈ cluster with distorted cubane topology:
structure, magnetism and density functional study**

Himanshu Arora, Joan Cano, Francesc Lloret and Rabindranath Mukherjee*

Dalton Trans

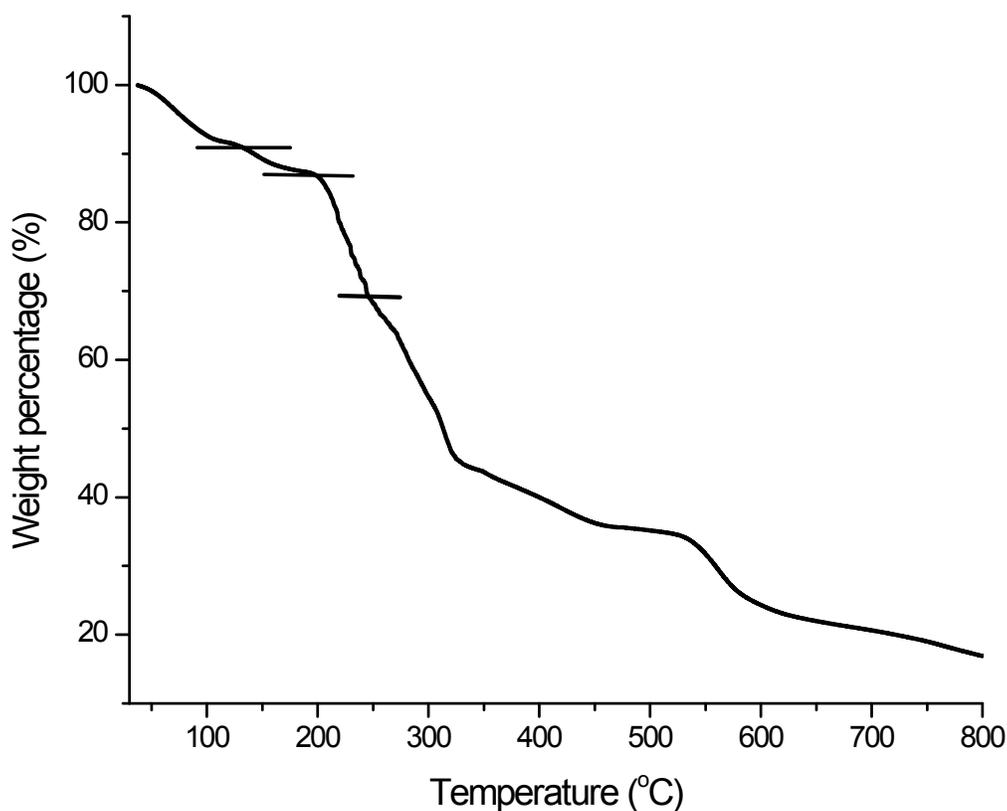


Fig. S1 The curve of TGA of $[\text{Ni}^{\text{II}}_8(\text{L}^4)_6(\text{H}_2\text{O})_6(\text{CH}_3\text{OH})_2(\text{DMF})_2][\text{ClO}_4]_4 \cdot 2\text{CH}_3\text{OH} \cdot 2\text{CH}_3\text{CO}_2 \cdot \text{C}_2\text{H}_5$ (1).

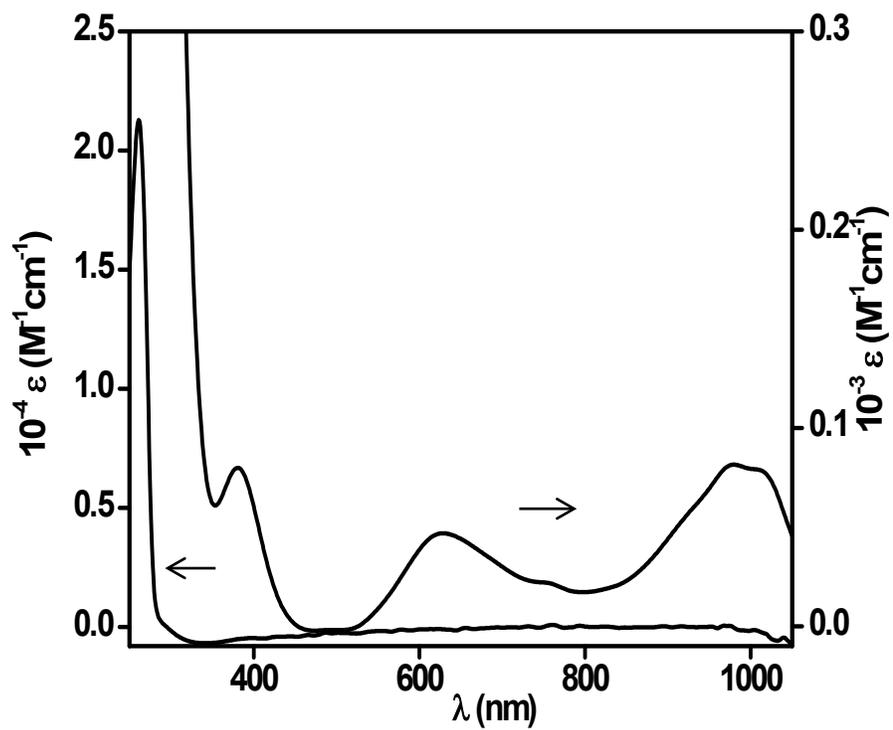


Fig. S2 UV-VIS spectra (in DMF) of $[\text{Ni}^{\text{II}}_8(\text{L}^4)_6(\text{H}_2\text{O})_6(\text{CH}_3\text{OH})_2(\text{DMF})_2][\text{ClO}_4]_4 \cdot 2\text{CH}_3\text{OH} \cdot 2\text{CH}_3\text{CO}_2\text{C}_2\text{H}_5$ (**1**).

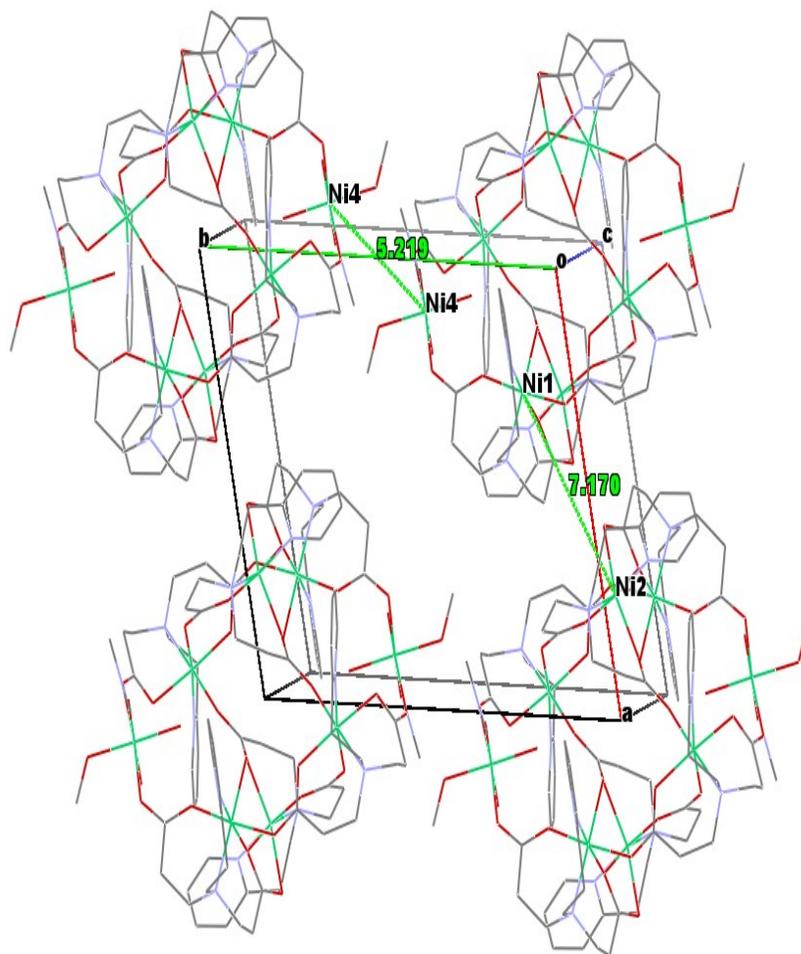


Fig. S3 Packing diagram of $[\text{Ni}^{\text{II}}_8(\text{L}^4)_6(\text{H}_2\text{O})_6(\text{CH}_3\text{OH})_2(\text{DMF})_2][\text{ClO}_4]_4 \cdot 2\text{CH}_3\text{OH} \cdot 2\text{CH}_3\text{CO}_2\text{C}_2\text{H}_5$ (1).

Table S1. Calculated spin configurations, their relative energies (E_i , in cm^{-1}) as a function of different J_i constants and their found S^2 parameter. The spin configuration used as a reference is that with the maximum multiplicity generated from the parallel alignment of all local spin moments of the Ni^{II} ions that shows a calculated energy equal to -18737.9021753 a.u. Only the centres with an antiparallel (negative) alignment of their spin moment are noted.

