

```

data_gazeevite_DE
#=====

# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common ?
_chemical_formula_moiety ?
_chemical_formula_structural ?
_chemical_formula_analytical ?
_chemical_formula_iupac ?
_chemical_formula_sum 'Ba0.917 Ca6 K0.083 O17 S2 Si2'
_chemical_formula_weight 761.9
_chemical_melting_point ?
_chemical_compound_source 'carbonate-silicate xenolith
from the Bellerberg volcano'
_chemical_absolute_configuration .

#=====

# 6. CRYSTAL DATA

_symmetry_cell_setting trigonal
_symmetry_space_group_name_H-M 'R -3 m'
_symmetry_space_group_name_Hall '-R 3;-2'
_symmetry_Int_Tables_number 166

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1 x,y,z
2 -y,x-y,z
3 -x+y,-x,z
4 y,x,-z
5 x-y,-y,-z
6 -x,-x+y,-z
7 -x,-y,-z
8 y,-x+y,-z
9 x-y,x,-z
10 -y,-x,z
11 -x+y,y,z
12 x,x-y,z
13 x+2/3,y+1/3,z+1/3
14 -y+2/3,x-y+1/3,z+1/3
15 -x+y+2/3,-x+1/3,z+1/3
16 y+2/3,x+1/3,-z+1/3
17 x-y+2/3,-y+1/3,-z+1/3
18 -x+2/3,-x+y+1/3,-z+1/3
19 -x+2/3,-y+1/3,-z+1/3
20 y+2/3,-x+y+1/3,-z+1/3
21 x-y+2/3,x+1/3,-z+1/3
22 -y+2/3,-x+1/3,z+1/3
23 -x+y+2/3,y+1/3,z+1/3
24 x+2/3,x-y+1/3,z+1/3
25 x+1/3,y+2/3,z+2/3
26 -y+1/3,x-y+2/3,z+2/3

```

```

27  -x+y+1/3,-x+2/3,z+2/3
28  y+1/3,x+2/3,-z+2/3
29  x-y+1/3,-y+2/3,-z+2/3
30  -x+1/3,-x+y+2/3,-z+2/3
31  -x+1/3,-y+2/3,-z+2/3
32  y+1/3,-x+y+2/3,-z+2/3
33  x-y+1/3,x+2/3,-z+2/3
34  -y+1/3,-x+2/3,z+2/3
35  -x+y+1/3,y+2/3,z+2/3
36  x+1/3,x-y+2/3,z+2/3

```

```

_cell_length_a      7.14040(10)
_cell_length_b      7.14040(10)
_cell_length_c      25.1675(5)
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    120
_cell_volume         1111.26(3)
_cell_formula_units_Z 3

```

```

_cell_measurement_reflns_used 4377
_cell_measurement_theta_min 2.42
_cell_measurement_theta_max 34.5
_cell_measurement_temperature 293
_cell_special_details
; ?
;

```

```

_exptl_crystal_density_diffn 3.4157
_exptl_crystal_density_meas ?
_exptl_crystal_density_method ?
_exptl_crystal_F_000 1107

```

```

_exptl_absorpt_coefficient_mu 5.001
_exptl_crystal_description fragment
_exptl_crystal_size_max ?
_exptl_crystal_size_mid ?
_exptl_crystal_size_min ?
_exptl_crystal_size_rad ?
_exptl_crystal_colour ?
_exptl_absorpt_correction_type 'none'
_exptl_absorpt_process_details ?
_exptl_absorpt_correction_T_min ?
_exptl_absorpt_correction_T_max ?

```

```

#=====

```

7. EXPERIMENTAL DATA

```

_exptl_special_details ?

_diffn_ambient_temperature 293
_diffn_source 'synchrotron'
_diffn_source_power ?
_diffn_source_voltage ?
_diffn_source_current ?
_diffn_radiation_type 'X-ray'
_diffn_radiation_source ?

```

```

_diffrn_radiation_wavelength      0.70848
_diffrn_radiation_monochromator    'synchrotron'
_diffrn_measurement_device        'four-circle diffractometer'
_diffrn_measurement_device_type
;
'dectris-CrysAlisPro-abstract goniometer imported dectris images'
;
_diffrn_detector                  'CCD plate'
_diffrn_detector_area_resol_mean  5.8140
_diffrn_measurement_method        '\f scans'
_diffrn_measurement_specimen_support ?

_diffrn_reflns_number             6362
_diffrn_reflns_theta_min          2.42
_diffrn_reflns_theta_max          34.51
_diffrn_reflns_theta_full         33.69
_diffrn_measured_fraction_theta_max 0.95
_diffrn_measured_fraction_theta_full 0.98
_diffrn_reflns_av_R_equivalents   0.1246
_diffrn_reflns_av_unetI/netI      0.0241
_diffrn_reflns_limit_h_min        -10
_diffrn_reflns_limit_h_max        10
_diffrn_reflns_limit_k_min        -11
_diffrn_reflns_limit_k_max        11
_diffrn_reflns_limit_l_min        -39
_diffrn_reflns_limit_l_max        40
_diffrn_reflns_reduction_process  ?
_diffrn_radiation_probe           X-ray

```

#=====

8. REFINEMENT DATA

```

_refine_special_details
; ?
;

_reflns_number_total             608
_reflns_number_gt                539
_reflns_threshold_expression      'I>3\s(I) '

_refine_ls_structure_factor_coef  F
_refine_ls_R_factor_gt            0.0309
_refine_ls_wR_factor_gt           0.0360
_refine_ls_R_factor_all           0.0334
_refine_ls_wR_factor_ref           0.0364
_refine_ls_goodness_of_fit_ref     1.68
_refine_ls_goodness_of_fit_gt      1.78
_refine_ls_restrained_S_gt         ?
_refine_ls_restrained_S_all        ?
_refine_ls_number_reflns           608
_refine_ls_number_parameters       39
_refine_ls_number_restraints       0
_refine_ls_number_constraints      2
_refine_ls_weighting_scheme         sigma
_refine_ls_weighting_details        'w=1/(\s^2^(F)+0.0001F^2^)'
_refine_ls_hydrogen_treatment      ?
_refine_ls_shift/su_max             0.0000

```

```

_refine_ls_shift/su_mean      0.0000
_refine_diff_density_max      1.16
_refine_diff_density_min     -1.41
_refine_ls_extinction_method   'none'
_refine_ls_extinction_coef     ?
_refine_ls_extinction_expression ?
_refine_ls_abs_structure_details ?
_refine_ls_abs_structure_Flack ?
_refine_ls_abs_structure_Rogers ?

