

```

data_zadovite
#=====

# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common ?
_chemical_formula_moiety ?
_chemical_formula_structural ?
_chemical_formula_analytical ?
_chemical_formula_iupac ?
_chemical_formula_sum 'Ba1 Ca6 F1 O16 P2 Si2'
_chemical_formula_weight 770.9
_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          7.08960(10)
_cell_length_b          7.08960(10)
_cell_length_c          25.4317(5)
_cell_angle_alpha       90
_cell_angle_beta        90
_cell_angle_gamma       120
_cell_volume            1107.00(3)
_cell_formula_units_Z   3

_cell_measurement_reflns_used    3235
_cell_measurement_theta_min     2.39
_cell_measurement_theta_max     34.71
_cell_measurement_temperature   293
_cell_special_details
; ?
;

_exptl_crystal_density_diffrn    3.4692
_exptl_crystal_density_meas      ?
_exptl_crystal_density_method    ?
_exptl_crystal_F_000            1113

_exptl_absorpt_coefficient_mu    5.16
_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   'multi-scan'
_exptl_absorpt_process_details
;
CrysAlisPro 1.171.40.67a (Rigaku Oxford Diffraction, 2019)
Empirical absorption correction using spherical harmonics,
implemented in SCALE3 ABSPACK scaling algorithm.
;
_exptl_absorpt_correction_T_min    0.982
_exptl_absorpt_correction_T_max    1
#####

# 7. EXPERIMENTAL DATA

_exptl_special_details            ?

_diffraction_radiation_type       synchrotron
_diffraction_radiation_probe      x-ray
_diffraction_radiation_source     'SLS super-bending magnet 2.9T, X06DA'

```

```

_diffrn_ambient_temperature      293(2)
_diffrn_radiation_wavelength     0.70848
_diffrn_radiation_monochromator
;Bartels Monochromator with dual channel cut crystals (DCCM)
  in (+--+) geometry
;
_diffrn_measurement_device        'multi-axis goniometer'
_diffrn_measurement_device_type   PRIGo
_diffrn_detector                  'hybrid pixel CMOS'
_diffrn_detector_type             PILATUS2M-F
_diffrn_detector_area_resol_mean  5.81
_diffrn_measurement_method        '\w scans'
_diffrn_measurement_specimen_support 'litho-loop'
_diffrn_measurement_details
;
  Swiss Light Source, Paul Scherrer Insitute, Villigen, Switzerland
  Beamline X06DA (PXIII)
  single omega-scan
  3600 frames, detector distance = 90 mm
  Detector threshold setting 8750 eV
  oscillation 0.1 deg, 0.1 sec exposure
  vertical detector offset 55 mm
;

```

```

_diffrn_reflns_number            4861
_diffrn_reflns_theta_min         2.39
_diffrn_reflns_theta_max         34.68
_diffrn_reflns_theta_full        34.24
_diffrn_measured_fraction_theta_max 0.96
_diffrn_measured_fraction_theta_full 0.98
_diffrn_reflns_av_R_equivalents  0.0393
_diffrn_reflns_av_unetI/netI     0.0193
_diffrn_reflns_limit_h_min       -11
_diffrn_reflns_limit_h_max       11
_diffrn_reflns_limit_k_min       -10
_diffrn_reflns_limit_k_max       10
_diffrn_reflns_limit_l_min       -40
_diffrn_reflns_limit_l_max       40
_diffrn_reflns_reduction_process ?

```

```

_diffrn_standards_number         ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        ?
loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
  ? ? ?

```

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#=====

```

``` # 8. REFINEMENT DATA ```

```

_refine_special_details
; ?