Spin conf.	S	J_1	J_2	J_3	J_4	J_5	J_6	S^2	E_i
{1}	6	3	0	3	3	0	0	44.021	-62.35
{2}	6	0	0	0	3	3	3	44.020	-95.38
{3A}	6	0	3	3	0	3	3	44.025	-17.29
{4}	6	3	3	0	0	0	0	44.019	+7.81
{1,4}	4	0	3	3	3	0	0	24.021	-58.62
{2,3A}	4	0	3	3	3	6	0	24.021	-49.97
{1,3A,4A}	2	6	6	6	3	3	3	12.019	-71.77
{1,3A,4}	2	0	0	6	3	3	3	12.020	-87.68
{1,2,4}	2	0	3	3	0	3	3	12.025	-17.05
{1,2,3A,4}	0	0	0	6	0	6	0	8.027	+16.57

X-ray crystallographic data (cif file)

data_17sepam

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

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

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H35B H 0.261266 0.350518 0.196979 0.032 Uiso 1 1 calc R U ...
C36 C 0.2299(5) 0.4266(5) 0.3028(4) 0.0200(12) Uani 1 1 d ...
C37 C 0.1102(6) 0.1134(4) 0.2357(5) 0.0242(13) Uani 1 1 d ...
H37A H 0.162278 0.088055 0.216488 0.029 Uiso 1 1 calc R U ...
H37B H 0.039083 0.075749 0.193722 0.029 Uiso 1 1 calc R U ...
C38 C 0.1187(6) 0.1043(5) 0.3309(5) 0.0267(14) Uani 1 1 d ...
H38A H 0.184953 0.148452 0.375005 0.032 Uiso 1 1 calc R U ...
H38B H 0.122830 0.043426 0.332223 0.032 Uiso 1 1 calc R U ...
C39 C 0.0234(5) 0.1198(4) 0.3598(5) 0.0231(13) Uani 1 1 d ...
C40 C 0.0376(6) 0.8608(5) 0.3283(5) 0.0317(15) Uani 1 1 d ...
H40 H 0.103730 0.851181 0.331266 0.038 Uiso 1 1 calc R U ...
C41 C 0.0047(8) 0.8455(7) 0.1671(6) 0.046(2) Uani 1 1 d ...
H41A H 0.074357 0.835924 0.181816 0.069 Uiso 1 1 calc R U ...
H41B H 0.007362 0.898005 0.144326 0.069 Uiso 1 1 calc R U ...
H41C H -0.047655 0.792251 0.120934 0.069 Uiso 1 1 calc R U ...
C42 C -0.1284(7) 0.8773(7) 0.2400(6) 0.050(2) Uani 1 1 d ...
H42A H -0.142509 0.880856 0.296560 0.075 Uiso 1 1 calc R U ...
H42B H -0.184095 0.827661 0.191796 0.075 Uiso 1 1 calc R U ...
H42C H -0.127185 0.933886 0.225108 0.075 Uiso 1 1 calc R U ...
C43 C 0.2651(7) 1.0830(6) 0.5536(7) 0.044(2) Uani 1 1 d ...

H43A H 0.271749 1.074172 0.493818 0.066 Uiso 1 1 calc R U . . .
H43B H 0.317889 1.062623 0.591618 0.066 Uiso 1 1 calc R U . . .
H43C H 0.276553 1.147021 0.580741 0.066 Uiso 1 1 calc R U . . .
O3S O 0.1285(10) 0.9838(8) 0.0391(9) 0.135(4) Uani 1 1 d D
H5S H 0.176743 0.980585 0.083813 0.203 Uiso 1 1 d R U . . .
O1S O 0.4622(10) 1.1809(10) 0.9091(10) 0.148(5) Uani 1 1 d
O2S O 0.3493(9) 1.0773(8) 0.7816(7) 0.123(4) Uani 1 1 d
C3S C 0.4508(17) 1.2610(12) 0.8784(16) 0.152(8) Uani 1 1 d
H0AA H 0.379833 1.267764 0.871828 0.183 Uiso 1 1 calc R U . . .
H0AB H 0.462929 1.256850 0.820304 0.183 Uiso 1 1 calc R U . . .
C4S C 0.5381(17) 1.3401(13) 0.9550(12) 0.139(7) Uani 1 1 d
H4SA H 0.518525 1.348663 1.009324 0.208 Uiso 1 1 calc R U . . .
H4SB H 0.545330 1.395267 0.936521 0.208 Uiso 1 1 calc R U . . .
H4SC H 0.605374 1.326405 0.967636 0.208 Uiso 1 1 calc R U . . .
C2S C 0.4064(12) 1.0953(12) 0.8573(11) 0.100(4) Uani 1 1 d
C1S C 0.431(2) 1.0292(18) 0.9100(19) 0.208(12) Uani 1 1 d
H1SA H 0.402319 1.036438 0.959318 0.312 Uiso 1 1 calc R U . . .
H1SB H 0.507387 1.041101 0.934487 0.312 Uiso 1 1 calc R U . . .
H1SC H 0.398097 0.967586 0.869898 0.312 Uiso 1 1 calc R U . . .

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_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
NI1 0.0178(4) 0.0271(5) 0.0242(4) 0.0088(4) 0.0088(3) 0.0067(4)
NI2 0.0179(4) 0.0282(5) 0.0215(4) 0.0087(3) 0.0079(3) 0.0080(4)
NI3 0.0188(4) 0.0262(5) 0.0221(4) 0.0070(3) 0.0090(3) 0.0073(4)
NI4 0.0208(4) 0.0281(5) 0.0284(5) 0.0112(4) 0.0110(4) 0.0089(4)
CL1 0.0414(11) 0.0495(12) 0.0438(12) 0.0211(10) 0.0140(9) 0.0088(10)
CL2 0.0411(12) 0.0607(14) 0.0469(13) 0.0277(11) 0.0065(10) 0.0082(10)
O1 0.021(2) 0.023(2) 0.029(2) 0.0046(19) 0.017(2) 0.0069(18)
O2 0.020(2) 0.029(2) 0.041(3) 0.011(2) 0.018(2) 0.009(2)
O3 0.018(2) 0.032(3) 0.024(2) 0.0099(19) 0.0106(18) 0.0110(19)
O4 0.022(2) 0.042(3) 0.026(2) 0.016(2) 0.0145(19) 0.018(2)
O5 0.018(2) 0.036(3) 0.022(2) 0.007(2) 0.0055(18) 0.007(2)
O6 0.023(2) 0.036(3) 0.028(3) 0.012(2) 0.016(2) 0.015(2)
O7 0.025(2) 0.023(2) 0.024(2) 0.0047(18) 0.0085(19) 0.0058(19)
O8 0.019(2) 0.029(2) 0.017(2) 0.0065(17) 0.0055(17) 0.0091(19)
O9 0.022(2) 0.024(2) 0.027(2) 0.009(2) 0.0096(19) 0.0031(19)
O10 0.022(2) 0.026(2) 0.027(2) 0.0042(19) 0.010(2) 0.0042(19)
O11 0.023(2) 0.022(2) 0.029(3) 0.0086(19) 0.008(2) 0.0042(19)
O12 0.023(2) 0.033(3) 0.034(3) 0.015(2) 0.016(2) 0.011(2)

O13 0.016(2) 0.026(2) 0.025(2) 0.0050(19) 0.0100(18) 0.0039(19)
O14 0.029(3) 0.025(2) 0.031(3) 0.010(2) 0.011(2) 0.009(2)
O15 0.023(2) 0.048(3) 0.023(2) 0.015(2) 0.0071(19) 0.010(2)
O16 0.027(2) 0.030(3) 0.036(3) 0.014(2) 0.012(2) 0.013(2)
O17 0.025(2) 0.040(3) 0.019(2) 0.009(2) 0.0083(19) 0.009(2)
O18 0.060(5) 0.071(5) 0.097(6) 0.055(5) -0.010(4) -0.011(4)
O19 0.194(12) 0.121(8) 0.093(7) 0.041(6) 0.086(8) 0.091(8)
O20 0.187(10) 0.060(5) 0.051(4) 0.030(4) 0.000(5) -0.022(6)
O21 0.051(4) 0.104(7) 0.209(11) 0.093(8) 0.060(6) 0.026(5)
O22 0.064(5) 0.150(9) 0.120(8) 0.085(7) -0.030(5) -0.036(5)
O23 0.075(5) 0.097(6) 0.073(5) 0.057(5) 0.027(4) 0.037(5)
O24 0.113(7) 0.120(8) 0.067(5) 0.026(5) 0.041(5) 0.063(6)
O25 0.057(4) 0.073(5) 0.048(3) 0.033(3) 0.018(3) 0.018(4)
C5S 0.149(14) 0.080(10) 0.056(8) 0.010(6) -0.009(7) 0.038(10)
N1 0.021(3) 0.037(3) 0.025(3) 0.011(3) 0.009(2) 0.010(3)
N2 0.013(2) 0.027(3) 0.028(3) 0.005(2) 0.008(2) 0.003(2)
N3 0.023(3) 0.028(3) 0.023(3) 0.007(2) 0.006(2) 0.003(2)
N4 0.016(2) 0.033(3) 0.026(3) 0.016(2) 0.007(2) 0.011(2)
N5 0.018(2) 0.029(3) 0.021(3) 0.004(2) 0.000(2) 0.011(2)
N6 0.023(3) 0.024(3) 0.024(3) 0.002(2) 0.011(2) 0.007(2)
N7 0.034(3) 0.038(4) 0.024(3) 0.005(3) 0.008(2) 0.012(3)
C1 0.023(3) 0.041(4) 0.034(4) 0.017(3) 0.006(3) 0.010(3)
C2 0.028(4) 0.046(5) 0.041(4) 0.022(4) 0.004(3) 0.006(4)
C3 0.038(4) 0.053(5) 0.031(4) 0.020(4) 0.003(3) 0.003(4)
C4 0.050(4) 0.046(5) 0.023(3) 0.010(3) 0.015(3) 0.014(4)
C5 0.029(3) 0.032(4) 0.025(3) 0.011(3) 0.012(3) 0.006(3)
C6 0.036(4) 0.049(5) 0.035(4) 0.011(3) 0.017(3) 0.017(4)
C7 0.030(4) 0.034(4) 0.040(4) 0.020(3) 0.017(3) 0.006(3)
C8 0.019(3) 0.025(3) 0.035(4) 0.012(3) 0.010(3) 0.001(3)
C9 0.016(3) 0.034(4) 0.043(4) 0.015(3) 0.020(3) 0.007(3)
C10 0.016(3) 0.032(3) 0.027(3) 0.010(3) 0.010(3) 0.007(2)
C11 0.012(3) 0.037(4) 0.028(3) 0.008(3) 0.008(3) 0.007(3)
C12 0.019(3) 0.038(4) 0.033(4) 0.010(3) 0.015(3) 0.007(3)
C13 0.013(3) 0.030(3) 0.019(3) 0.006(3) 0.001(2) 0.003(2)
C14 0.032(4) 0.030(3) 0.030(4) 0.011(3) 0.007(3) 0.011(3)
C15 0.038(4) 0.036(4) 0.039(4) 0.010(3) 0.014(3) 0.005(3)
C16 0.034(4) 0.033(4) 0.038(4) -0.002(3) 0.008(3) 0.001(3)
C17 0.018(3) 0.043(4) 0.034(4) 0.006(3) 0.007(3) 0.007(3)
C18 0.024(3) 0.039(4) 0.023(3) 0.005(3) 0.009(2) 0.007(3)
C19 0.020(3) 0.042(4) 0.033(4) 0.015(3) 0.005(3) 0.010(3)
C20 0.020(3) 0.038(4) 0.028(3) 0.012(3) 0.007(3) 0.011(3)
C21 0.024(3) 0.030(3) 0.025(3) 0.014(3) 0.011(3) 0.007(3)
C22 0.026(3) 0.030(3) 0.023(3) 0.011(3) 0.010(3) 0.011(3)
C23 0.014(3) 0.024(3) 0.021(3) -0.001(2) 0.009(2) 0.007(2)
C24 0.021(3) 0.032(4) 0.029(4) 0.014(3) 0.013(3) 0.005(3)
C25 0.026(3) 0.027(3) 0.021(3) 0.007(3) 0.004(3) 0.008(3)