```

```

loop_
  _atom_type_symbol
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
Ba  -0.2823  2.2981
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
Ca   0.2282  0.3092
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
K    0.2016  0.2519
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
O    0.0113  0.0062
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
S    0.1258  0.1248
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
Si   0.0833  0.0715
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'

```

```

_computing_data_collection
'CrysAlisPro 1.171.40.53 (Rigaku OD, 2019)'
_computing_cell_refinement
'CrysAlisPro 1.171.40.53 (Rigaku OD, 2019)'
_computing_data_reduction
'CrysAlisPro 1.171.40.53 (Rigaku OD, 2019)'
_computing_structure_solution      ?
_computing_structure_refinement    ?
_computing_molecular_graphics      ?
_computing_publication_material    ?

```

```

#=====

```

``` # 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS ```

```

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_site_symmetry_multiplicity
  _atom_site_occupancy
  _atom_site_calc_flag
  _atom_site_refinement_flags
  _atom_site_disorder_assembly
  _atom_site_disorder_group
Ba1 Ba 0.333333 0.666667 0.166667 Uani 0.01746(16) 3 0.917(5) d . . .

```

```

K1 K 0.333333 0.666667 0.166667 Uani 0.01746(16) 3 0.083(5) d . . .
Ca1 Ca 0.84283(5) 0.68566(11) 0.05907(3) Uani 0.0147(2) 18 1 d . . .
T1 Si 0.333333 0.666667 0.03414(6) Uani 0.0071(3) 6 1 d . . .
T2 S 0.666667 0.333333 0.15503(5) Uani 0.0115(3) 6 1 d . . .
O1 O 0.333333 0.666667 0.96922(16) Uani 0.0171(10) 6 1 d . . .
O2 O 0.2085(2) 0.7915(2) 0.05328(13) Uani 0.0259(9) 18 1 d . . .
O3 O 0.5870(11) 0.1120(5) 0.13495(13) Uani 0.022(2) 36 0.5 d . . .
O4 O 0.666667 0.333333 0.21458(15) Uani 0.0160(10) 6 1 d . . .
O5 O 0 0 0 Uani 0.0114(12) 3 1 d . . .

```

loop_

```

_atom_site_aniso_label
_atom_site_aniso_type_symbol
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23

```

```

Ba1 Ba 0.0201(2) 0.0201(2) 0.0122(2) 0.01004(10) 0 0
K1 K 0.0201(2) 0.0201(2) 0.0122(2) 0.01004(10) 0 0
Ca1 Ca 0.0115(3) 0.0122(3) 0.0205(4) 0.00609(16) -0.00022(12) -0.0004(2)
T1 Si 0.0069(4) 0.0069(4) 0.0076(6) 0.00343(19) 0 0
T2 S 0.0135(4) 0.0135(4) 0.0076(5) 0.00675(19) 0 0
O1 O 0.0208(13) 0.0208(13) 0.0099(17) 0.0104(6) 0 0
O2 O 0.0146(9) 0.0146(9) 0.0493(18) 0.0080(10) 0.0074(6) -0.0074(6)
O3 O 0.033(5) 0.0133(13) 0.0149(12) 0.0095(16) 0.0040(15) -0.0002(10)
O4 O 0.0211(13) 0.0211(13) 0.0056(16) 0.0106(6) 0 0
O5 O 0.0133(15) 0.0133(15) 0.008(2) 0.0066(8) 0 0

```

#=====

10. MOLECULAR GEOMETRY

loop_

```

_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_distance
_geom_bond_publ_flag
Ba1 K1 . . 0 ?
Ba1 O2 . . 3.245(3) ?
Ba1 O2 . 2_665 3.245(3) ?
Ba1 O2 . 3_565 3.245(3) ?
Ba1 O2 . 16_455 3.245(3) ?
Ba1 O2 . 17_565 3.245(3) ?
Ba1 O2 . 18_555 3.245(3) ?
Ba1 O3 . 1_565 2.876(3) ?
Ba1 O3 . 2_555 2.876(3) ?
Ba1 O3 . 3_665 2.876(10) ?
Ba1 O3 . 16_555 2.876(3) ?
Ba1 O3 . 17_455 2.876(3) ?
Ba1 O3 . 18_565 2.876(10) ?
Ba1 O3 . 19_555 2.876(3) ?
Ba1 O3 . 20_565 2.876(3) ?

```

Ba1 O3 . 21_455 2.876(10) ?
 Ba1 O3 . 10_565 2.876(3) ?
 Ba1 O3 . 11_665 2.876(3) ?
 Ba1 O3 . 12_555 2.876(10) ?
 K1 O2 . . 3.245(3) ?
 K1 O2 . 2_665 3.245(3) ?
 K1 O2 . 3_565 3.245(3) ?
 K1 O2 . 16_455 3.245(3) ?
 K1 O2 . 17_565 3.245(3) ?
 K1 O2 . 18_555 3.245(3) ?
 K1 O3 . 1_565 2.876(3) ?
 K1 O3 . 2_555 2.876(3) ?
 K1 O3 . 3_665 2.876(10) ?
 K1 O3 . 16_555 2.876(3) ?
 K1 O3 . 17_455 2.876(3) ?
 K1 O3 . 18_565 2.876(10) ?
 K1 O3 . 19_555 2.876(3) ?
 K1 O3 . 20_565 2.876(3) ?
 K1 O3 . 21_455 2.876(10) ?
 K1 O3 . 10_565 2.876(3) ?
 K1 O3 . 11_665 2.876(3) ?
 K1 O3 . 12_555 2.876(10) ?
 Ca1 T1 . 4_555 3.2016(12) ?
 Ca1 T2 . . 3.2526(12) ?
 Ca1 O1 . 4_556 2.2921(14) ?
 Ca1 O2 . 1_655 2.3312(15) ?
 Ca1 O2 . 3_565 2.331(2) ?
 Ca1 O2 . 6_655 2.898(3) ?
 Ca1 O3 . 2_655 2.549(6) ?
 Ca1 O3 . 3_665 2.858(5) ?
 Ca1 O3 . 10_665 2.858(7) ?
 Ca1 O3 . 12_555 2.549(5) ?
 Ca1 O4 . 16_555 2.456(2) ?
 Ca1 O5 . 1_665 2.4472(7) ?
 T1 O1 . 1_554 1.634(4) ?
 T1 O2 . . 1.618(2) ?
 T1 O2 . 2_665 1.618(2) ?
 T1 O2 . 3_565 1.618(2) ?
 T2 O1 . 4_556 3.127(4) ?
 T2 O3 . . 1.476(4) ?
 T2 O3 . 2_655 1.476(3) ?
 T2 O3 . 3_665 1.476(10) ?
 T2 O3 . 10_665 1.476(4) ?
 T2 O3 . 11_655 1.476(3) ?
 T2 O3 . 12_555 1.476(10) ?
 T2 O4 . . 1.499(4) ?
 O1 O2 . 1_556 2.619(4) ?
 O1 O2 . 2_666 2.619(4) ?
 O1 O2 . 3_566 2.619(4) ?
 O1 O3 . 4_556 2.966(5) ?
 O1 O3 . 5_566 2.966(5) ?
 O1 O3 . 6_666 2.966(7) ?
 O1 O3 . 7_666 2.966(5) ?
 O1 O3 . 8_566 2.966(5) ?
 O1 O3 . 9_556 2.966(7) ?
 O2 O2 . 2_665 2.675(3) ?
 O2 O2 . 3_565 2.675(3) ?
 O2 O3 . 1_565 3.253(5) ?

