

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_caznp4
_shelx_title ' CaZnSi2O6 data collection i n DAC by Xcaliber-I at VT'
_shelx_refl_list_code      4
_shelx_F_calc_maximum     202.50
_exptl_crystal_F_000      504.00
_reflns_d_resolution_high  0.7134
```

```
loop_
_symmetry_equiv_pos_as_xyz
'x, y, z'
'-x, y, -z+1/2'
'x+1/2, y+1/2, z'
'-x+1/2, y+1/2, -z+1/2'
'-x, -y, -z'
'x, -y, z-1/2'
'-x+1/2, -y+1/2, -z'
'x+1/2, -y+1/2, z-1/2'
```

```
_cell_length_a    9.6914
_cell_length_b    8.8293
_cell_length_c    5.1862
_cell_angle_alpha 90.000
_cell_angle_beta  105.140
_cell_angle_gamma 90.000

_shelx_F_squared_multiplier 1.000
```

```
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
  4  0  0   6313.65   5587.93   131.32 o
  6  0  0   18907.94   19905.73   849.21 o
  8  0  0   14753.37   14691.47   337.32 o
 10  0  0    7340.54    7464.65   247.66 o
 12  0  0    345.66    207.26    97.62 o
  1  1  0    3133.79    3322.24   101.64 o
  3  1  0   16734.99   17173.13   754.77 o
  5  1  0    384.59    435.41    63.96 o
  7  1  0   5856.46   6283.18   183.18 o
  9  1  0    554.80    587.70    67.30 o
 11  1  0    2817.94    2863.47   198.04 o
  0  2  0    2280.62    2237.15   150.60 o
  2  2  0    1440.43    1562.72    87.58 o
  6  2  0     58.59    114.20    41.20 o
  8  2  0     27.07     48.06    47.43 o
```

12	2	0	200.85	250.94	90.97 o
3	3	0	3202.28	3519.38	122.67 o
5	3	0	1559.31	1567.19	98.69 o
7	3	0	180.22	180.59	83.60 o
9	3	0	791.25	861.20	132.07 o
11	3	0	316.95	222.91	100.33 o
0	4	0	2811.80	2475.01	194.73 o
2	4	0	539.48	612.63	44.67 o
4	4	0	10083.19	10365.27	470.80 o
8	4	0	182.90	203.57	41.01 o
10	4	0	4863.63	4988.92	250.12 o
1	5	0	22300.56	22159.63	798.28 o
3	5	0	14477.52	14266.74	745.42 o
5	5	0	1011.89	1061.54	59.48 o
7	5	0	23242.71	24161.05	1095.42 o
9	5	0	1955.25	1928.61	112.51 o
11	5	0	4881.45	4771.74	298.74 o
0	6	0	20523.11	17989.89	2256.30 o
4	6	0	2414.77	2425.73	144.71 o
6	6	0	732.29	747.50	108.98 o
8	6	0	1694.68	1800.44	174.98 o
10	6	0	2855.00	3001.69	198.55 o
1	7	0	647.06	614.78	54.10 o
3	7	0	88.91	111.03	54.71 o
5	7	0	673.48	680.36	85.02 o
7	7	0	1924.16	2122.35	169.83 o
0	8	0	54.81	91.83	48.00 o
2	8	0	1393.08	1342.02	101.42 o
4	8	0	2083.13	2145.32	143.91 o
6	8	0	138.82	179.29	46.16 o
10	8	0	1192.02	1285.19	80.82 o
1	9	0	292.61	336.51	44.69 o
3	9	0	1291.52	1265.34	71.37 o
7	9	0	1165.03	1275.13	85.86 o
0	10	0	10929.63	10901.45	380.08 o
2	10	0	1261.45	1272.35	155.13 o
4	10	0	6516.65	6951.41	280.16 o
6	10	0	1795.60	1811.83	285.41 o
-13	1	1	137.07	285.67	87.76 o
-11	1	1	222.14	181.20	45.29 o
-9	1	1	90.00	93.04	63.05 o
-5	1	1	2199.74	2330.37	241.88 o
-3	1	1	3034.78	3155.67	171.68 o
3	1	1	2446.52	2384.84	140.26 o
5	1	1	1001.40	4127.54	4506.80 o
9	1	1	346.90	335.61	49.15 o
11	1	1	777.59	701.21	136.17 o
-12	2	1	9181.33	9123.21	587.21 o
-10	2	1	994.31	951.89	84.22 o
-8	2	1	5423.41	5354.83	226.39 o
-6	2	1	9289.86	9341.53	346.61 o
-4	2	1	14098.81	14772.44	1446.15 o
-2	2	1	41008.02	41292.89	1124.15 o
0	2	1	473.21	410.03	47.98 o

2	2	1	30327.34	30709.41	1581.44 o