C26 0.008(3) 0.032(3) 0.019(3) 0.005(2) 0.008(2) 0.006(2)
 C27 0.020(3) 0.040(4) 0.031(3) 0.008(3) 0.007(3) 0.011(3)
 C28 0.026(3) 0.050(5) 0.033(4) 0.014(4) 0.007(3) 0.012(4)
 C29 0.033(4) 0.065(6) 0.030(4) 0.012(4) 0.006(3) 0.011(4)
 C30 0.040(4) 0.055(5) 0.025(3) 0.013(4) 0.011(3) 0.014(4)
 C31 0.029(3) 0.029(4) 0.024(3) 0.008(3) 0.011(3) 0.007(3)
 C32 0.032(3) 0.032(4) 0.021(3) 0.008(3) 0.010(3) 0.010(3)
 C33 0.027(3) 0.031(4) 0.021(3) 0.002(3) 0.008(3) 0.007(3)
 C34 0.014(3) 0.030(3) 0.029(3) 0.005(3) 0.011(2) 0.007(3)
 C35 0.031(4) 0.026(3) 0.027(3) 0.009(3) 0.014(3) 0.007(3)
 C36 0.020(3) 0.029(3) 0.013(3) 0.004(2) 0.009(2) 0.009(2)
 C37 0.024(3) 0.022(3) 0.028(3) 0.003(3) 0.015(3) 0.004(3)
 C38 0.025(3) 0.029(4) 0.030(3) 0.007(3) 0.014(3) 0.012(3)
 C39 0.022(3) 0.022(3) 0.029(3) 0.007(3) 0.014(3) 0.005(3)
 C40 0.035(4) 0.026(4) 0.032(3) 0.009(3) 0.010(3) 0.008(3)
 C41 0.059(6) 0.057(6) 0.027(4) 0.012(4) 0.022(4) 0.017(5)
 C42 0.046(5) 0.065(6) 0.045(5) 0.016(5) 0.018(4) 0.029(5)
 C43 0.038(4) 0.032(4) 0.069(6) 0.027(4) 0.024(4) 0.008(3)
 O3S 0.140(11) 0.114(9) 0.150(11) 0.031(8) 0.051(9) 0.041(8)
 O1S 0.116(10) 0.126(8) 0.139(10) -0.030(7) 0.026(8) 0.004(8)
 O2S 0.109(8) 0.107(8) 0.085(6) 0.002(6) -0.014(6) -0.014(6)
 C3S 0.162(17) 0.087(10) 0.22(2) -0.001(10) 0.148(15) 0.003(10)
 C4S 0.186(19) 0.141(13) 0.108(13) 0.021(10) 0.100(13) 0.039(12)
 C2S 0.077(9) 0.112(9) 0.074(7) -0.014(7) 0.015(6) 0.007(8)
 C1S 0.22(3) 0.20(2) 0.21(3) 0.10(2) 0.05(2) 0.09(2)

_geom_special_details

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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.

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 N11 O1 2.031(4) . ?
 N11 O3 2.049(5) . ?
 N11 N1 2.058(6) . ?
 N11 O10 2.067(5) . ?

NI1 O13 2.103(4) . ?
NI1 N2 2.117(5) . ?
NI2 O7 2.006(5) . ?
NI2 O5 2.014(5) . ?
NI2 N3 2.067(6) . ?
NI2 N4 2.067(5) . ?
NI2 O3 2.123(5) . ?
NI2 O4 2.154(4) . ?
NI2 C13 2.479(7) . ?
NI3 O9 2.053(5) . ?
NI3 O8 2.088(4) . ?
NI3 N5 2.092(5) . ?
NI3 O11 2.097(5) . ?
NI3 O6 2.100(4) 2_566 ?
NI3 N6 2.126(5) . ?
NI4 O2 2.030(5) . ?
NI4 O17 2.036(5) . ?
NI4 O14 2.059(5) . ?
NI4 O12 2.079(5) . ?
NI4 O16 2.084(5) . ?
NI4 O15 2.087(5) . ?
CL1 O19 1.373(9) . ?
CL1 O20 1.383(8) . ?
CL1 O21 1.397(9) . ?
CL1 O18 1.418(7) . ?
CL2 O22 1.395(9) . ?
CL2 O23 1.417(7) . ?
CL2 O25 1.426(7) . ?
CL2 O24 1.446(9) . ?
O1 C10 1.247(8) . ?
O2 C10 1.259(8) . ?
O3 C13 1.284(7) . ?
O4 C13 1.252(8) . ?
O5 C26 1.269(7) . ?
O6 C26 1.251(7) . ?
O6 NI3 2.100(4) 2_566 ?
O7 C23 1.246(8) . ?
O8 C23 1.253(7) . ?
O9 C36 1.264(8) . ?
O10 C36 1.241(8) . ?
O11 C39 1.271(8) . ?
O12 C39 1.254(8) 2_566 ?
O16 C43 1.442(9) . ?
O17 C40 1.235(9) . ?
C5S O3S 1.480(14) . ?
N1 C1 1.338(9) . ?

N1 C5 1.356(9) . ?
N2 C11 1.477(8) . ?
N2 C8 1.485(9) . ?
N2 C7 1.486(9) . ?
N3 C14 1.328(9) . ?
N3 C18 1.340(9) . ?
N4 C21 1.489(9) . ?
N4 C24 1.501(8) . ?
N4 C20 1.500(9) . ?
N5 C31 1.342(9) . ?
N5 C27 1.350(9) . ?
N6 C34 1.466(8) . ?
N6 C33 1.480(8) . ?
N6 C37 1.500(8) . ?
N7 C40 1.304(10) . ?
N7 C42 1.441(10) . ?
N7 C41 1.468(10) . ?
C1 C2 1.403(11) . ?
C2 C3 1.361(12) . ?
C3 C4 1.387(12) . ?
C4 C5 1.382(10) . ?
C5 C6 1.524(10) . ?
C6 C7 1.522(11) . ?
C8 C9 1.531(9) . ?
C9 C10 1.526(9) . ?
C11 C12 1.530(10) . ?
C12 C13 1.509(9) . ?
C14 C15 1.374(11) . ?
C15 C16 1.382(12) . ?
C16 C17 1.380(11) . ?
C17 C18 1.386(10) . ?
C18 C19 1.518(10) . ?
C19 C20 1.522(10) . ?
C21 C22 1.525(10) . ?
C22 C23 1.522(9) . ?
C24 C25 1.514(9) . ?
C25 C26 1.530(9) . ?
C27 C28 1.381(10) . ?
C28 C29 1.378(11) . ?
C29 C30 1.367(12) . ?
C30 C31 1.396(10) . ?
C31 C32 1.490(10) . ?
C32 C33 1.543(10) . ?
C34 C35 1.543(9) . ?
C35 C36 1.527(9) . ?
C37 C38 1.519(9) . ?

C38 C39 1.534(9) . ?
C39 O12 1.254(8) 2_566 ?
O1S C2S 1.332(19) . ?
O1S C3S 1.46(2) . ?
O2S C2S 1.168(17) . ?
C3S C4S 1.52(3) . ?
C2S C1S 1.49(3) . ?