```

02 03 . 2_555 3.065(5) ?
02 03 . 10_565 3.253(5) ?
02 03 . 11_665 3.065(5) ?
02 04 . 16_455 3.060(3) ?
02 05 . 1_565 2.906(2) ?
03 03 . 2_655 2.402(7) ?
03 03 . 3_665 2.402(12) ?
03 03 . 16_545 2.858(9) ?
03 03 . 20_555 3.191(10) ?
03 03 . 21_445 3.191(10) ?
03 03 . 10_665 2.150(6) ?
03 03 . 11_655 0.442(12) ?
03 03 . 12_555 2.592(11) ?
03 04 . . 2.437(5) ?
04 05 . 13_555 2.989(4) ?

```

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11. STRUCTURE-FACTOR LIST

```

loop_
  _refln_index_h
  _refln_index_k
  _refln_index_l
  _refln_F_squared_calc
  _refln_F_squared_meas
  _refln_F_squared_sigma
  _refln_observed_status
-1 2 0 67796.20 63805.40 419.04 o
 0 3 0 17265.60 16346.90 211.27 o
-2 4 0 224655.00 200466.00 1062.68 o
-1 5 0 26266.00 24850.70 253.62 o
-3 6 0 42219.30 40735.10 519.49 o
 0 6 0 58951.50 54648.40 548.99 o
-2 7 0 7953.27 7726.44 147.32 o
-4 8 0 39648.80 41470.00 585.97 o
-1 8 0 9902.90 9489.90 218.27 o
-3 9 0 3922.68 3899.69 152.21 o
 0 9 0 3366.90 3417.48 270.21 o
-5 10 0 7941.45 6422.68 510.50 o
-2 10 0 16221.30 20288.50 919.22 o
-1 1 1 1634.62 1593.39 55.14 o
 0 2 1 86313.90 81272.10 451.20 o
-2 3 1 2617.31 2628.87 63.53 o
-4 4 1 51419.00 48047.30 408.97 o
-1 4 1 393.82 395.03 26.91 o
-3 5 1 652.39 774.56 47.90 o
 0 5 1 1354.12 1356.24 78.13 o
-5 6 1 1238.52 1255.86 59.66 o
-2 6 1 32302.30 31554.20 279.62 o
-7 7 1 44.41 34.93 27.51 <
-4 7 1 1740.56 1747.77 70.52 o
-1 7 1 159.25 143.88 25.28 o
-6 8 1 9954.23 10221.30 194.68 o
-3 8 1 1075.28 1046.52 78.43 o
 0 8 1 9452.44 9051.67 368.55 o
-8 9 1 2285.54 2429.61 185.99 o

```

-5	9	1	263.40	461.39	48.26	o
-2	9	1	913.38	802.19	75.65	o
-7	10	1	1090.90	1091.16	119.63	o
-4	10	1	6208.44	6093.29	288.25	o
-1	10	1	76.20	147.08	58.70	<
-6	11	1	1465.43	1370.12	235.88	o
0	1	2	2686.28	3105.22	59.73	o
-2	2	2	1535.82	1360.59	50.56	o
-1	3	2	9325.83	9767.35	112.51	o
-3	4	2	658.30	659.99	35.65	o
0	4	2	11091.60	11274.20	228.76	o
-5	5	2	232.48	196.79	32.64	o
-2	5	2	5942.98	5743.81	114.62	o
-4	6	2	3996.79	4024.63	110.76	o
-1	6	2	387.20	571.67	39.15	o
-6	7	2	3860.35	3490.30	98.82	o
-3	7	2	308.46	307.37	34.81	o
0	7	2	5413.86	5195.54	186.41	o
-8	8	2	1252.27	1174.29	158.48	o
-5	8	2	118.14	176.46	31.67	o
-2	8	2	3858.25	4103.66	126.03	o
-7	9	2	1834.16	1867.53	140.62	o
-4	9	2	5187.25	5267.51	159.33	o
-1	9	2	221.52	362.94	79.57	o
-9	10	2	711.75	787.77	137.91	o
-6	10	2	937.71	909.27	117.04	o
-3	10	2	39.64	114.14	55.38	<
-5	11	2	790.11	774.98	182.31	o
0	0	3	1249.94	1077.22	52.18	o
-1	2	3	29122.30	25236.10	152.45	o
-3	3	3	133.59	293.92	30.65	o
0	3	3	68303.30	64813.10	443.29	o
-2	4	3	201.23	264.72	23.95	o
-4	5	3	22629.00	20811.10	211.57	o
-1	5	3	3004.00	3095.27	87.72	o
-6	6	3	1379.24	1190.22	80.72	o
-3	6	3	7266.15	6870.44	125.30	o
0	6	3	525.38	430.14	51.70	o
-5	7	3	515.13	503.08	39.27	o
-2	7	3	17846.20	17683.60	218.81	o
-7	8	3	2424.52	2574.15	202.40	o
-4	8	3	50.23	54.96	28.05	<
-1	8	3	762.29	934.85	67.51	o
-9	9	3	14.68	4.77	47.24	<
-6	9	3	4649.00	4460.32	163.07	o
-3	9	3	671.66	771.84	63.22	o
0	9	3	7268.40	7909.17	407.76	o
-8	10	3	444.72	563.23	106.36	o
-5	10	3	441.44	452.40	79.21	o
-2	10	3	8.38	5.43	56.77	<
-1	1	4	8605.34	8735.91	155.23	o
0	2	4	37958.90	36720.50	287.52	o
-2	3	4	26162.60	25080.50	180.14	o
-4	4	4	8524.15	8209.25	235.28	o
-1	4	4	2853.54	2780.54	70.40	o
-3	5	4	591.93	625.73	35.84	o
0	5	4	13813.80	13321.30	282.64	o