```

;

```
_reflns_number_total          618
_reflns_number_gt             547
_reflns_threshold_expression   'I>3\s(I) '

_refine_ls_structure_factor_coef      F
_refine_ls_R_factor_gt               0.0188
_refine_ls_wR_factor_gt              0.0227
_refine_ls_R_factor_all              0.0217
_refine_ls_wR_factor_ref              0.0231
_refine_ls_goodness_of_fit_ref        1.25
_refine_ls_goodness_of_fit_gt         1.31
_refine_ls_restrained_S_gt            ?
_refine_ls_restrained_S_all           ?
_refine_ls_number_reflns              618
_refine_ls_number_parameters           35
_refine_ls_number_restraints           0
_refine_ls_number_constraints           0
_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                0.0031
_refine_ls_shift/su_mean               0.0011
_refine_diff_density_max               0.45
_refine_diff_density_min              -0.43
_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'
F    0.0178  0.0106
'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'
P    0.1035  0.0955
'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 1.171.40.67a (Rigaku OD, 2019)'
_computing_cell_refinement
'CrysAlisPro 1.171.40.67a (Rigaku OD, 2019)'
_computing_data_reduction
'CrysAlisPro 1.171.40.67a (Rigaku OD, 2019)'
_computing_structure_solution          ?
```

```

_computing_structure_refinement
;
Jana2006
Petricek, V., Dusek, M. & Palatinus L. (2014). Z. Kristallogr. 229(5),
345-352
;
_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 0.01581(9) 3 1 d . . .
Ca1 Ca 0.83874(3) 0.67749(6) 0.065327(18) Uani 0.01479(13) 18 1 d . . .
Si1/p1 Si 0.333333 0.666667 0.03220(3) Uani 0.00601(18) 6 1 d . . .
P2/s2 P 0.666667 0.333333 0.15400(3) Uani 0.00825(18) 6 1 d . . .
O1 O 0.333333 0.666667 0.96911(10) Uani 0.0169(6) 6 1 d . . .
O2 O 0.20963(12) 0.79037(12) 0.05042(7) Uani 0.0212(5) 18 1 d . . .
O3 O 0.55001(11) 0.1000(2) 0.13222(6) Uani 0.0162(4) 18 1 d . . .
O4 O 0.666667 0.333333 0.21486(10) Uani 0.0148(6) 6 1 d . . .
F1 F 0 0 0 Uani 0.0249(9) 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 0.01368(11) 0.01368(11) 0.02006(15) 0.00684(5) 0 0
Ca1 Ca 0.00959(14) 0.00925(17) 0.0254(2) 0.00462(9) -0.00002(7) -
0.00003(15)
Si1/p1 Si 0.0052(2) 0.0052(2) 0.0077(3) 0.00259(11) 0 0
P2/s2 P 0.0089(2) 0.0089(2) 0.0070(3) 0.00443(11) 0 0
O1 O 0.0190(8) 0.0190(8) 0.0127(11) 0.0095(4) 0 0
O2 O 0.0123(5) 0.0123(5) 0.0384(10) 0.0058(6) 0.0047(3) -0.0047(3)
O3 O 0.0194(5) 0.0111(6) 0.0153(6) 0.0056(3) 0.0003(3) 0.0007(5)
O4 O 0.0163(7) 0.0163(7) 0.0119(10) 0.0081(3) 0 0
F1 F 0.0247(10) 0.0247(10) 0.0254(18) 0.0124(5) 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 O2 . . 3.3239(17) ?
Ba1 O2 . 2_665 3.3239(17) ?
Ba1 O2 . 3_565 3.3239(17) ?
Ba1 O2 . 16_455 3.3239(17) ?
Ba1 O2 . 17_565 3.3238(17) ?
Ba1 O2 . 18_555 3.3238(17) ?
Ba1 O3 . 1_565 2.8012(14) ?
Ba1 O3 . 2_555 2.8012(14) ?
Ba1 O3 . 3_665 2.8012(17) ?
Ba1 O3 . 16_555 2.8012(14) ?
Ba1 O3 . 17_455 2.8012(14) ?
Ba1 O3 . 18_565 2.8012(17) ?
Ca1 O1 . 4_556 2.2873(11) ?
Ca1 O2 . 1_655 2.3651(9) ?
Ca1 O2 . 3_565 2.3651(14) ?
Ca1 O2 . 6_655 3.0029(19) ?
Ca1 O3 . 2_655 2.5267(19) ?
Ca1 O3 . 3_665 2.5267(14) ?
Ca1 O4 . 16_555 2.3974(15) ?
Ca1 F1 . 1_665 2.5848(4) ?
Si1/p1 O1 . 1_554 1.604(3) ?
Si1/p1 O2 . . 1.5881(12) ?
Si1/p1 O2 . 2_665 1.5881(12) ?
Si1/p1 O2 . 3_565 1.5881(12) ?
P2/s2 O1 . 4_556 3.131(3) ?
P2/s2 O3 . . 1.5358(14) ?
P2/s2 O3 . 2_655 1.5358(14) ?
P2/s2 O3 . 3_665 1.5358(17) ?
P2/s2 O4 . . 1.548(3) ?
F1 O2 . 1_545 2.8758(13) ?
F1 O2 . 2_665 2.8758(13) ?
F1 O2 . 3_455 2.8758(13) ?
F1 O2 . 4_455 2.8758(13) ?
F1 O2 . 5_665 2.8758(13) ?
F1 O2 . 6_545 2.8758(13) ?
F1 O4 . 25_444 3.013(3) ?
F1 O4 . 16_445 3.013(3) ?
```

#####

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	68122.20	73587.90	596.04	o
0	3	0	18949.70	19556.70	226.10	o
-2	4	0	255649.00	251154.00	1988.38	o
-1	5	0	27293.50	27728.50	227.92	o
-3	6	0	49532.70	47746.00	463.68	o
0	6	0	69009.10	67315.70	587.69	o
-2	7	0	10278.10	10550.80	125.32	o
-4	8	0	52357.40	49974.30	549.57	o
-1	8	0	11704.00	11132.20	164.22	o
-3	9	0	4415.71	4471.77	116.96	o
0	9	0	7152.89	7147.84	330.27	o
-5	10	0	8794.62	9368.84	317.21	o
-2	10	0	23913.40	24791.90	439.66	o
-4	11	0	3122.34	2685.99	293.98	o
-1	1	1	3533.38	3540.50	55.35	o
0	2	1	91032.00	93720.00	684.81	o
-2	3	1	2589.63	2365.38	36.81	o
-4	4	1	59008.00	59206.60	512.76	o
-1	4	1	575.33	535.47	22.71	o
-3	5	1	1852.47	1846.36	45.95	o
0	5	1	2347.67	2407.94	64.49	o
-5	6	1	994.70	1051.37	42.82	o
-2	6	1	39930.00	40076.80	279.36	o
-7	7	1	115.94	131.06	43.86	<
-4	7	1	2126.70	2040.60	44.64	o
-1	7	1	609.58	598.40	34.20	o
-6	8	1	18189.30	18042.20	226.36	o
-3	8	1	495.50	443.83	37.33	o
0	8	1	16608.60	16948.20	443.57	o
-8	9	1	1606.92	1542.98	114.88	o
-5	9	1	87.92	88.24	29.50	<
-2	9	1	922.30	803.86	68.40	o
-7	10	1	871.76	901.51	91.90	o
-4	10	1	10866.20	11013.10	244.89	o
-1	10	1	164.20	192.68	56.65	o
-6	11	1	1360.62	1325.24	208.34	o
0	1	2	2166.84	1922.07	34.20	o
-2	2	2	5404.39	4605.45	81.20	o
-1	3	2	14829.80	15649.60	129.50	o
-3	4	2	386.17	312.77	19.06	o
0	4	2	19634.50	20177.00	211.74	o
-5	5	2	4081.37	3583.58	87.20	o
-2	5	2	2258.03	2367.47	48.30	o
-4	6	2	6282.48	6360.16	94.51	o
-1	6	2	30.25	16.71	15.66	<
-6	7	2	3417.25	3388.29	72.84	o
-3	7	2	66.72	76.24	18.28	o
0	7	2	2300.78	2496.44	86.68	o
-8	8	2	1844.43	1739.31	136.54	o
-5	8	2	51.27	58.74	25.06	<
-2	8	2	8630.21	9038.84	159.00	o
-7	9	2	410.57	363.16	53.00	o
-4	9	2	4398.06	4085.11	91.90	o
-1	9	2	127.35	123.23	60.83	<
-9	10	2	648.92	561.58	108.61	o