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O1 NI1 O3 89.21(19) . . ?
O1 NI1 N1 93.5(2) . . ?
O3 NI1 N1 176.2(2) . . ?
O1 NI1 O10 174.12(18) . . ?
O3 NI1 O10 87.91(19) . . ?
N1 NI1 O10 89.1(2) . . ?
O1 NI1 O13 84.79(18) . . ?
O3 NI1 O13 87.30(18) . . ?
N1 NI1 O13 90.3(2) . . ?
O10 NI1 O13 89.96(18) . . ?
O1 NI1 N2 92.3(2) . . ?
O3 NI1 N2 88.1(2) . . ?
N1 NI1 N2 94.4(2) . . ?
O10 NI1 N2 92.7(2) . . ?
O13 NI1 N2 174.6(2) . . ?
O7 NI2 O5 90.0(2) . . ?
O7 NI2 N3 171.2(2) . . ?
O5 NI2 N3 93.6(2) . . ?
O7 NI2 N4 94.3(2) . . ?
O5 NI2 N4 96.0(2) . . ?
N3 NI2 N4 93.3(2) . . ?
O7 NI2 O3 85.76(19) . . ?
O5 NI2 O3 94.64(18) . . ?
N3 NI2 O3 86.0(2) . . ?
N4 NI2 O3 169.33(19) . . ?
O7 NI2 O4 88.78(19) . . ?
O5 NI2 O4 156.12(19) . . ?
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O3 NI2 O4 61.49(17) . . ?

O7 NI2 C13 87.9(2) . . ?
O5 NI2 C13 125.8(2) . . ?
N3 NI2 C13 83.5(2) . . ?
N4 NI2 C13 138.1(2) . . ?
O3 NI2 C13 31.20(18) . . ?
O4 NI2 C13 30.32(19) . . ?
O9 NI3 O8 90.48(18) . . ?
O9 NI3 N5 101.2(2) . . ?
O8 NI3 N5 167.3(2) . . ?
O9 NI3 O11 171.86(19) . . ?
O8 NI3 O11 81.60(18) . . ?
N5 NI3 O11 86.6(2) . . ?
O9 NI3 O6 90.12(19) . 2_566 ?
O8 NI3 O6 84.93(18) . 2_566 ?
N5 NI3 O6 90.1(2) . 2_566 ?
O11 NI3 O6 87.36(19) . 2_566 ?
O9 NI3 N6 91.9(2) . . ?
O8 NI3 N6 93.4(2) . . ?
N5 NI3 N6 91.1(2) . . ?
O11 NI3 N6 90.5(2) . . ?
O6 NI3 N6 177.4(2) 2_566 . ?
O2 NI4 O17 93.8(2) . . ?
O2 NI4 O14 93.52(19) . . ?
O17 NI4 O14 90.3(2) . . ?
O2 NI4 O12 173.4(2) . . ?
O17 NI4 O12 86.6(2) . . ?
O14 NI4 O12 93.11(19) . . ?
O2 NI4 O16 87.18(19) . . ?
O17 NI4 O16 88.3(2) . . ?
O14 NI4 O16 178.5(2) . . ?
O12 NI4 O16 86.20(19) . . ?
O2 NI4 O15 87.2(2) . . ?
O17 NI4 O15 178.8(2) . . ?
O14 NI4 O15 89.1(2) . . ?
O12 NI4 O15 92.46(19) . . ?
O16 NI4 O15 92.3(2) . . ?
O19 CL1 O20 108.5(7) . . ?
O19 CL1 O21 105.9(8) . . ?
O20 CL1 O21 112.0(7) . . ?
O19 CL1 O18 111.8(7) . . ?
O20 CL1 O18 110.9(5) . . ?
O21 CL1 O18 107.8(5) . . ?
O22 CL2 O23 114.1(6) . . ?
O22 CL2 O25 110.4(5) . . ?
O23 CL2 O25 110.4(5) . . ?
O22 CL2 O24 110.1(8) . . ?

O23 CL2 O24 105.5(5) .. ?
O25 CL2 O24 105.9(5) .. ?
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C24 C25 C26 116.3(6) .. ?
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N6 C33 C32 116.3(6) . . ?
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N6 C37 C38 116.8(5) . . ?
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O14 H14B O1 0.87 1.91 2.674(6) 145.8 .
O14 H14A O6 0.87 2.02 2.809(7) 150.7 .
O15 H15B O11_\$1 0.85 1.92 2.629(7) 139.5 2_566
O15 H15A O2S 0.84 2.08 2.798(12) 143.0 .
O16 H16 O12_\$2 0.85 2.01 2.863(7) 180.0 2_576
O3S H5S O20 0.84 1.96 2.779(17) 165.8 .

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shelx.res created by SHELXL-2016/4 at 12:53:45 on 26-Jul-2016
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DISP C 0.003 0.002
DISP Cl 0.148 0.159
DISP H 0 0
DISP N 0.006 0.003
DISP Ni 0.339 1.112
DISP O 0.011 0.006
UNIT 96 154 4 14 8 56
MERG 2
EQIV $1 -X,1-Y,1-Z
EQIV $2 -X,2-Y,1-Z
RIGU
HTAB O13 O5
HTAB O13 O9
HTAB O14 O1
HTAB O14 O6
HTAB O15 O11_$1
HTAB O15 O2S
HTAB O16 O12_$2
HTAB O3S O20
DFIX 1.450 0.020 O3S C5S
FMAP 2 53 53
PLAN 20
SIZE 0.100 0.200 0.500
ACTA
L.S. 4
TEMP 0.00
WGHT 0.136100 7.993200
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0.02422 0.00876 0.00885 0.00672
NI2 5 0.286236 0.550646 0.613489 11.00000 0.01790 0.02820 =
0.02150 0.00875 0.00786 0.00797
NI3 5 0.041295 0.278227 0.293713 11.00000 0.01882 0.02619 =
0.02213 0.00704 0.00900 0.00728
NI4 5 0.116800 0.889834 0.526743 11.00000 0.02084 0.02807 =
0.02842 0.01116 0.01104 0.00894
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0.04378 0.02112 0.01396 0.00884
CL2 3 0.263343 0.374110 -0.020636 11.00000 0.04106 0.06070 =

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		0.04691	0.02771	0.00649	0.00816		
O1	6	0.247464	0.745669	0.461234	11.00000	0.02127	0.02266 =
		0.02932	0.00463	0.01696	0.00694		
O2	6	0.245478	0.890321	0.484519	11.00000	0.02014	0.02894 =
		0.04064	0.01143	0.01757	0.00902		
O3	6	0.344315	0.615048	0.523872	11.00000	0.01769	0.03160 =
		0.02392	0.00986	0.01056	0.01097		
O4	6	0.439835	0.544488	0.602836	11.00000	0.02190	0.04188 =
		0.02617	0.01627	0.01451	0.01821		
O5	6	0.149359	0.586384	0.586576	11.00000	0.01807	0.03566 =
		0.02247	0.00671	0.00549	0.00677		
O6	6	0.044194	0.656822	0.635187	11.00000	0.02336	0.03600 =
		0.02794	0.01202	0.01593	0.01528		
O7	6	0.214458	0.439102	0.504163	11.00000	0.02492	0.02276 =
		0.02446	0.00469	0.00849	0.00581		
O8	6	0.145610	0.292742	0.424068	11.00000	0.01872	0.02950 =
		0.01670	0.00647	0.00553	0.00914		
O9	6	0.131306	0.403537	0.294896	11.00000	0.02205	0.02357 =
		0.02726	0.00870	0.00963	0.00312		
O10	6	0.292016	0.505980	0.339533	11.00000	0.02198	0.02648 =
		0.02747	0.00423	0.01011	0.00417		
O11	6	-0.038230	0.155690	0.312481	11.00000	0.02342	0.02190 =
		0.02939	0.00857	0.00818	0.00417		
O12	6	-0.008998	0.905827	0.573476	11.00000	0.02321	0.03329 =
		0.03432	0.01487	0.01642	0.01109		
O13	6	0.125035	0.561510	0.403824	11.00000	0.01646	0.02581 =
		0.02463	0.00501	0.00996	0.00392		
AFIX	3						
H13A	2	0.128255	0.571490	0.458884	11.00000	-1.50000	
H13B	2	0.110155	0.503420	0.380904	11.00000	-1.50000	
AFIX	0						
O14	6	0.071686	0.750005	0.505838	11.00000	0.02876	0.02457 =
		0.03096	0.00968	0.01125	0.00896		
AFIX	3						
H14A	2	0.081926	0.738575	0.558478	11.00000	-1.50000	
H14B	2	0.110716	0.726424	0.478068	11.00000	-1.50000	
AFIX	0						
O15	6	0.219428	0.906394	0.658364	11.00000	0.02284	0.04805 =
		0.02256	0.01477	0.00705	0.00995		
AFIX	3						
H15A	2	0.270078	0.955214	0.675613	11.00000	-1.50000	
H15B	2	0.184738	0.890624	0.692692	11.00000	-1.50000	
AFIX	0						
O16	6	0.158604	1.030962	0.545312	11.00000	0.02662	0.02956 =
		0.03591	0.01447	0.01186	0.01315		
AFIX	3						