-5	6	4	3254.42	3112.58	100.27	o

-2	6	4	9109.74	9310.12	172.96	o
-7	7	4	202.35	212.60	74.87	<
-4	7	4	4551.16	4511.06	111.12	o
-1	7	4	1016.53	956.02	53.93	o
-6	8	4	3499.65	3036.99	127.71	o
-3	8	4	1396.90	1552.43	92.42	o
0	8	4	6888.35	6646.80	272.02	o
-8	9	4	911.29	1037.53	108.65	o
-5	9	4	237.13	261.83	36.74	o
-2	9	4	3040.59	3158.92	179.42	o
-7	10	4	550.66	585.12	89.53	o
-4	10	4	3111.13	3164.41	289.39	o
-1	10	4	63.12	11.64	40.36	<
0	1	5	3299.04	3723.77	99.24	o
-2	2	5	7676.77	6686.68	238.60	o
-1	3	5	39663.20	39277.10	243.12	o
-3	4	5	15469.10	15502.50	168.07	o
0	4	5	7110.20	6702.67	179.84	o
-5	5	5	11406.60	11231.00	299.29	o
-2	5	5	1061.87	1099.61	50.43	o
-4	6	5	13393.40	12951.90	166.69	o
-1	6	5	6693.22	6508.23	137.97	o
-6	7	5	2974.23	2883.82	134.96	o
-3	7	5	3681.61	3903.91	101.83	o
0	7	5	1862.04	1905.05	118.36	o
-8	8	5	5723.91	5928.47	343.93	o
-5	8	5	3387.58	3361.02	100.57	o
-2	8	5	3130.10	3259.06	122.53	o
-7	9	5	3015.46	3435.10	268.94	o
-4	9	5	1588.45	1732.57	88.08	o
-1	9	5	453.20	494.87	91.88	o
-9	10	5	72.75	103.22	43.80	<
-6	10	5	2781.57	2785.36	183.04	o
-3	10	5	506.83	599.30	107.08	o
0	0	6	5304.80	5195.00	226.11	o
-1	2	6	77360.30	79312.60	386.10	o
-3	3	6	72523.10	71696.10	649.98	o
0	3	6	35465.90	34457.00	338.20	o
-2	4	6	2002.66	1936.30	58.22	o
-4	5	6	15905.80	15800.30	244.75	o
-1	5	6	43059.00	41375.40	315.46	o
-6	6	6	1335.52	1217.61	107.02	o
-3	6	6	18121.50	17693.30	224.78	o
0	6	6	2229.14	2051.53	124.88	o
-5	7	6	35007.70	31796.30	368.06	o
-2	7	6	4488.78	4735.60	118.06	o
-7	8	6	3800.88	4053.71	201.20	o
-4	8	6	1136.41	1155.95	66.72	o
-1	8	6	9593.32	9933.85	242.76	o
-9	9	6	11196.50	13135.30	592.79	o
-6	9	6	3465.93	3331.15	211.57	o
-3	9	6	12489.10	13451.50	231.30	o
0	9	6	920.23	1028.42	156.01	o
-8	10	6	86.78	122.35	46.33	<
-5	10	6	3051.85	2821.92	214.59	o
-2	10	6	1240.64	1380.55	247.89	o
-1	1	7	47918.60	51997.30	376.27	o
0	2	7	122.34	61.53	18.82	o

-2	3	7	8780.26	8652.54	110.52	o
-4	4	7	9377.91	9336.97	423.02	o
-1	4	7	4535.23	4422.98	91.94	o
-3	5	7	26526.90	25481.00	246.86	o
0	5	7	3285.76	3243.74	138.27	o
-5	6	7	666.29	695.47	57.25	o
-2	6	7	10038.20	9071.34	157.34	o
-7	7	7	11112.70	11842.80	957.29	o
-4	7	7	1170.52	1333.14	60.09	o
-1	7	7	8211.44	8036.83	154.50	o
-6	8	7	4187.06	4100.88	200.83	o
-3	8	7	1363.06	1530.23	85.24	o
0	8	7	2680.59	2692.28	167.65	o
-8	9	7	384.74	420.01	90.67	o
-5	9	7	8891.53	8921.79	274.31	o
-2	9	7	93.61	95.32	32.88	<
-7	10	7	534.84	790.60	164.70	o
-4	10	7	1711.86	1743.13	220.92	o
-1	10	7	2563.64	2541.51	272.38	o
0	1	8	1939.36	2722.92	87.05	o
-2	2	8	99604.00	101883.00	524.43	o
-1	3	8	4792.50	5150.72	91.88	o
-3	4	8	8169.82	8869.84	174.59	o
0	4	8	30000.40	29407.80	354.79	o
-5	5	8	2296.58	2396.24	142.01	o
-2	5	8	881.91	1118.79	54.42	o
-4	6	8	19152.70	18027.80	271.72	o
-1	6	8	5101.72	5003.15	126.75	o
-6	7	8	196.34	293.50	60.09	o
-3	7	8	3584.81	3723.83	104.25	o
0	7	8	26.71	16.41	28.35	<
-8	8	8	9512.37	10635.80	530.41	o
-5	8	8	1739.59	1711.21	102.38	o
-2	8	8	7747.70	7826.28	176.88	o
-7	9	8	3103.46	3314.56	184.18	o
-4	9	8	88.79	92.54	30.77	o
-1	9	8	2030.32	2068.54	152.81	o
-9	10	8	15.95	59.24	59.91	<
-6	10	8	5808.50	6025.30	249.16	o
-3	10	8	880.50	892.50	142.50	o
0	0	9	232983.00	277085.00	1500.85	o
-1	2	9	3596.75	3286.81	69.02	o
-3	3	9	58.93	102.20	33.12	o
0	3	9	6584.27	6006.29	157.15	o
-2	4	9	91690.80	85383.50	404.92	o
-4	5	9	3154.83	2991.02	126.57	o