-6	10	2	1818.77	1797.53	109.92	o
-3	10	2	31.36	-14.36	45.43	<
-5	11	2	417.50	416.16	94.25	o
0	0	3	3464.47	3401.61	96.08	o
-1	2	3	24600.80	24408.30	154.04	o
-3	3	3	55.61	132.37	20.63	o
0	3	3	59288.70	61661.80	541.48	o
-2	4	3	527.70	494.22	21.15	o
-4	5	3	19770.80	19981.70	194.50	o
-1	5	3	4188.79	4411.72	65.27	o
-6	6	3	3079.21	3271.85	117.75	o
-3	6	3	10324.80	10047.70	116.96	o
0	6	3	239.42	184.84	27.94	o
-5	7	3	1348.08	1268.33	45.17	o
-2	7	3	15571.30	16364.50	155.08	o
-7	8	3	4208.00	4243.59	124.01	o
-4	8	3	479.08	450.36	38.38	o
-1	8	3	2561.27	2695.91	80.67	o
-9	9	3	486.39	462.11	99.73	o
-6	9	3	3541.45	3557.21	99.99	o
-3	9	3	2534.26	2523.07	90.07	o
0	9	3	7091.99	7149.67	332.09	o
-8	10	3	755.79	726.06	75.97	o
-5	10	3	1841.81	1764.64	106.78	o
-2	10	3	23.21	-12.53	43.34	<
-7	11	3	549.76	392.92	139.94	<
-4	11	3	3966.72	3625.61	342.54	o
-1	1	4	11352.00	10509.50	121.92	o
0	2	4	32930.50	34387.30	301.02	o
-2	3	4	30324.50	30399.30	218.79	o
-4	4	4	6817.64	6857.26	143.85	o
-1	4	4	4506.05	4245.42	59.00	o
-3	5	4	1661.29	1638.80	40.73	o
0	5	4	15986.40	15887.20	192.42	o
-5	6	4	4077.92	4102.35	79.89	o
-2	6	4	7783.18	7980.68	109.39	o
-7	7	4	311.67	268.65	68.40	o
-4	7	4	6288.74	6369.04	99.21	o
-1	7	4	2292.30	2268.52	53.00	o
-6	8	4	2284.26	2272.44	87.72	o
-3	8	4	1706.93	1691.80	51.95	o
0	8	4	5328.65	5005.16	184.58	o
-8	9	4	1630.17	1497.03	100.25	o
-5	9	4	965.49	1001.24	63.70	o
-2	9	4	3030.81	3022.26	113.57	o
-7	10	4	1622.72	1329.42	127.41	o
-4	10	4	3570.25	3545.46	147.77	o
-1	10	4	588.13	485.35	108.35	o
0	1	5	6173.92	5693.36	104.17	o
-2	2	5	5423.98	4707.27	83.02	o
-1	3	5	38770.70	40348.80	292.67	o
-3	4	5	22213.70	22396.20	178.84	o
0	4	5	6519.82	6640.30	118.53	o
-5	5	5	13218.70	12759.00	340.71	o
-2	5	5	1767.72	1769.08	44.91	o
-4	6	5	15613.70	15492.20	152.47	o
-1	6	5	12395.90	12436.00	125.58	o
-6	7	5	6618.73	6782.59	136.81	o