H16	2	0.114204	1.049741	0.510042	11.00000	-1.50000	
AFIX 0							
O17	6	0.014121	0.872282	0.398950	11.00000	0.02520	0.03977 =
		0.01861	0.00915	0.00827	0.00914		
O18	6	0.272577	0.858151	0.235678	11.00000	0.05992	0.07100 =
		0.09676	0.05537	-0.01003	-0.01134		
O19	6	0.321823	1.011973	0.314401	11.00000	0.19374	0.12113 =
		0.09288	0.04074	0.08583	0.09141		
O20	6	0.308952	0.972108	0.166866	11.00000	0.18662	0.05957 =
		0.05080	0.03002	-0.00006	-0.02163		
O21	6	0.444085	0.952501	0.279756	11.00000	0.05121	0.10361 =
		0.20885	0.09255	0.05957	0.02571		
O22	6	0.363174	0.441438	0.011278	11.00000	0.06403	0.15032 =
		0.12031	0.08503	-0.02991	-0.03648		
O23	6	0.266250	0.293556	0.006303	11.00000	0.07481	0.09673 =
		0.07349	0.05735	0.02719	0.03662		
O24	6	0.188421	0.408624	0.015698	11.00000	0.11300	0.11983 =
		0.06693	0.02571	0.04054	0.06300		
O25	6	0.217318	0.351780	-0.117985	11.00000	0.05748	0.07265 =
		0.04797	0.03296	0.01815	0.01802		
C5S	1	0.175049	1.020588	-0.024944	11.00000	0.14898	0.07983 =
		0.05558	0.01049	-0.00856	0.03817		
AFIX 137							
H3SA	2	0.187725	0.972112	-0.064872	11.00000	-1.50000	
H3SB	2	0.241970	1.068070	0.009387	11.00000	-1.50000	
H3SC	2	0.125641	1.045443	-0.060862	11.00000	-1.50000	
AFIX 0							
N1	4	0.198872	0.636690	0.268371	11.00000	0.02133	0.03698 =
		0.02458	0.01125	0.00891	0.00963		
N2	4	0.429669	0.704802	0.405407	11.00000	0.01260	0.02681 =
		0.02781	0.00526	0.00778	0.00301		
N3	4	0.375165	0.672405	0.715200	11.00000	0.02264	0.02826 =
		0.02286	0.00669	0.00590	0.00310		
N4	4	0.255930	0.481307	0.705727	11.00000	0.01602	0.03309 =
		0.02585	0.01572	0.00673	0.01142		
N5	4	-0.087481	0.243607	0.170848	11.00000	0.01847	0.02924 =
		0.02077	0.00374	0.00039	0.01082		
N6	4	0.127782	0.208376	0.225385	11.00000	0.02261	0.02449 =
		0.02367	0.00249	0.01069	0.00744		
N7	4	-0.025567	0.861356	0.249744	11.00000	0.03357	0.03810 =
		0.02375	0.00506	0.00834	0.01218		
C1	1	0.095512	0.635124	0.244702	11.00000	0.02318	0.04094 =
		0.03411	0.01728	0.00624	0.00980		
AFIX 43							
H1	2	0.065392	0.644541	0.290663	11.00000	-1.20000	
AFIX 0							

C2 1 0.030393 0.619943 0.153796 11.00000 0.02843 0.04634 =
0.04062 0.02197 0.00387 0.00557
AFIX 43
H2 2 -0.041282 0.619228 0.139282 11.00000 -1.20000
AFIX 0
C3 1 0.076137 0.606306 0.087692 11.00000 0.03787 0.05250 =
0.03115 0.01963 0.00342 0.00271
AFIX 43
H3 2 0.034769 0.594292 0.026505 11.00000 -1.20000
AFIX 0
C4 1 0.183963 0.610184 0.110843 11.00000 0.04990 0.04611 =
0.02334 0.01001 0.01507 0.01359
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H4 2 0.215371 0.601529 0.065686 11.00000 -1.20000
AFIX 0
C5 1 0.244086 0.627081 0.201922 11.00000 0.02939 0.03176 =
0.02527 0.01107 0.01203 0.00645
C6 1 0.364111 0.636544 0.232918 11.00000 0.03599 0.04881 =
0.03479 0.01113 0.01658 0.01712
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H6B 2 0.390649 0.641958 0.182745 11.00000 -1.20000
AFIX 0
C7 1 0.428598 0.719878 0.315682 11.00000 0.03029 0.03396 =
0.03977 0.01966 0.01673 0.00611
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H7A 2 0.502377 0.738633 0.316646 11.00000 -1.20000
H7B 2 0.399010 0.769981 0.308366 11.00000 -1.20000
AFIX 0
C8 1 0.468819 0.793758 0.478407 11.00000 0.01862 0.02549 =
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AFIX 23
H8A 2 0.541946 0.824543 0.483632 11.00000 -1.20000
H8B 2 0.471760 0.781061 0.536250 11.00000 -1.20000
AFIX 0
C9 1 0.401981 0.859990 0.464794 11.00000 0.01593 0.03356 =
0.04320 0.01517 0.02000 0.00681
AFIX 23
H9A 2 0.441389 0.918760 0.510672 11.00000 -1.20000
H9B 2 0.394547 0.869478 0.405068 11.00000 -1.20000
AFIX 0
C10 1 0.289675 0.828420 0.471021 11.00000 0.01550 0.03213 =
0.02666 0.00969 0.00987 0.00747
C11 1 0.504793 0.651170 0.428904 11.00000 0.01241 0.03728 =
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AFIX 23

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H11B	2	0.477002	0.592327	0.382090	11.00000	-1.20000	
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AFIX	23						
H12A	2	0.570937	0.592219	0.525213	11.00000	-1.20000	
H12B	2	0.568837	0.690721	0.569083	11.00000	-1.20000	
AFIX	0						
C13	1	0.430984	0.592251	0.548472	11.00000	0.01343	0.03032 =
		0.01936	0.00559	0.00073	0.00254		
C14	1	0.375910	0.751671	0.696955	11.00000	0.03232	0.03027 =
		0.02975	0.01119	0.00720	0.01113		
AFIX	43						
H14	2	0.320872	0.752510	0.646975	11.00000	-1.20000	
AFIX	0						
C15	1	0.455055	0.832485	0.749252	11.00000	0.03777	0.03571 =
		0.03865	0.01047	0.01360	0.00452		
AFIX	43						
H15	2	0.453112	0.886938	0.734862	11.00000	-1.20000	
AFIX	0						
C16	1	0.537551	0.832061	0.823423	11.00000	0.03389	0.03344 =
		0.03773	-0.00164	0.00763	0.00086		
AFIX	43						
H16A	2	0.593254	0.885498	0.858674	11.00000	-1.20000	
AFIX	0						
C17	1	0.534913	0.750075	0.843689	11.00000	0.01752	0.04284 =
		0.03394	0.00593	0.00651	0.00694		
AFIX	43						
H17	2	0.587671	0.748050	0.894639	11.00000	-1.20000	
AFIX	0						
C18	1	0.453313	0.670755	0.787802	11.00000	0.02352	0.03873 =
		0.02293	0.00516	0.00923	0.00679		
C19	1	0.445160	0.577756	0.804847	11.00000	0.02030	0.04163 =
		0.03310	0.01474	0.00549	0.01031		
AFIX	23						
H19A	2	0.496823	0.586088	0.864484	11.00000	-1.20000	
H19B	2	0.464260	0.539751	0.758954	11.00000	-1.20000	
AFIX	0						
C20	1	0.333094	0.528102	0.801753	11.00000	0.02046	0.03770 =
		0.02759	0.01174	0.00668	0.01135		
AFIX	23						
H20A	2	0.338544	0.482721	0.834816	11.00000	-1.20000	
H20B	2	0.304721	0.572003	0.832698	11.00000	-1.20000	
AFIX	0						
C21	1	0.270281	0.389301	0.676215	11.00000	0.02414	0.02983 =

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 H21B 2 0.343482 0.398759 0.675863 11.00000 -1.20000
 AFIX 0
 C22 1 0.194513 0.323455 0.583453 11.00000 0.02617 0.02992 =
 0.02258 0.01114 0.00969 0.01148
 AFIX 23
 H22A 2 0.216735 0.268400 0.574040 11.00000 -1.20000
 H22B 2 0.122837 0.305814 0.587379 11.00000 -1.20000
 AFIX 0
 C23 1 0.185661 0.355882 0.498288 11.00000 0.01427 0.02391 =
 0.02108 -0.00064 0.00909 0.00657
 C24 1 0.142942 0.471112 0.705535 11.00000 0.02085 0.03191 =
 0.02862 0.01391 0.01323 0.00539
 AFIX 23
 H24A 2 0.132511 0.442870 0.752664 11.00000 -1.20000
 H24B 2 0.093009 0.429914 0.646855 11.00000 -1.20000
 AFIX 0
 C25 1 0.115639 0.560548 0.721932 11.00000 0.02584 0.02701 =
 0.02082 0.00660 0.00415 0.00835
 AFIX 23
 H25A 2 0.172757 0.604782 0.775184 11.00000 -1.20000
 H25B 2 0.049951 0.550207 0.736907 11.00000 -1.20000
 AFIX 0
 C26 1 0.100096 0.603276 0.642604 11.00000 0.00814 0.03153 =
 0.01892 0.00545 0.00811 0.00588
 C27 1 -0.189124 0.219474 0.172364 11.00000 0.01982 0.04031 =
 0.03122 0.00846 0.00684 0.01107
 AFIX 43
 H27 2 -0.199318 0.217105 0.227604 11.00000 -1.20000
 AFIX 0
 C28 1 -0.278509 0.198179 0.094863 11.00000 0.02567 0.04984 =
 0.03350 0.01438 0.00667 0.01187
 AFIX 43
 H28 2 -0.347634 0.183301 0.098053 11.00000 -1.20000
 AFIX 0
 C29 1 -0.263037 0.199458 0.012689 11.00000 0.03294 0.06458 =
 0.03009 0.01157 0.00571 0.01101
 AFIX 43
 H29 2 -0.321715 0.185894 -0.040494 11.00000 -1.20000
 AFIX 0
 C30 1 -0.160381 0.220909 0.010361 11.00000 0.04017 0.05526 =
 0.02479 0.01281 0.01130 0.01377
 AFIX 43
 H30 2 -0.149143 0.220656 -0.044978 11.00000 -1.20000