-1	5	9	3316.54	3086.46	93.69	o
-6	6	9	33890.80	32370.30	543.62	o
-3	6	9	6899.30	6637.33	127.65	o
0	6	9	24374.70	24338.80	431.95	o
-5	7	9	1551.06	1592.85	101.11	o
-2	7	9	271.46	270.03	34.99	o
-7	8	9	1825.42	1965.08	141.47	o
-4	8	9	19674.40	20111.10	294.64	o
-1	8	9	3803.22	4010.33	134.11	o
-9	9	9	587.78	750.18	185.69	o
-6	9	9	209.01	269.37	86.81	o
-3	9	9	1241.83	1369.76	96.10	o

0	9	9	128.62	147.62	84.76	<
-8	10	9	7028.28	7893.13	355.58	o
-5	10	9	2748.78	2898.42	201.56	o
-2	10	9	6685.61	7303.48	545.43	o
-1	1	10	23678.80	28334.40	284.39	o
0	2	10	112174.00	123088.00	710.49	o
-2	3	10	707.29	705.84	40.42	o
-4	4	10	48040.70	47253.80	601.66	o
-1	4	10	3237.58	3039.83	81.62	o
-3	5	10	4117.84	3850.64	88.20	o
0	5	10	859.09	749.22	67.45	o
-5	6	10	2990.96	2952.11	115.65	o
-2	6	10	40164.70	38978.00	338.62	o
-7	7	10	52.48	52.73	56.71	<
-4	7	10	2564.03	2458.86	98.64	o
-1	7	10	90.74	132.96	26.54	o
-6	8	10	9288.71	9840.71	392.44	o
-3	8	10	1138.41	1188.83	67.51	o
0	8	10	11308.90	11814.40	406.55	o
-8	9	10	1996.48	2085.25	148.05	o
-5	9	10	352.52	385.02	88.44	o
-2	9	10	795.59	724.54	89.53	o
-7	10	10	1340.97	1343.27	120.84	o
-4	10	10	6513.33	4823.44	455.30	o
-1	10	10	262.76	313.41	182.43	<
0	1	11	277.47	317.69	41.93	o
-2	2	11	7898.53	9049.08	170.79	o
-1	3	11	960.35	1210.85	55.92	o
-3	4	11	21.95	31.67	17.01	<
0	4	11	2110.97	2274.74	112.03	o
-5	5	11	2635.76	2669.53	153.23	o
-2	5	11	162.31	163.79	23.83	o
-4	6	11	1153.42	1286.56	76.50	o
-1	6	11	1031.71	1307.80	67.87	o
-6	7	11	37.13	39.03	52.24	<
-3	7	11	2011.07	2095.45	84.46	o
0	7	11	409.39	428.99	63.71	o
-8	8	11	763.77	702.71	179.78	o
-5	8	11	414.80	376.51	73.36	o
-2	8	11	1097.32	1204.58	77.46	o
-7	9	11	3087.83	3141.66	205.54	o
-4	9	11	508.26	402.15	63.22	o
-1	9	11	1787.42	2018.35	216.22	o
-6	10	11	278.60	331.20	75.59	o
-3	10	11	828.82	733.65	183.28	o
0	0	12	8085.18	9379.50	300.13	o
-1	2	12	8878.73	8935.42	128.32	o
-3	3	12	128.51	72.39	23.41	o
0	3	12	42739.40	42740.00	423.51	o
-2	4	12	111.32	234.62	27.15	o
-4	5	12	8751.27	8584.97	190.46	o
-1	5	12	318.14	298.63	31.85	o
-6	6	12	2227.33	2143.29	202.95	o
-3	6	12	510.08	551.40	40.24	o
0	6	12	11.31	10.92	24.92	<
-5	7	12	35.04	79.51	38.13	<
-2	7	12	9749.68	9793.29	197.70	o
-7	8	12	1237.03	1349.18	127.05	o

-4	8	12	386.50	354.55	45.67	o
-1	8	12	248.14	298.20	49.17	o
-9	9	12	458.68	558.46	114.56	o
-6	9	12	3149.53	3232.03	181.65	o
-3	9	12	207.68	225.63	56.47	o
0	9	12	3795.84	3224.13	537.71	o
-8	10	12	217.62	291.14	89.95	o
-5	10	12	195.93	257.18	74.87	o
-2	10	12	12.46	13.27	53.33	<
-1	1	13	24803.00	26865.30	341.40	o
0	2	13	503.69	521.72	46.75	o
-2	3	13	18624.30	18669.80	189.55	o
-4	4	13	1235.61	1116.50	135.62	o
-1	4	13	14140.20	13907.10	194.62	o
-3	5	13	5078.27	4808.35	104.67	o
0	5	13	18010.10	17276.80	307.98	o
-5	6	13	11959.70	11992.40	271.24	o
-2	6	13	608.74	662.34	46.75	o
-7	7	13	1087.48	1161.50	156.49	o
-4	7	13	12006.10	10661.40	249.46	o
-1	7	13	1973.27	1985.59	88.38	o
-6	8	13	316.95	235.46	56.35	o
-3	8	13	3574.84	3987.83	143.34	o
0	8	13	759.73	682.13	107.63	o
-8	9	13	2454.56	2879.29	199.69	o
-5	9	13	691.63	709.28	90.85	o
-2	9	13	8302.45	8853.86	329.94	o
-7	10	13	1632.22	1934.19	164.46	o
-4	10	13	252.78	170.43	74.69	<
0	1	14	13303.00	14740.60	235.10	o
-2	2	14	1841.17	1672.18	80.96	o
-1	3	14	10568.00	10904.20	163.91	o
-3	4	14	15587.60	15481.10	190.76	o
0	4	14	5584.99	5603.66	183.70	o