-3	7	5	3802.88	3910.19	66.58	o
0	7	5	3520.18	3607.60	99.73	o
-8	8	5	9162.78	9125.78	381.44	o
-5	8	5	8229.00	8244.38	142.29	o
-2	8	5	3908.66	3806.02	75.71	o
-7	9	5	3464.58	3394.56	114.35	o
-4	9	5	3703.73	3484.11	92.16	o
-1	9	5	807.58	785.07	88.51	o
-9	10	5	1038.57	1090.53	137.85	o
-6	10	5	3776.57	3596.89	149.08	o
-3	10	5	2786.34	2774.76	151.43	o
-5	11	5	394.17	306.25	90.33	o
0	0	6	926.05	869.92	66.05	o
-1	2	6	90093.70	91398.50	578.81	o
-3	3	6	68761.80	71968.20	725.80	o
0	3	6	55371.10	56041.00	539.13	o
-2	4	6	664.02	730.50	26.63	o
-4	5	6	28296.70	29137.50	234.45	o
-1	5	6	43283.30	44980.90	306.77	o
-6	6	6	706.89	700.74	55.09	o
-3	6	6	27334.20	28029.50	228.97	o
0	6	6	437.97	476.47	36.81	o
-5	7	6	29855.60	30202.70	282.23	o
-2	7	6	13191.20	13469.40	138.11	o
-7	8	6	9518.98	9519.23	220.87	o
-4	8	6	367.08	345.67	37.33	o
-1	8	6	13412.80	13974.60	180.67	o
-6	9	6	7000.27	6994.59	142.03	o
-3	9	6	15121.00	15235.80	212.00	o
0	9	6	3982.00	4305.47	255.34	o
-8	10	6	9.41	5.22	48.04	<
-5	10	6	6889.40	6507.67	224.01	o
-2	10	6	210.72	171.79	59.00	<
-4	11	6	3349.82	3018.34	221.92	o
-1	1	7	63873.20	64544.40	782.98	o
0	2	7	2984.16	3891.39	84.07	o
-2	3	7	17891.60	17896.20	141.24	o
-4	4	7	2616.52	2951.24	110.44	o
-1	4	7	8101.12	7888.00	84.33	o
-3	5	7	34642.70	35181.80	222.70	o
0	5	7	9307.71	9323.42	141.51	o
-5	6	7	2250.87	2273.74	57.44	o
-2	6	7	6410.99	6451.28	96.08	o
-7	7	7	11748.50	12488.00	361.86	o
-4	7	7	6833.79	6914.17	108.87	o
-1	7	7	9957.85	10211.90	126.10	o
-6	8	7	3072.56	3220.94	121.92	o
-3	8	7	1867.08	1901.70	59.79	o
0	8	7	3346.47	3274.72	137.33	o
-8	9	7	2744.60	2658.84	119.31	o
-5	9	7	10481.40	10470.60	207.04	o
-2	9	7	696.94	638.60	54.04	o
-7	10	7	1477.01	1285.56	93.47	o
-4	10	7	1045.59	1056.33	88.51	o
-1	10	7	4130.76	3431.37	329.74	o
0	1	8	8563.43	8423.21	153.51	o
-2	2	8	72075.00	72985.40	768.36	o
-1	3	8	6250.42	5889.70	72.58	o

-3	4	8	12048.90	12083.80	125.84	o
0	4	8	21549.10	21605.40	243.59	o
-5	5	8	4000.17	4098.95	119.31	o
-2	5	8	3100.34	2994.58	54.57	o
-4	6	8	14745.50	14702.70	170.49	o
-1	6	8	7809.29	7944.66	96.34	o
-6	7	8	916.96	934.40	60.31	o
-3	7	8	4449.34	4747.73	96.86	o
0	7	8	976.93	960.25	64.23	o
-8	8	8	7233.89	7079.96	475.17	o
-5	8	8	3298.94	3414.14	89.55	o
-2	8	8	5608.62	5891.00	100.78	o
-7	9	8	4658.08	4581.17	151.69	o
-4	9	8	76.58	110.44	33.94	o
-1	9	8	2490.89	2491.74	142.55	o
-6	10	8	5878.07	5625.75	234.45	o
-3	10	8	1356.42	1325.76	108.35	o
0	0	9	178939.00	165817.00	2792.77	o
-1	2	9	4220.74	4009.14	62.92	o
-3	3	9	34.36	38.12	22.19	<
0	3	9	10538.30	10386.50	150.64	o
-2	4	9	77931.90	77384.80	496.57	o
-4	5	9	3989.36	3863.72	78.06	o
-1	5	9	3737.25	3969.72	73.36	o
-6	6	9	40749.00	41215.30	604.92	o
-3	6	9	5959.41	5997.00	105.74	o
0	6	9	22229.60	23212.10	310.42	o
-5	7	9	2535.79	2552.31	80.67	o
-2	7	9	1227.44	1281.90	48.56	o
-7	8	9	1515.02	1554.21	90.33	o
-4	8	9	22686.60	22641.90	258.21	o
-1	8	9	3667.90	3820.12	93.73	o
-9	9	9	2127.87	1673.26	164.48	o
-6	9	9	42.63	39.68	39.16	<
-3	9	9	3640.40	3823.25	127.15	o
-8	10	9	11654.40	11773.70	277.01	o
-5	10	9	2098.92	1937.21	125.58	o
-2	10	9	8723.22	8308.08	301.29	o
-1	1	10	22191.80	24092.20	308.07	o
0	2	10	140233.00	137963.00	1384.24	o
-2	3	10	61.86	57.18	14.36	o
-4	4	10	55399.60	54726.50	608.84	o
-1	4	10	4643.63	4426.35	78.32	o
-3	5	10	8636.66	8359.77	118.01	o
0	5	10	34.66	46.21	27.41	<
-5	6	10	1789.21	1683.70	56.39	o
-2	6	10	52732.80	52757.70	439.66	o
-7	7	10	703.79	692.38	93.73	o
-4	7	10	1438.59	1520.01	59.79	o
-1	7	10	294.34	268.13	31.85	o
-6	8	10	14409.50	14217.90	241.76	o
-3	8	10	1007.02	963.12	56.13	o
0	8	10	22455.10	23263.50	422.17	o
-8	9	10	1396.31	1300.70	87.72	o
-5	9	10	8.75	2.09	29.76	<
-2	9	10	279.74	279.88	50.39	o
-7	10	10	414.14	369.95	60.31	o
-4	10	10	12800.20	13174.60	332.88	o