AFIX 0

C31 1 -0.072313 0.243196 0.090628 11.00000 0.02929 0.02892 =
0.02412 0.00848 0.01062 0.00716

C32 1 0.041387 0.267272 0.092388 11.00000 0.03178 0.03221 =
0.02136 0.00755 0.01012 0.00969

AFIX 23

H32A 2 0.080249 0.328985 0.132627 11.00000 -1.20000

H32B 2 0.042250 0.266317 0.031202 11.00000 -1.20000

AFIX 0

C33 1 0.098567 0.199604 0.126130 11.00000 0.02683 0.03073 =
0.02090 0.00212 0.00781 0.00651

AFIX 23

H33A 2 0.052084 0.137636 0.092433 11.00000 -1.20000

H33B 2 0.163894 0.207400 0.110645 11.00000 -1.20000

AFIX 0

C34 1 0.242415 0.259228 0.272482 11.00000 0.01424 0.02966 =
0.02851 0.00500 0.01128 0.00708

AFIX 23

H34A 2 0.284456 0.223414 0.249654 11.00000 -1.20000

H34B 2 0.259433 0.264654 0.337356 11.00000 -1.20000

AFIX 0

C35 1 0.278571 0.356173 0.261915 11.00000 0.03077 0.02605 =
0.02682 0.00929 0.01437 0.00680

AFIX 23

H35A 2 0.356405 0.380113 0.290045 11.00000 -1.20000

H35B 2 0.261266 0.350518 0.196979 11.00000 -1.20000

AFIX 0

C36 1 0.229869 0.426644 0.302833 11.00000 0.02046 0.02870 =
0.01285 0.00426 0.00882 0.00921

C37 1 0.110188 0.113380 0.235705 11.00000 0.02368 0.02179 =
0.02816 0.00331 0.01540 0.00402

AFIX 23

H37A 2 0.162278 0.088055 0.216488 11.00000 -1.20000

H37B 2 0.039083 0.075749 0.193722 11.00000 -1.20000

AFIX 0

C38 1 0.118687 0.104310 0.330857 11.00000 0.02493 0.02930 =
0.03026 0.00685 0.01437 0.01209

AFIX 23

H38A 2 0.184953 0.148452 0.375005 11.00000 -1.20000

H38B 2 0.122830 0.043426 0.332223 11.00000 -1.20000

AFIX 0

C39 1 0.023445 0.119839 0.359828 11.00000 0.02186 0.02157 =
0.02865 0.00683 0.01411 0.00539

C40 1 0.037647 0.860759 0.328295 11.00000 0.03511 0.02622 =
0.03243 0.00938 0.01037 0.00753

AFIX 43

H40 2 0.103730 0.851181 0.331266 11.00000 -1.20000
AFIX 0
C41 1 0.004746 0.845514 0.167053 11.00000 0.05860 0.05715 =
0.02679 0.01246 0.02158 0.01678
AFIX 137
H41A 2 0.074357 0.835924 0.181816 11.00000 -1.50000
H41B 2 0.007362 0.898005 0.144326 11.00000 -1.50000
H41C 2 -0.047655 0.792251 0.120934 11.00000 -1.50000
AFIX 0
C42 1 -0.128428 0.877268 0.239987 11.00000 0.04646 0.06544 =
0.04493 0.01603 0.01768 0.02892
AFIX 137
H42A 2 -0.142509 0.880856 0.296560 11.00000 -1.50000
H42B 2 -0.184095 0.827661 0.191796 11.00000 -1.50000
H42C 2 -0.127185 0.933886 0.225108 11.00000 -1.50000
AFIX 0
C43 1 0.265093 1.083045 0.553561 11.00000 0.03797 0.03231 =
0.06926 0.02728 0.02388 0.00753
AFIX 137
H43A 2 0.271749 1.074172 0.493818 11.00000 -1.50000
H43B 2 0.317889 1.062623 0.591618 11.00000 -1.50000
H43C 2 0.276553 1.147021 0.580741 11.00000 -1.50000
AFIX 0
O3S 6 0.128513 0.983805 0.039053 11.00000 0.13981 0.11402 =
0.15041 0.03142 0.05107 0.04099
AFIX 3
H5S 2 0.176743 0.980585 0.083813 11.00000 -1.50000
AFIX 0
O1S 6 0.462221 1.180926 0.909077 11.00000 0.11598 0.12642 =
0.13890 -0.03044 0.02628 0.00412
O2S 6 0.349330 1.077254 0.781579 11.00000 0.10937 0.10705 =
0.08467 0.00158 -0.01354 -0.01399
C3S 1 0.450828 1.260993 0.878365 11.00000 0.16235 0.08662 =
0.22152 -0.00080 0.14788 0.00267
AFIX 23
H0AA 2 0.379833 1.267764 0.871828 11.00000 -1.20000
H0AB 2 0.462929 1.256850 0.820304 11.00000 -1.20000
AFIX 0
C4S 1 0.538070 1.340141 0.955042 11.00000 0.18647 0.14146 =
0.10809 0.02076 0.09956 0.03939
AFIX 137
H4SA 2 0.518525 1.348663 1.009324 11.00000 -1.50000
H4SB 2 0.545330 1.395267 0.936521 11.00000 -1.50000
H4SC 2 0.605374 1.326405 0.967636 11.00000 -1.50000
AFIX 0
C2S 1 0.406447 1.095277 0.857311 11.00000 0.07695 0.11180 =

0.07389 -0.01411 0.01513 0.00740
C1S 1 0.430734 1.029191 0.909961 11.00000 0.22228 0.20408 =
0.21336 0.10079 0.05052 0.08740

AFIX 137

HISA 2 0.402319 1.036438 0.959318 11.00000 -1.50000

HISB 2 0.507387 1.041101 0.934487 11.00000 -1.50000

HISC 2 0.398097 0.967586 0.869898 11.00000 -1.50000

AFIX 0

HKLF 4

REM 17SEPAM OLEX2: imported from CIF

REM R1 = 0.0814 for 8925 Fo > 4sig(Fo) and 0.1320 for all 14286 data

REM 808 parameters refined using 820 restraints

END

WGHT 0.1362 8.0422

REM Highest difference peak 1.733, deepest hole -1.335, 1-sigma level 0.202

Q1 1 0.2474 0.4806 0.5552 11.00000 0.05 1.46
Q2 1 0.3214 0.6205 0.6643 11.00000 0.05 1.42
Q3 1 0.2837 0.9784 0.7205 11.00000 0.05 1.34
Q4 1 0.0986 0.8177 0.4773 11.00000 0.05 1.04
Q5 1 0.1444 0.9601 0.5715 11.00000 0.05 1.03
Q6 1 0.3259 0.5173 0.5581 11.00000 0.05 1.01
Q7 1 0.1774 0.9788 0.5549 11.00000 0.05 0.99
Q8 1 -0.0222 0.2972 0.2408 11.00000 0.05 0.99
Q9 1 0.2354 0.5750 0.3592 11.00000 0.05 0.97
Q10 1 0.4053 0.5428 0.7031 11.00000 0.05 0.97
Q11 1 0.2633 0.7037 0.4022 11.00000 0.05 0.96
Q12 1 0.2909 0.5661 0.5560 11.00000 0.05 0.94
Q13 1 0.2979 0.4363 0.0403 11.00000 0.05 0.89
Q14 1 0.2380 0.6609 0.4578 11.00000 0.05 0.88
Q15 1 0.0818 0.3451 0.3410 11.00000 0.05 0.87
Q16 1 0.3688 0.5624 0.5849 11.00000 0.05 0.86
Q17 1 0.1791 0.6398 0.3768 11.00000 0.05 0.86
Q18 1 0.3203 1.0206 0.2598 11.00000 0.05 0.86
Q19 1 0.3521 0.6269 0.4608 11.00000 0.05 0.84
Q20 1 0.3794 1.0045 0.3234 11.00000 0.05 0.83

;

_shelx_res_checksum 8065

_shelx_hkl_file

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-2 0 0 1250.41 38.04 2
-3 0 0 22.20 3.20 2
-4 0 0 940.57 32.09 2
-5 0 0 1346.69 45.34 2
5 0 0 1373.44 39.56 1
-6 0 0 472.85 21.00 2
-7 0 0 1402.83 49.10 2
-8 0 0 213.94 14.33 2
-9 0 0 29.99 7.26 2
-10 0 0 173.35 14.13 2
-11 0 0 107.99 13.31 2
-12 0 0 486.82 28.14 2
-13 0 0 552.64 31.59 2
-14 0 0 5.67 6.69 2
-15 0 0 10.60 7.12 2
-16 0 0 1.68 6.60 3
-16 1 0 -0.82 6.36 3
-15 1 0 6.06 6.55 2
-14 1 0 210.35 18.93 2
-13 1 0 73.84 13.05 2
-12 1 0 5.07 4.62 2
-11 1 0 101.71 13.03 2
-10 1 0 127.69 13.29 2
-9 1 0 1425.97 52.73 2
-8 1 0 112.23 10.20 2
-7 1 0 89.91 9.12 2
-6 1 0 1212.20 42.35 2
-5 1 0 95.21 7.48 2
-4 1 0 1461.49 46.72 2
-3 1 0 19.20 2.98 2
-2 1 0 4411.42 126.18 2
2 1 0 369.26 12.27 1
3 1 0 228.05 8.85 1
-3 -1 0 233.62 10.83 2
4 1 0 139.58 6.63 1
-4 -1 0 144.72 9.03 2
5 1 0 215.22 9.24 1
-5 -1 0 218.05 12.24 2
-6 -1 0 2.54 2.13 1
-6 -1 0 2.12 1.69 4
-6 -1 0 3.06 2.68 2
-7 -1 0 428.90 16.11 1
-7 -1 0 439.23 15.85 4
-7 -1 0 433.54 21.23 2
-8 -1 0 2.73 3.33 2