-5	5	14	6255.36	6343.89	239.14	o
-2	5	14	6024.47	6176.90	128.14	o
-4	6	14	4657.16	4339.30	141.23	o
-1	6	14	8631.84	8635.10	166.21	o
-6	7	14	3329.93	3393.29	182.55	o
-3	7	14	4943.94	5011.18	147.32	o
0	7	14	3216.92	3284.76	212.24	o
-8	8	14	1610.79	1539.34	207.59	o
-5	8	14	3749.47	3691.07	191.90	o
-2	8	14	2010.72	2075.18	124.10	o
-7	9	14	3474.32	3477.93	187.50	o
-4	9	14	2363.62	2328.43	157.28	o
-1	9	14	840.02	877.96	146.42	o
-6	10	14	1107.50	1085.43	110.58	o
-3	10	14	1057.24	1030.11	153.72	o
0	0	15	2141.22	2830.55	181.65	o
-1	2	15	43403.90	46652.60	326.44	o
-3	3	15	66829.20	67747.10	533.24	o
0	3	15	26706.00	26955.10	352.92	o
-2	4	15	1577.95	1505.50	65.40	o
-4	5	15	12477.00	12610.50	235.94	o
-1	5	15	27713.40	28616.60	305.14	o
-3	6	15	9732.88	9696.28	163.67	o
0	6	15	2450.88	2504.65	126.09	o

-5	7	15	23780.60	26334.50	817.63	o
-2	7	15	5813.71	5781.69	180.50	o
-7	8	15	4898.08	4657.17	301.46	o
-4	8	15	819.01	710.73	84.22	o
-1	8	15	7948.20	8248.22	241.25	o
-6	9	15	4779.00	5092.80	225.99	o
-3	9	15	9750.90	10450.00	329.45	o
-5	10	15	3434.35	3364.94	200.17	o
-2	10	15	345.88	441.00	121.20	o
-1	1	16	58186.00	66326.20	528.96	o
0	2	16	19342.20	20163.70	298.87	o
-2	3	16	20033.70	21684.20	247.10	o
-4	4	16	10677.60	10372.30	298.69	o
-1	4	16	29112.00	29501.70	290.90	o
-3	5	16	36349.80	35653.20	299.53	o
0	5	16	7918.41	7912.01	235.10	o
-5	6	16	9260.63	9334.79	296.45	o
-2	6	16	9652.69	9671.43	165.42	o
-7	7	16	17326.40	19637.00	714.77	o
-4	7	16	5587.45	5699.34	271.36	o
-1	7	16	12947.80	12952.20	268.76	o
-6	8	16	4669.76	4417.79	344.84	o
-3	8	16	5602.23	5787.48	199.57	o
0	8	16	4801.93	5275.36	305.32	o
-8	9	16	1349.62	1344.60	119.87	o
-5	9	16	12664.90	13404.00	587.84	o
-2	9	16	1077.82	1123.56	116.07	o
-7	10	16	1768.13	1899.62	204.27	o
-4	10	16	2775.55	2906.38	218.87	o
0	1	17	26.24	56.17	23.83	<
-2	2	17	6435.41	6789.12	174.05	o
-1	3	17	1667.87	1605.58	65.21	o
-3	4	17	74.25	110.34	20.51	o
0	4	17	1157.59	1115.23	87.36	o
-5	5	17	33.67	42.17	49.17	<
-2	5	17	408.69	377.54	35.77	o
-4	6	17	2779.58	2751.10	162.22	o
-1	6	17	137.70	147.56	30.04	o
-6	7	17	1661.72	1659.63	130.25	o
-3	7	17	431.63	423.08	55.92	o
0	7	17	2081.92	1891.54	203.43	o
-8	8	17	1668.47	1911.51	281.92	o
-5	8	17	218.65	282.16	64.67	o
-2	8	17	348.17	316.00	50.62	o
-7	9	17	722.99	780.77	106.90	o
-4	9	17	2568.47	2364.09	182.85	o
-1	9	17	252.37	299.95	132.48	<
-6	10	17	676.81	642.44	125.72	o
-3	10	17	6.34	63.47	77.04	<
0	0	18	42032.80	46216.70	789.64	o
-1	2	18	452.53	505.25	39.21	o
-3	3	18	1591.53	1551.53	98.03	o
0	3	18	10.92	3.14	25.28	<
-2	4	18	30520.30	30414.00	276.91	o
-4	5	18	51.74	61.72	31.55	<
-1	5	18	325.98	347.85	38.85	o
-6	6	18	9928.46	10639.90	524.01	o
-3	6	18	445.93	412.35	41.63	o

0	6	18	12295.20	11721.80	335.73	o
-5	7	18	57.29	100.69	44.40	<
-2	7	18	83.46	101.65	33.42	o
-7	8	18	274.56	242.58	61.05	o
-4	8	18	7662.25	7710.57	297.84	o
-1	8	18	572.94	585.79	76.62	o
-6	9	18	16.21	18.46	39.52	<
-3	9	18	80.15	99.66	46.15	<
-5	10	18	578.78	457.35	156.37	<
-1	1	19	319.77	381.21	45.55	o
0	2	19	51276.10	55921.10	687.56	o
-2	3	19	29.73	77.22	20.63	o
-4	4	19	19666.50	18223.20	339.77	o
-1	4	19	1475.02	1622.47	70.04	o
-3	5	19	98.87	93.21	22.02	o
0	5	19	44.10	33.12	26.12	<
-5	6	19	1256.42	1404.99	118.49	o
-2	6	19	14746.90	14269.10	284.15	o
-7	7	19	126.62	109.80	64.73	<
-4	7	19	241.85	255.43	62.62	o
-1	7	19	6.04	66.48	29.56	<
-6	8	19	5371.07	5516.07	233.23	o