-1	10	10	325.24	333.40	137.85	<
0	1	11	2590.97	2794.07	83.02	o
-2	2	11	29829.10	29089.00	343.58	o
-1	3	11	1558.62	1629.40	46.21	o
-3	4	11	452.11	468.38	22.71	o
0	4	11	12982.80	12740.40	196.07	o
-5	5	11	1518.66	1524.71	75.97	o
-2	5	11	867.52	850.34	33.94	o
-4	6	11	7147.98	7186.48	106.00	o
-1	6	11	702.09	726.85	34.98	o
-6	7	11	232.49	222.18	45.43	o
-3	7	11	1532.97	1501.47	56.13	o
0	7	11	68.36	65.27	31.59	<
-8	8	11	2761.04	2726.98	166.05	o
-5	8	11	315.41	265.78	37.07	o
-2	8	11	4966.65	5018.47	118.01	o
-7	9	11	1217.40	1007.25	77.54	o
-4	9	11	40.51	41.51	28.72	<
-1	9	11	1204.27	1072.25	114.35	o
-6	10	11	2778.47	2634.56	128.97	o
-3	10	11	600.40	385.88	98.17	o
0	0	12	110.26	284.84	56.13	o
-1	2	12	5261.55	5016.65	85.63	o
-3	3	12	599.36	571.77	39.68	o
0	3	12	29760.80	29981.30	343.32	o
-2	4	12	6380.65	6527.25	92.68	o
-4	5	12	5157.35	5252.92	86.16	o
-1	5	12	383.51	417.20	26.37	o
-6	6	12	11884.40	11826.60	268.39	o
-3	6	12	31.33	41.51	21.67	<
0	6	12	3790.87	3910.45	112.26	o
-5	7	12	150.05	136.28	30.29	o
-2	7	12	6387.94	6702.44	107.83	o
-7	8	12	654.90	562.63	61.61	o
-4	8	12	4703.07	4780.63	110.44	o
-1	8	12	121.05	137.33	31.07	o
-9	9	12	549.94	528.42	101.30	o
-6	9	12	1910.17	1983.16	103.13	o
-3	9	12	908.59	951.90	84.33	o
0	9	12	997.08	903.60	186.67	o
-8	10	12	2365.13	2392.53	160.56	o
-5	10	12	95.18	79.63	69.97	<
-1	1	13	17618.60	17240.90	258.73	o
0	2	13	4255.26	4485.61	107.57	o
-2	3	13	16839.40	16821.90	159.52	o
-4	4	13	788.47	876.97	55.09	o
-1	4	13	14872.50	14895.90	159.26	o
-3	5	13	5647.26	5362.58	84.07	o
0	5	13	13750.40	13688.10	220.09	o
-5	6	13	12703.40	12887.20	188.50	o
-2	6	13	841.93	849.55	35.51	o
-7	7	13	1832.83	1966.19	140.46	o
-4	7	13	11716.20	11874.40	177.27	o
-1	7	13	2875.41	2937.41	73.10	o
-6	8	13	277.53	273.87	49.61	o
-3	8	13	5959.51	6099.87	127.67	o
0	8	13	156.26	174.40	53.78	o
-8	9	13	4425.33	4413.29	183.54	o

-5	9	13	935.32	849.55	66.58	o
-2	9	13	8571.57	8494.23	262.65	o
-7	10	13	2965.49	2732.20	130.28	o
-4	10	13	249.80	255.34	71.01	o
0	1	14	17012.90	16452.50	254.29	o
-2	2	14	7.91	53.00	27.15	<
-1	3	14	7132.89	6968.22	104.95	o
-3	4	14	20061.50	19803.20	178.06	o
0	4	14	2947.22	3080.74	92.16	o
-5	5	14	2375.27	2472.69	103.39	o
-2	5	14	10795.90	10692.30	166.31	o
-4	6	14	2098.47	2137.20	57.44	o
-1	6	14	10617.10	10782.30	146.47	o
-6	7	14	5508.72	5723.13	165.79	o
-3	7	14	3283.22	3386.73	101.04	o
0	7	14	7178.08	7575.75	180.41	o
-8	8	14	1198.42	869.66	123.49	o
-5	8	14	8314.16	8150.91	167.09	o
-2	8	14	2580.94	2668.76	100.52	o
-7	9	14	2456.05	2417.60	112.26	o
-4	9	14	3554.59	3315.45	145.68	o
-1	9	14	1575.27	1023.69	201.55	o
-6	10	14	663.45	648.78	71.80	o
0	0	15	6102.61	6036.95	240.98	o
-1	2	15	48226.60	48132.70	389.79	o
-3	3	15	67031.80	66439.80	698.91	o
0	3	15	31665.90	31495.60	464.72	o
-2	4	15	3.52	9.92	16.19	<
-4	5	15	20867.70	20789.00	217.22	o
-1	5	15	28494.40	28919.50	261.86	o
-6	6	15	2.80	74.41	92.16	<
-3	6	15	12758.80	12585.10	189.02	o
0	6	15	1204.51	1191.05	85.11	o
-5	7	15	20188.70	20487.70	320.87	o
-2	7	15	13461.30	13885.80	179.10	o
-7	8	15	9376.39	9129.70	237.58	o
-4	8	15	50.02	85.37	33.42	<
-1	8	15	8770.93	9006.47	236.54	o
-6	9	15	11917.70	11748.80	252.20	o
-3	9	15	9000.69	8761.31	261.86	o
0	9	15	3835.62	3460.35	332.88	o
-5	10	15	5838.31	5644.54	207.56	o
-1	1	16	65684.00	66405.10	747.99	o
0	2	16	3971.60	4015.14	116.44	o
-2	3	16	30544.90	29970.40	268.39	o
-4	4	16	1464.23	1501.47	65.53	o
-1	4	16	36555.00	36198.20	312.25	o
-3	5	16	38980.10	38550.80	295.54	o
0	5	16	14172.00	14902.70	223.74	o
-5	6	16	16158.40	15296.90	227.92	o
-2	6	16	2354.29	2427.00	63.70	o
-7	7	16	18357.10	18144.00	460.28	o
-4	7	16	12552.10	12846.70	236.02	o
-1	7	16	14338.30	14684.40	193.72	o
-6	8	16	451.43	415.38	68.66	o
-3	8	16	10373.60	10719.90	195.81	o
0	8	16	1316.76	1062.59	140.20	o
-8	9	16	5373.63	5294.96	162.91	o