-9 -1 0 114.40 12.39 2
-10 -1 0 28.70 6.90 2
-11 -1 0 149.68 15.77 2
-12 -1 0 250.07 19.19 2
-13 -1 0 -1.03 4.32 2
-14 -1 0 94.61 15.88 2
-16 2 0 -0.86 6.66 3
-15 2 0 128.66 18.06 2
-15 2 0 102.50 17.19 3
-14 2 0 294.47 22.90 2
-13 2 0 17.86 6.91 2
-12 2 0 97.95 13.20 2
-11 2 0 9.15 4.14 2
-10 2 0 3.97 3.70 2
-9 2 0 33.55 7.04 2
-8 2 0 200.77 13.64 2
-7 2 0 686.48 28.32 2
-6 2 0 4.98 2.87 2
-5 2 0 470.83 19.83 2
-4 2 0 272.50 12.95 2
-3 2 0 1506.93 46.88 2
2 -2 0 5257.66 147.44 1
-2 2 0 5394.49 152.13 2
1 -2 0 729.92 21.72 4
-1 2 0 713.79 22.77 2
1 -2 0 697.53 21.78 1
0 2 0 39.17 3.19 2
1 2 0 202.57 8.39 1
3 2 0 266.56 10.95 1
4 2 0 747.33 24.89 1
-4 -2 0 738.82 27.99 2
-5 -2 0 171.06 11.18 2
-6 -2 0 703.17 24.28 4
-6 -2 0 718.05 29.73 2
-6 -2 0 706.57 24.60 1
-7 -2 0 129.84 7.89 4
-7 -2 0 131.45 11.04 2
-7 -2 0 142.81 8.75 1
-8 -2 0 6.42 4.04 2
-9 -2 0 313.86 19.76 2
-10 -2 0 482.52 26.70 2
-11 -2 0 28.97 7.71 2
-12 -2 0 16.89 7.38 2
-13 -2 0 25.16 8.42 2
-14 -2 0 27.61 9.23 2
-17 3 0 -1.93 5.69 3

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-15	3	0	4.09	6.94	3
-14	3	0	40.02	10.06	2
-14	3	0	48.85	12.60	3
-13	3	0	0.04	4.05	2
-13	3	0	3.00	5.72	3
-12	3	0	2.63	4.84	2
-11	3	0	106.30	13.26	2
-10	3	0	636.92	30.71	2
-9	3	0	539.65	26.56	2
-8	3	0	493.92	24.13	2
-7	3	0	762.15	31.17	2
-6	3	0	501.72	22.08	2
5	-3	0	11.52	1.86	1
-5	3	0	5.71	2.81	2
-4	3	0	488.50	18.59	3
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-4	3	0	453.39	19.20	2
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-2	3	0	435.93	15.96	2
1	-3	0	2188.91	62.87	1
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-1	3	0	2158.30	64.72	2
0	-3	0	344.37	12.66	4
0	-3	0	308.69	12.48	1
0	3	0	316.68	13.18	2
1	3	0	63.04	4.95	1
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-7	-3	0	26.66	4.23	4
-8	-3	0	3.28	3.90	2
-9	-3	0	27.76	7.28	2
-10	-3	0	-0.07	3.74	2
-11	-3	0	123.11	15.67	2
-12	-3	0	182.81	19.33	2
-13	-3	0	172.39	20.24	2

-14 -3 0 38.33 10.70 2
-17 4 0 -0.24 5.88 3
-16 4 0 7.60 7.20 3
-15 4 0 0.20 6.74 3
-15 4 0 11.26 7.08 2
-14 4 0 -4.71 5.12 3
-14 4 0 -1.62 4.38 2
-13 4 0 100.15 13.79 2
-13 4 0 114.50 15.58 3
-12 4 0 50.48 10.86 3
-12 4 0 74.34 11.56 2
-11 4 0 44.48 9.55 3
-11 4 0 40.50 8.76 2
-10 4 0 497.55 26.07 2
-9 4 0 81.59 10.37 2
-8 4 0 0.19 2.80 2
-7 4 0 5.38 3.16 3
-7 4 0 6.13 3.12 2
-6 4 0 30.41 5.12 3
-6 4 0 34.00 6.01 2
6 -4 0 39.53 3.40 1
-5 4 0 167.26 10.66 2
5 -4 0 156.68 7.31 1
-5 4 0 156.14 9.41 3
4 -4 0 9.48 2.18 1
-4 4 0 5.09 2.56 2
3 -4 0 -1.08 0.68 1
-3 4 0 0.01 1.24 3
-3 4 0 2.57 2.04 2
2 -4 0 343.19 13.21 4
-2 4 0 274.25 13.38 2
2 -4 0 326.47 13.01 1
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1 -4 0 16.81 3.07 1
1 -4 0 17.16 3.12 4
-1 4 0 16.13 3.50 2
0 -4 0 2843.09 82.36 4
0 -4 0 2804.44 82.92 1
0 4 0 2879.90 85.46 2
-1 -4 0 1671.19 50.76 1
-1 -4 0 1618.80 50.12 4
-4 -4 0 652.86 24.20 4
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-5 -4 0 105.28 8.43 1
-5 -4 0 98.70 7.72 4
-6 -4 0 203.21 12.20 1

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-9	-4	0	26.38	7.14	2
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-11	5	0	455.24	26.01	3
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-4	-5	0	1.76	2.30	4
-5	-5	0	312.23	15.51	4
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-7	-5	0	1.28	3.40	1
-7	-5	0	2.24	3.37	2
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5	-6	0	11.03	2.83	1
-4	6	0	4.72	2.35	3
-4	6	0	5.38	2.95	2
4	-6	0	2.40	1.92	1
3	-6	0	79.38	6.93	1
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0	-6	0	849.35	30.29	4
-1	-6	0	208.94	12.10	4
-1	-6	0	216.63	12.62	1
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-2	-6	0	6.03	2.55	4
-3	-6	0	26.14	4.95	4
-3	-6	0	26.68	5.22	1
-4	-6	0	603.50	24.93	4
-4	-6	0	601.60	25.47	1
-5	-6	0	44.22	6.55	4
-5	-6	0	37.92	6.64	1
-6	-6	0	959.74	37.35	1
-6	-6	0	1039.09	37.91	4
-7	-6	0	281.38	16.66	4
-7	-6	0	285.83	17.35	1
-7	-6	0	276.31	19.79	2
-8	-6	0	19.02	6.74	2
-9	-6	0	6.59	5.21	2
-10	-6	0	3.73	5.04	2

-11	-6	0	6.56	6.19	2
-12	-6	0	3.07	6.31	2
-13	-6	0	18.70	9.13	2
-17	7	0	61.75	15.16	3
-16	7	0	-1.75	6.72	3
-16	7	0	0.95	5.70	2
-15	7	0	126.79	18.29	3
-15	7	0	178.05	20.52	2
-14	7	0	3.38	4.92	2
-14	7	0	-2.95	6.29	3
-13	7	0	38.13	10.12	3
-13	7	0	45.09	10.66	2
-12	7	0	207.97	17.96	2
-12	7	0	198.84	17.67	3
-11	7	0	691.40	34.75	2
-11	7	0	717.90	34.41	3
-10	7	0	28.48	7.08	3
-10	7	0	33.47	7.76	2
-9	7	0	0.47	3.79	3
-9	7	0	-4.16	3.10	2
-8	7	0	491.42	23.12	3
8	-7	0	487.58	18.97	1
-8	7	0	480.13	24.88	2
-7	7	0	30.51	6.75	2
7	-7	0	42.18	5.11	1
6	-7	0	59.48	5.93	1
-6	7	0	65.55	8.87	2
-6	7	0	67.04	6.95	3
5	-7	0	-2.25	1.17	1
-5	7	0	-0.86	2.22	2
-5	7	0	3.06	2.41	3
-4	7	0	383.72	19.10	2
4	-7	0	375.57	17.04	1
-4	7	0	389.06	15.92	3
-3	7	0	47.10	7.09	2
-3	7	0	51.01	5.04	3
3	-7	0	47.05	6.34	1
3	-7	0	38.68	6.01	4
2	-7	0	3949.55	116.02	1
-2	7	0	3876.70	119.47	2
2	-7	0	3969.08	115.42	4
1	-7	0	818.89	30.38	1
1	-7	0	779.04	29.91	4
-1	7	0	790.17	31.54	2
0	-7	0	55.12	6.91	4
0	-7	0	47.23	6.73	1