-3	8	19	469.42	501.93	73.36	o
0	8	19	6679.61	6763.36	545.01	o
-5	9	19	245.03	182.25	75.77	<
-2	9	19	113.19	146.05	54.66	<
0	1	20	1483.47	1591.10	119.45	o
-2	2	20	6325.95	6445.43	216.28	o
-1	3	20	434.14	480.27	40.48	o
-3	4	20	31.78	76.74	21.30	o
0	4	20	4944.70	4804.31	183.52	o
-2	5	20	899.72	852.44	55.56	o
-4	6	20	5130.28	4786.70	215.43	o
-1	6	20	288.78	277.45	45.01	o
-6	7	20	59.70	61.84	72.94	<
-3	7	20	313.98	262.55	43.26	o
0	7	20	100.93	51.82	52.55	<
-8	8	20	1407.53	1221.11	185.27	o
-5	8	20	118.78	135.44	47.60	<
-2	8	20	1866.22	1323.06	244.15	o
-7	9	20	1402.12	1493.85	177.85	o
-4	9	20	183.55	168.38	66.66	<
0	0	21	3257.11	3397.76	229.79	o
-1	2	21	11024.20	11264.50	171.70	o
-3	3	21	7473.37	7543.88	199.14	o
0	3	21	14580.90	14787.90	315.76	o
-2	4	21	5125.27	5155.18	123.92	o
-4	5	21	8575.10	8926.37	290.42	o
-1	5	21	2131.92	2170.56	92.00	o
-6	6	21	2995.92	2844.18	236.55	o
-3	6	21	2536.38	2736.13	121.38	o
0	6	21	3020.29	3043.75	225.51	o
-5	7	21	323.08	291.81	61.84	o
-2	7	21	9711.38	9188.13	234.56	o
-7	8	21	2612.34	2833.62	168.68	o
-4	8	21	2282.82	2300.80	155.04	o
-1	8	21	431.68	503.32	93.15	o
-6	9	21	4002.78	4335.08	222.73	o

-3	9	21	239.43	286.68	105.94	<
-1	1	22	15023.70	16616.00	361.85	o
0	2	22	5043.91	5255.21	170.31	o
-2	3	22	25679.50	26272.60	267.86	o
-4	4	22	1601.43	1509.18	105.15	o
-1	4	22	18552.00	18324.70	265.45	o
-3	5	22	6093.95	5969.19	179.90	o
0	5	22	19402.20	19315.90	384.05	o
-5	6	22	13994.30	14277.90	372.47	o
-2	6	22	355.35	375.24	58.22	o
-7	7	22	3095.89	2814.92	237.15	o
-4	7	22	12760.90	13084.30	383.75	o
-1	7	22	4655.27	4617.11	189.37	o
-6	8	22	935.85	870.42	140.38	o
-3	8	22	5928.64	5787.42	243.18	o
0	8	22	216.83	186.54	149.01	<
-5	9	22	2494.89	2455.61	159.15	o
-2	9	22	9529.67	9935.30	527.63	o
0	1	23	10769.60	10954.70	245.36	o
-2	2	23	2780.98	2625.43	135.07	o
-1	3	23	5670.62	5816.50	129.28	o
-3	4	23	4632.89	4453.02	132.00	o
0	4	23	1246.53	1228.04	97.37	o
-5	5	23	3995.58	4123.81	284.27	o
-2	5	23	5906.84	6085.45	181.17	o
-4	6	23	911.46	843.09	95.50	o
-1	6	23	2865.05	2771.55	122.83	o
-6	7	23	2658.18	2609.75	161.44	o
-3	7	23	2477.03	2471.90	158.48	o
0	7	23	2425.90	2165.73	220.68	o
-5	8	23	1761.42	1497.95	144.91	o
-2	8	23	873.12	835.97	100.21	o
-4	9	23	1948.35	1845.14	140.75	o
0	0	24	36.99	0.06	37.40	<
-1	2	24	12996.30	13174.40	194.32	o
-3	3	24	22549.90	22159.10	424.17	o
0	3	24	3789.34	4053.10	171.03	o
-2	4	24	10.59	30.83	22.32	<
-4	5	24	4647.16	4568.73	210.73	o
-1	5	24	9818.39	9957.32	232.69	o
-6	6	24	379.53	271.48	84.76	o
-3	6	24	5075.18	4455.37	146.60	o
0	6	24	158.24	101.89	76.62	<
-5	7	24	7384.27	7523.31	271.05	o
-2	7	24	2708.03	2428.10	160.65	o
-4	8	24	17.02	6.64	34.51	<
-1	8	24	2184.12	2252.30	221.16	o
-3	9	24	2801.91	2765.51	488.42	o
-1	1	25	7704.31	8232.35	269.07	o
0	2	25	1476.33	1811.36	115.41	o
-2	3	25	6766.07	6652.17	170.61	o
-4	4	25	1187.00	1232.57	109.86	o
-1	4	25	7129.89	7459.67	186.23	o
-3	5	25	8249.67	8079.90	191.00	o
0	5	25	1671.14	1674.35	153.54	o
-5	6	25	1696.13	1825.30	193.35	o
-2	6	25	379.15	437.32	54.11	o
-7	7	25	6717.53	8027.42	452.16	o

-4	7	25	684.15	571.37	81.20	o
-1	7	25	4950.62	5206.16	234.74	o
-6	8	25	607.92	733.53	103.04	o
-3	8	25	1654.36	1626.39	143.22	o
0	1	26	1086.01	1039.88	85.12	o
-2	2	26	1614.37	1618.25	121.68	o
-1	3	26	879.42	891.23	67.21	o
-3	4	26	21.01	20.99	21.18	<
0	4	26	2005.26	2076.68	129.28	o