-5	9	16	11524.70	11490.60	273.61	o
-2	9	16	5408.77	4998.37	289.54	o
-7	10	16	3891.46	3687.49	239.15	o
-4	10	16	620.75	624.76	112.00	o
0	1	17	1652.64	1512.70	80.15	o
-2	2	17	1286.23	1235.43	62.14	o
-1	3	17	496.68	461.59	29.76	o
-3	4	17	110.22	109.13	19.84	o
0	4	17	2183.42	2214.48	87.20	o
-5	5	17	27.47	24.54	26.89	<
-2	5	17	767.07	816.14	36.03	o
-4	6	17	17.20	-16.71	25.06	<
-1	6	17	187.56	204.95	28.20	o
-6	7	17	482.11	391.62	54.57	o
-3	7	17	1088.99	945.89	66.31	o
0	7	17	48.67	43.60	41.25	<
-8	8	17	259.06	157.43	109.65	<
-5	8	17	32.66	45.43	33.94	<
-2	8	17	847.30	783.50	67.10	o
-7	9	17	1164.04	1263.36	121.14	o
-4	9	17	725.44	607.27	91.12	o
-1	9	17	1100.20	1227.07	149.08	o
-6	10	17	5.97	19.58	60.83	<
0	0	18	15779.90	14561.70	611.97	o
-1	2	18	1250.86	1176.43	45.69	o
-3	3	18	3326.65	3059.85	98.69	o
0	3	18	77.89	85.63	32.90	<
-2	4	18	10840.50	10986.20	138.89	o
-4	5	18	208.54	195.03	21.67	o
-1	5	18	1252.82	1250.57	47.52	o
-6	6	18	4253.49	4102.08	196.59	o
-3	6	18	471.76	454.28	34.46	o
0	6	18	6074.76	6450.76	192.15	o
-5	7	18	1031.76	875.14	61.61	o
-2	7	18	8.37	3.39	29.76	<
-7	8	18	95.74	74.93	40.47	<
-4	8	18	3574.42	3634.49	125.32	o
-1	8	18	582.83	557.14	59.00	o
-6	9	18	8.42	46.47	54.83	<
-3	9	18	516.74	423.21	80.15	o
-5	10	18	252.81	342.80	89.81	o
-1	1	19	326.60	355.59	43.60	o
0	2	19	53510.10	51681.80	773.06	o
-2	3	19	34.29	25.32	21.67	<
-4	4	19	20950.90	21021.10	248.55	o
-1	4	19	2787.54	2761.96	69.45	o
-3	5	19	676.55	603.88	35.77	o
0	5	19	331.41	337.32	46.21	o
-5	6	19	1671.93	1516.09	74.15	o
-2	6	19	15238.60	15813.90	210.43	o
-7	7	19	849.16	682.46	93.99	o
-4	7	19	8.99	-3.66	29.76	<
-1	7	19	408.52	411.98	52.22	o
-6	8	19	6250.96	6318.39	194.50	o
-3	8	19	1854.10	1765.94	91.64	o
0	8	19	7096.71	7350.96	480.65	o
-8	9	19	34.29	18.80	95.82	<
-5	9	19	120.93	140.98	44.91	o