-1	-7	0	139.37	10.12	4
-1	-7	0	156.21	11.21	1
-2	-7	0	0.88	2.79	1
-2	-7	0	2.22	2.46	4
-3	-7	0	3.90	3.67	1
-3	-7	0	2.44	2.58	4
-4	-7	0	28.36	5.74	4
-4	-7	0	23.71	5.77	1
-5	-7	0	295.11	17.00	4
-5	-7	0	282.98	17.12	1
-6	-7	0	9.25	4.88	4
-6	-7	0	9.98	5.62	1
-7	-7	0	428.34	23.46	1
-7	-7	0	479.90	23.54	4
-8	-7	0	54.43	11.34	2
-9	-7	0	24.28	8.03	2
-10	-7	0	13.72	7.44	2
-11	-7	0	75.00	15.14	2
-12	-7	0	67.69	15.01	2
-13	-7	0	-3.29	7.08	2
-17	8	0	62.90	15.23	3
-16	8	0	2.11	7.87	3
-16	8	0	17.18	8.45	2
-15	8	0	4.25	7.41	3
-15	8	0	-5.16	4.98	2
-14	8	0	142.27	18.26	2
-14	8	0	181.45	19.42	3
-13	8	0	281.94	22.03	2
-13	8	0	279.44	21.69	3
-12	8	0	18.14	6.58	2
-12	8	0	18.81	7.97	3
-11	8	0	177.11	15.77	2
-11	8	0	158.56	15.55	3
-10	8	0	13.70	5.93	2
-10	8	0	15.90	5.88	3
-9	8	0	7.77	4.37	3
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-8	8	0	654.93	29.62	3
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-7	8	0	4.77	3.31	3
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7	-8	0	9.44	3.38	1
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6	-8	0	143.87	9.61	1

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3	-8	0	72.27	8.02	4
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2	-8	0	93.81	9.52	4
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-1	-8	0	92.21	9.93	1
-2	-8	0	160.73	12.01	4
-2	-8	0	149.64	12.30	1
-3	-8	0	24.24	6.69	1
-3	-8	0	23.77	5.96	4
-4	-8	0	3.28	3.75	4
-4	-8	0	14.43	5.52	1
-5	-8	0	127.05	12.86	1
-5	-8	0	119.68	12.26	4
-6	-8	0	111.22	12.32	4
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-7	-8	0	3.85	5.08	1
-7	-8	0	8.95	4.38	4
-8	-8	0	18.72	7.80	2
-9	-8	0	101.25	16.92	2
-10	-8	0	9.20	7.29	2
-11	-8	0	11.79	8.49	2
-12	-8	0	16.38	10.17	2
-13	-8	0	7.42	10.09	2
-17	9	0	141.48	20.48	3
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-15	9	0	13.30	7.21	2
-15	9	0	20.87	10.02	3
-14	9	0	70.44	13.73	2
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-12	9	0	257.17	20.25	3
-11	9	0	2.22	4.18	2
-11	9	0	0.78	4.43	3
-10	9	0	774.26	37.33	2
-9	9	0	297.56	20.48	2
-9	9	0	305.36	18.11	3
8	-9	0	106.30	8.41	1
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7	-9	0	119.06	8.94	1
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-5	9	0	143.62	12.49	2
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0	-9	0	6.94	4.54	1
-1	-9	0	384.27	20.69	1
-1	-9	0	364.52	20.15	4
-2	-9	0	41.13	7.98	4
-2	-9	0	52.57	8.93	1
-3	-9	0	299.99	18.81	4
-3	-9	0	364.19	20.48	1
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-8	-9	0	129.29	19.18	2

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-10	-9	0	109.88	20.35	2
-11	-9	0	32.18	11.84	2
-12	-9	0	0.31	8.72	2
-16	10	0	111.73	18.31	2
-15	10	0	106.58	17.15	2
-14	10	0	13.01	7.64	2
-13	10	0	26.95	9.82	3
-13	10	0	39.59	10.78	2
-12	10	0	45.19	10.39	3
-12	10	0	43.36	10.15	2
-11	10	0	73.51	12.48	2
-10	10	0	19.92	7.04	2
-10	10	0	24.52	7.04	3
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-9	10	0	3.45	4.42	3
-8	10	0	53.75	10.14	2
8	-10	0	49.82	6.89	1
-8	10	0	46.79	7.41	3
-7	10	0	22.63	6.73	2
-7	10	0	14.54	4.98	3
7	-10	0	9.21	3.90	1
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-6	10	0	5.56	3.33	3
-6	10	0	0.61	3.94	2
-5	10	0	33.31	5.69	3
-5	10	0	32.21	7.66	2
5	-10	0	40.95	7.23	1
-4	10	0	424.32	23.77	2
4	-10	0	465.16	22.38	1
3	-10	0	1187.79	44.98	1
3	-10	0	1256.22	45.52	4
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1	-10	0	103.40	11.70	1
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0	-10	0	97.31	11.41	4
-1	-10	0	132.91	13.57	1
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-2	-10	0	174.84	14.80	1
-2	-10	0	159.10	13.54	4
-3	-10	0	-7.32	2.52	4
-3	-10	0	2.25	4.37	1

-4	-10	0	108.32	13.30	1
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-5	-10	0	20.87	6.57	4
-5	-10	0	24.19	8.02	1
-6	-10	0	3.66	5.57	1
-7	-10	0	37.85	10.18	1
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-10	-10	0	16.31	10.26	2
-11	-10	0	10.94	11.48	2
-16	11	0	22.49	10.31	2
-15	11	0	-3.20	6.05	2
-14	11	0	35.47	11.32	2
-13	11	0	292.59	23.96	2
-12	11	0	353.26	25.49	2
-11	11	0	-3.56	3.53	2
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-9	11	0	64.09	11.50	2
8	-11	0	288.92	16.48	1
-8	11	0	299.14	20.65	2
7	-11	0	151.73	11.84	1
-7	11	0	148.05	15.33	2
-6	11	0	121.18	13.78	2
6	-11	0	110.49	11.03	1
5	-11	0	109.19	11.23	1
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4	-11	0	1072.10	41.75	1
-4	11	0	1074.39	44.72	2
-3	11	0	315.84	20.93	2
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2	-11	0	33.32	8.03	4
-2	11	0	49.42	9.72	2
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-1	-11	0	3.72	4.11	4
-1	-11	0	2.53	5.29	1
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-3	-11	0	-2.11	5.02	1
-3	-11	0	6.08	4.64	4
-4	-11	0	84.39	12.81	1
-4	-11	0	102.55	13.35	4
-5	-11	0	74.38	11.95	1
-6	-11	0	94.34	14.35	1

-7	-11	0	13.19	8.21	1
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-10	-11	0	3.91	9.64	2
-11	-11	0	30.34	17.54	2
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-12	12	0	-0.11	4.57	2
-11	12	0	107.16	15.79	2
-10	12	0	9.59	5.80	2
-9	12	0	52.20	10.78	2
-8	12	0	53.52	11.09	2
7	-12	0	9.36	4.73	1
-7	12	0	1.64	4.82	2
6	-12	0	642.84	29.11	1
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5	-12	0	214.88	15.58	1
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4	-12	0	18.78	6.43	1
3	-12	0	1.84	4.54	1
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2	-12	0	81.79	11.98	1
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1	-12	0	56.17	10.46	4
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-2	-12	0	132.62	15.13	4
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-5	-12	0	14.30	7.84	1
-6	-12	0	217.32	19.12	1
-7	-12	0	530.44	31.95	1
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-16	13	0	6.68	7.97	2
-15	13	0	132.43	20.35	2
-14	13	0	28.78	9.93	2
-13	13	0	6.20	6.89	2
-12	13	0	260.90	22.33	2
-11	13	0	126.51	17.10	2

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-9	13	0	115.61	15.64	2
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8	-13	0	6.28	5.12	1
7	-13	0	16.16	6.71	1
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6	-13	0	135.79	14.11	1
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-7	-13	0	22.36	10.02	1
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8	-14	0	286.39	19.78	1
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7	-14	0	5.95	6.42	1
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6	-14	0	39.70	9.74	1
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-3	-14	0	-5.40	5.87	1
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6	-15	0	5.50	6.65	1
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3	-15	0	23.96	8.70	1
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-5	-15	0	18.73	9.68	1
-6	-15	0	35.47	12.03	1
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8	-16	0	9.58	8.24	1
7	-16	0	1.27	6.93	1
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-12	17	0	8.78	8.20	2
-11	17	0	-2.34	7.43	2
-10	17	0	1.54	7.07	2
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6	-17	0	24.20	9.98	1
5	-17	0	24.07	10.09	1
-5	17	0	13.80	9.36	2
4	-17	0	166.34	19.78	1
3	-17	0	38.66	11.59	1
2	-17	0	4.66	8.08	1
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-7	11	4	18.81	7.75	3
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9	6	-12	224.83	19.54	1
8	6	-12	58.42	11.47	1
-8	-6	12	62.32	10.96	3
-7	-6	12	104.40	12.91	3
7	6	-12	106.75	14.50	1
-6	-6	12	315.39	20.91	3
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5	6	-12	832.95	38.21	1
-5	-6	12	776.09	36.17	3
4	6	-12	31.65	7.59	1
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-11	6	-12	-5.71	3.92	2
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9	7-19	3.43	7.07	1
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7	7-19	5.66	8.57	1
6	7-19	-13.43	6.69	1
5	7-19	-6.85	6.23	1
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11	6-19	12.06	7.40	1
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7	6-19	-4.00	7.18	1
6	6-19	21.38	9.86	1
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4	6-19	-0.39	7.31	1
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10	5-19	0.08	6.52	1
9	5-19	-3.08	7.49	1
8	5-19	-1.15	7.52	1
7	5-19	11.61	8.83	1
6	5-19	111.74	18.82	1
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4	5-19	9.49	8.18	1
3	5-19	94.22	16.72	1
2	5-19	9.60	7.11	1
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