-5	5	26	1352.43	1426.53	170.43	o
-2	5	26	15.64	10.50	23.17	<
-4	6	26	1876.62	1812.39	156.79	o
-1	6	26	192.72	213.62	46.39	o
-6	7	26	112.77	105.09	42.89	<
-3	7	26	893.50	702.34	89.89	o
0	7	26	474.10	488.18	153.23	o
-5	8	26	5.45	38.61	34.33	<
-2	8	26	434.39	538.37	102.14	o
0	0	27	12602.90	12302.60	477.32	o
-1	2	27	368.39	420.67	43.32	o
-3	3	27	94.13	101.65	41.02	<
0	3	27	2663.67	2383.45	137.37	o
-2	4	27	4721.43	4542.67	174.35	o
-4	5	27	436.56	409.03	55.62	o
-1	5	27	49.03	50.37	27.39	<
-6	6	27	1152.10	1092.97	152.33	o
-3	6	27	24.80	13.33	32.88	<
0	6	27	2042.30	2045.92	212.12	o
-5	7	27	148.02	232.32	79.87	<
-2	7	27	821.33	693.96	130.67	o
-4	8	27	1123.92	1205.90	113.42	o
-1	1	28	1126.79	1018.46	101.29	o
0	2	28	25074.70	25080.70	521.60	o
-2	3	28	2327.29	2229.44	138.57	o
-4	4	28	17582.90	17975.30	572.58	o
-1	4	28	1621.44	1499.46	94.84	o
-3	5	28	717.20	582.71	68.53	o
0	5	28	618.13	744.51	133.75	o
-5	6	28	1049.80	1114.99	116.07	o
-2	6	28	10975.40	11191.80	357.81	o
-4	7	28	533.91	588.62	103.52	o
-1	7	28	814.95	825.65	123.79	o
-3	8	28	1105.86	1346.83	200.59	o
0	1	29	2051.98	2192.82	169.82	o
-2	2	29	9220.77	8860.55	291.14	o
-1	3	29	1512.41	1361.91	87.23	o
-3	4	29	558.55	562.14	56.23	o
0	4	29	10335.00	10270.10	652.63	o
-5	5	29	380.10	389.30	95.08	o
-2	5	29	1506.90	1347.25	98.09	o
-4	6	29	6889.69	6297.74	249.04	o
-1	6	29	98.79	97.61	87.72	<
-3	7	29	46.95	66.66	49.83	<
0	0	30	8139.77	7463.95	540.97	o
-1	2	30	3491.52	3714.60	163.61	o
-3	3	30	929.79	1038.25	112.15	o
0	3	30	4089.74	4115.24	236.55	o
-2	4	30	3391.95	2771.37	119.39	o

-4	5	30	3711.06	3777.82	194.32	o
-1	5	30	1062.17	1059.19	98.88	o
-6	6	30	2147.76	1611.61	181.77	o
-3	6	30	2270.55	2319.51	222.55	o
0	6	30	1583.57	1274.50	231.48	o
-2	7	30	3734.94	3979.86	591.40	o
-1	1	31	10531.20	11360.40	387.55	o
0	2	31	3608.09	3065.65	224.00	o
-2	3	31	16689.00	16417.10	295.79	o
-4	4	31	3614.97	3034.70	284.93	o
-1	4	31	7742.55	7519.39	227.38	o
-3	5	31	4442.12	4675.03	216.34	o
0	5	31	12185.10	12575.80	581.69	o
-5	6	31	5998.39	5975.77	240.23	o
-2	6	31	1712.66	1395.09	124.10	o
-4	7	31	7389.12	6541.59	512.19	o
0	1	32	3556.86	3639.07	223.03	o
-2	2	32	346.97	481.60	97.31	o
-1	3	32	4474.96	4304.31	213.14	o
-3	4	32	2740.13	2666.33	165.66	o
0	4	32	51.64	55.62	46.27	<
-5	5	32	2079.88	2064.38	204.82	o
-2	5	32	2684.80	2516.30	235.76	o
-4	6	32	299.04	337.24	65.82	o
0	0	33	2854.13	2714.42	338.50	o
-1	2	33	87.70	72.88	42.59	<
-3	3	33	81.17	54.66	43.44	<
0	3	33	18.93	18.40	40.90	<
-2	4	33	3915.23	3584.23	192.15	o
-4	5	33	14.59	30.16	37.10	<
-1	5	33	207.98	199.99	63.71	o
-3	6	33	91.00	40.60	52.00	<
-1	1	34	5663.54	4931.30	262.55	o
0	2	34	117.37	245.84	68.71	o
-2	3	34	3863.87	3089.60	161.56	o
-4	4	34	512.67	701.38	126.45	o
-1	4	34	2613.06	2541.27	187.56	o
-3	5	34	4863.31	4613.73	214.65	o
-2	6	34	353.65	522.87	231.18	<
0	1	35	139.36	133.87	57.49	<
-2	2	35	775.65	1043.62	139.60	o
-1	3	35	1192.64	1157.22	108.65	o
-3	4	35	263.40	209.22	63.16	o
0	4	35	604.63	986.25	207.95	o
-2	5	35	6.20	31.13	61.53	<
-1	2	36	238.07	194.50	48.69	o
-3	3	36	39.08	30.95	49.11	<
0	3	36	100.49	41.87	63.89	<
-2	4	36	3145.31	3222.32	228.46	o
-1	1	37	3818.69	3121.21	260.32	o
0	2	37	12512.00	12687.70	513.40	o
-2	3	37	2450.25	2428.82	171.70	o
0	1	38	700.87	675.68	130.43	o
-2	2	38	7502.39	6873.46	375.61	o
-1	3	38	1002.21	888.76	299.65	<
-1	2	39	288.35	299.71	75.17	o
-1	1	40	3224.99	3453.80	388.03	o