-2	9	19	31.98	55.61	107.30	<
0	1	20	394.23	398.41	45.17	o
-2	2	20	17174.20	16425.80	307.03	o
-1	3	20	12.90	19.58	21.67	<
-3	4	20	357.99	307.55	26.63	o
0	4	20	15372.80	14969.00	238.63	o
-5	5	20	7.31	6.79	25.06	<
-2	5	20	58.87	49.61	23.76	<
-4	6	20	14048.40	14345.30	233.40	o
-1	6	20	388.88	400.50	39.16	o
-6	7	20	89.98	58.22	93.73	<
-3	7	20	10.22	14.36	30.02	<
0	7	20	211.06	168.13	56.65	<
-8	8	20	5814.26	5910.84	241.76	o
-5	8	20	404.74	329.48	51.69	o
-2	8	20	7448.24	7654.86	175.97	o
-7	9	20	259.75	282.49	70.49	o
-4	9	20	61.70	50.65	40.99	<
0	0	21	23780.10	22747.40	603.88	o
-1	2	21	5851.92	5669.87	112.53	o
-3	3	21	7771.62	7583.32	168.13	o
0	3	21	4759.08	4968.87	133.93	o
-2	4	21	21874.10	22092.80	208.08	o
-4	5	21	3552.67	3432.41	76.76	o
-1	5	21	2357.46	2469.29	74.41	o
-6	6	21	12014.70	12414.30	362.38	o
-3	6	21	1120.72	1062.33	58.22	o
0	6	21	17057.10	17793.10	322.17	o
-5	7	21	1112.63	1107.50	71.80	o
-2	7	21	3445.24	3555.12	122.71	o
-7	8	21	1346.30	1153.71	88.77	o
-4	8	21	10835.20	10602.20	221.66	o
-1	8	21	412.04	303.64	75.19	o
-6	9	21	2887.84	2696.69	127.93	o
-3	9	21	290.78	214.35	57.44	o
-1	1	22	8270.91	8669.67	212.78	o
0	2	22	25261.30	25427.90	355.07	o
-2	3	22	20297.10	19665.00	221.40	o
-4	4	22	16246.80	16155.10	282.49	o
-1	4	22	12675.20	12786.40	159.26	o
-3	5	22	2866.25	3028.26	79.11	o
0	5	22	15744.80	16362.60	366.82	o
-5	6	22	11206.80	11101.90	192.42	o
-2	6	22	7069.74	7231.39	136.54	o
-7	7	22	2178.27	2136.42	148.03	o
-4	7	22	8202.98	8405.98	178.58	o
-1	7	22	4378.47	4441.23	139.68	o
-6	8	22	7236.65	7480.19	212.26	o
-3	8	22	6163.56	6262.26	180.93	o
0	8	22	2259.47	2152.34	272.31	o
-5	9	22	2087.47	1980.03	112.79	o
0	1	23	6782.58	7339.73	195.81	o
-2	2	23	10.44	22.19	33.94	<
-1	3	23	2999.42	3143.14	75.71	o
-3	4	23	3576.13	3622.48	87.20	o
0	4	23	36.96	17.75	38.64	<
-5	5	23	1130.37	1265.71	67.36	o
-2	5	23	5990.08	6086.81	154.30	o

-4	6	23	76.51	70.75	22.45	o
-1	6	23	1561.47	1508.26	73.62	o
-6	7	23	3032.89	3016.25	133.41	o
-3	7	23	1068.19	928.66	83.02	o
0	7	23	3283.06	3356.70	324.78	o
-5	8	23	1750.55	1516.35	112.26	o
-2	8	23	5.01	32.90	43.34	<
-4	9	23	2683.58	2653.61	146.21	o
0	0	24	5.06	0.00	59.00	<
-1	2	24	8575.03	8536.52	139.94	o
-3	3	24	12190.40	11903.70	263.95	o
0	3	24	2243.13	2397.23	95.56	o
-2	4	24	276.66	237.84	31.59	o
-4	5	24	4869.84	4932.32	98.17	o
-1	5	24	5834.66	6076.37	132.11	o
-6	6	24	2078.01	2090.47	143.33	o
-3	6	24	5882.72	6119.45	123.49	o
0	6	24	3.54	12.27	42.82	<
-5	7	24	3071.48	3046.02	148.82	o
-2	7	24	3237.71	3322.76	144.38	o
-7	8	24	3247.13	3488.55	230.27	o
-4	8	24	481.47	404.67	56.13	o
-1	8	24	1810.93	1594.41	136.28	o
-3	9	24	461.76	277.01	127.41	<
-1	1	25	8752.73	8880.89	203.38	o
0	2	25	882.08	815.61	65.79	o
-2	3	25	10429.80	10523.10	184.58	o
-4	4	25	177.89	216.70	43.34	o
-1	4	25	6677.98	6815.75	139.15	o
-3	5	25	6060.53	6258.34	126.62	o
0	5	25	6418.92	6521.51	180.93	o
-5	6	25	3605.30	3132.43	200.77	o
-2	6	25	548.46	525.03	45.95	o
-7	7	25	4052.22	4032.38	198.68	o
-4	7	25	3178.21	3155.67	126.10	o
-1	7	25	4521.20	4614.84	155.60	o
-6	8	25	69.76	45.43	39.42	<
-3	8	25	2413.71	2340.58	139.94	o
0	1	26	3635.36	3834.74	142.29	o
-2	2	26	2926.15	2902.42	124.54	o
-1	3	26	2997.55	3156.71	88.24	o
-3	4	26	615.69	576.46	41.51	o
0	4	26	878.98	858.43	86.94	o
-5	5	26	2739.56	2639.52	136.54	o
-2	5	26	1521.52	1627.05	79.11	o
-4	6	26	343.88	308.60	44.12	o
-1	6	26	357.65	301.02	56.65	o
-6	7	26	277.34	363.68	53.00	o
-3	7	26	1891.23	1770.38	107.57	o
0	7	26	147.17	99.99	73.10	<
-5	8	26	27.42	45.95	38.64	<
-2	8	26	299.43	263.17	71.01	o
0	0	27	1047.14	879.32	117.22	o
-1	2	27	23.72	13.58	30.29	<
-3	3	27	16.41	62.40	41.25	<
0	3	27	424.31	387.18	58.74	o
-2	4	27	10.78	40.73	28.98	<
-4	5	27	9.75	26.89	24.54	<

-1	5	27	157.62	139.68	34.46	o
-6	6	27	209.88	258.99	84.85	o
-3	6	27	742.31	701.26	61.88	o
0	6	27	160.59	140.98	57.96	<
-5	7	27	149.57	93.73	70.23	<
-2	7	27	131.47	92.94	37.86	<
-4	8	27	72.23	42.56	44.91	<
-1	1	28	3283.06	3241.83	150.38	o
0	2	28	13597.50	14027.30	334.96	o
-2	3	28	3593.33	3678.09	107.30	o
-4	4	28	11074.60	11493.50	243.59	o
-1	4	28	3032.79	3019.91	105.21	o
-3	5	28	2529.64	2478.69	86.42	o
0	5	28	1504.84	1486.85	127.67	o
-5	6	28	1630.95	1589.19	90.59	o
-2	6	28	6619.31	6857.00	173.62	o
-4	7	28	707.14	741.73	68.40	o
-1	7	28	2452.81	2318.13	112.26	o
-3	8	28	1739.69	1697.02	245.41	o
0	1	29	1157.92	1291.82	142.03	o
-2	2	29	13479.10	14003.80	300.24	o
-1	3	29	3702.14	3711.77	122.97	o
-3	4	29	567.75	587.17	43.86	o
0	4	29	15021.50	15240.00	415.38	o
-5	5	29	3079.88	2859.87	167.87	o
-2	5	29	284.71	227.40	51.95	o
-4	6	29	8865.27	9138.83	235.76	o
-1	6	29	553.50	517.46	61.61	o
-6	7	29	801.39	681.16	162.91	o
-3	7	29	1068.43	974.35	83.55	o
-1	2	30	916.01	934.40	68.14	o
-3	3	30	238.93	187.19	47.78	o
0	3	30	857.47	744.34	115.92	o
-2	4	30	10592.00	10456.50	191.63	o
-4	5	30	650.54	556.62	51.95	o
-1	5	30	471.71	544.87	53.78	o
-6	6	30	6456.13	6720.97	311.47	o
-3	6	30	861.72	825.53	67.36	o
0	6	30	5270.81	5427.59	286.14	o
-5	7	30	223.58	276.48	72.06	o
-2	7	30	402.01	321.65	59.00	o
-1	1	31	4878.24	4991.58	269.17	o
0	2	31	11967.80	12312.00	314.34	o
-2	3	31	7878.48	7917.76	173.36	o
-4	4	31	12961.40	12903.10	310.16	o
-1	4	31	2818.75	2892.24	112.53	o
-3	5	31	2060.34	2102.74	103.65	o
0	5	31	6611.03	6490.70	227.40	o
-5	6	31	2211.20	1934.60	100.25	o
-2	6	31	8377.24	8570.72	197.90	o
-4	7	31	3330.48	3282.82	183.80	o
0	1	32	506.29	396.84	76.50	o
-2	2	32	1625.83	1635.66	114.35	o
-1	3	32	920.65	963.38	76.24	o
-3	4	32	977.87	884.28	67.36	o
0	4	32	1303.71	1048.76	87.20	o
-5	5	32	223.24	341.75	73.10	o
-2	5	32	547.62	496.83	55.35	o

-4	6	32	297.92	330.01	51.69	o
-1	6	32	435.63	459.76	58.22	o
-3	7	32	14.10	39.16	99.21	<
0	0	33	1279.08	1323.41	214.61	o
-1	2	33	172.10	149.60	37.33	o
-3	3	33	812.17	752.43	86.16	o
0	3	33	49.42	88.24	48.56	<
-2	4	33	1876.60	1676.91	84.07	o
-4	5	33	15.16	7.57	41.77	<
-1	5	33	194.73	217.22	49.08	o
-3	6	33	14.26	31.85	54.83	<
-1	1	34	5006.61	4964.95	222.96	o
0	2	34	406.71	351.41	66.05	o
-2	3	34	3577.58	3582.27	110.96	o
-4	4	34	30.24	30.55	54.57	<
-1	4	34	1837.86	1871.42	113.05	o
-3	5	34	3380.21	3409.18	131.06	o
0	5	34	2689.34	2987.80	310.68	o
-2	6	34	2.68	-40.21	99.73	<
0	1	35	1639.44	1439.07	126.36	o
-2	2	35	166.81	139.68	50.65	<
-1	3	35	2312.76	2187.33	94.25	o
-3	4	35	1808.89	1799.10	96.60	o
0	4	35	186.70	217.74	68.40	o
-2	5	35	971.63	982.97	110.70	o
0	0	36	12.11	96.08	100.25	<
-1	2	36	1196.99	1117.94	75.45	o
-3	3	36	325.32	265.78	68.93	o
0	3	36	1877.39	1947.92	112.79	o
-2	4	36	5.16	12.79	34.20	<
-1	1	37	5136.86	5061.81	196.33	o
0	2	37	3374.90	3124.08	159.26	o
-2	3	37	2523.34	2677.63	103.39	o
-1	4	37	2969.01	2707.14	175.71	o
0	1	38	509.90	429.48	100.25	o
-2	2	38	4948.09	4834.94	193.20	o
-1	3	38	1137.86	958.16	107.30	o
0	0	39	901.79	739.12	169.18	o
-1	2	39	11.64	14.36	50.91	<
-1	1	40	439.79	470.73	102.60	o
0	2	40	2873.43	3225.38	325.57	o