4	2	1	5656.29	5506.63	607.60 o
6	2	1	13824.48	13695.19	348.07 o
8	2	1	5373.39	5478.09	224.95 o
10	2	1	578.34	543.33	69.76 o
12	2	1	4810.52	4316.48	270.45 o
-13	3	1	1809.61	1900.60	119.52 o
-11	3	1	2832.38	2619.90	223.39 o
-9	3	1	12082.85	11929.69	577.19 o
-7	3	1	73.81	99.44	28.40 o
-5	3	1	24185.44	23359.53	2194.93 o
-3	3	1	22047.23	23581.70	569.81 o
-1	3	1	22330.23	21739.72	706.98 o
1	3	1	1275.69	929.74	176.83 o
3	3	1	8188.77	8143.75	307.69 o
5	3	1	38154.46	37372.02	975.10 o
7	3	1	207.54	227.56	37.40 o
9	3	1	5947.28	5997.39	314.50 o
11	3	1	1315.00	1155.73	91.63 o
-12	4	1	1756.37	1930.05	98.01 o
-10	4	1	220.60	225.57	76.15 o
-8	4	1	10.78	95.55	51.36 o
-6	4	1	300.46	325.98	30.91 o
-4	4	1	488.57	434.83	29.10 o
-2	4	1	2662.54	2778.05	119.06 o
0	4	1	3254.36	3297.06	195.67 o
2	4	1	3179.31	2930.52	292.66 o
4	4	1	113.98	134.70	38.99 o
6	4	1	935.92	952.66	62.50 o
10	4	1	306.04	239.19	79.36 o
-9	5	1	277.20	367.36	67.91 o
-7	5	1	371.89	351.55	55.86 o
-5	5	1	451.78	456.31	69.47 o
-1	5	1	2091.75	2092.24	100.54 o
1	5	1	570.66	512.14	39.23 o
5	5	1	997.01	1020.58	48.35 o
7	5	1	322.44	353.78	136.28 o
-10	6	1	254.08	224.76	76.93 o
-6	6	1	407.41	466.20	42.45 o
-4	6	1	520.46	499.41	35.63 o
-2	6	1	873.12	896.30	43.43 o
0	6	1	1773.80	1643.55	95.64 o
8	6	1	315.67	270.38	46.79 o
10	6	1	326.16	208.13	90.78 o
-11	7	1	1216.44	1151.38	87.64 o
-9	7	1	2677.77	2443.77	272.88 o
-7	7	1	601.98	620.02	48.70 o
-5	7	1	16160.75	16127.06	396.38 o
-3	7	1	767.89	642.00	75.79 o
-1	7	1	6417.43	6216.64	210.65 o
1	7	1	9308.48	8886.44	241.63 o
3	7	1	1578.77	1659.52	153.00 o
5	7	1	6738.40	6525.43	453.13 o
7	7	1	1427.11	1233.48	265.65 o

9	7	1	5629.99	5551.28	678.65 o
-10	8	1	556.53	443.90	116.97 o
-8	8	1	4140.13	3569.21	407.56 o
-6	8	1	2415.40	2227.59	137.46 o
-4	8	1	2623.19	2646.81	130.16 o
-2	8	1	18163.47	17844.09	501.51 o
2	8	1	7707.21	7514.67	459.69 o
4	8	1	2428.74	2213.41	217.01 o
6	8	1	7630.09	7432.87	447.25 o
8	8	1	1526.11	1574.52	155.37 o
-9	9	1	360.82	235.40	61.35 o
-7	9	1	1659.62	1444.05	98.59 o
-5	9	1	3567.18	3614.91	202.66 o
-3	9	1	116.80	134.42	58.79 o
1	9	1	16.15	95.53	62.10 o
3	9	1	56.65	145.64	72.25 o
5	9	1	2150.68	1997.22	118.77 o
-8	10	1	619.99	495.24	226.82 o
-4	10	1	301.14	247.94	85.61 o
-2	10	1	2827.23	3008.26	261.39 o
2	10	1	325.14	417.45	137.30 o
4	10	1	632.12	615.62	176.89 o
6	10	1	1241.22	1124.52	85.20 o
-5	11	1	478.80	385.69	86.94 o
-1	11	1	39.66	168.01	77.60 o
1	11	1	1195.63	1275.20	145.33 o
-2	12	1	2387.98	2556.58	151.25 o
2	12	1	4088.44	4217.74	501.73 o
-11	1	2	282.17	362.42	47.25 o
-12	2	2	740.70	719.70	91.68 o
-10	2	2	1161.28	1254.58	63.02 o
-8	2	2	198.69	159.15	51.63 o
-6	2	2	1164.73	1151.25	80.85 o
-13	3	2	357.76	162.11	91.00 o
-11	3	2	8.10	237.75	65.94 o
-9	3	2	297.48	295.56	71.42 o
-7	3	2	601.73	683.76	43.16 o
-5	3	2	706.72	813.75	36.31 o
5	3	2	921.21	1014.70	79.79 o
7	3	2	488.22	536.61	72.17 o
-10	4	2	1891.64	2097.55	167.38 o
-8	4	2	988.18	974.49	55.44 o
-6	4	2	1733.24	1830.16	160.80 o
-4	4	2	1123.52	1099.85	60.60 o
-2	4	2	264.50	349.73	103.94 o
0	4	2	10097.38	10480.72	908.49 o
2	4	2	144.26	165.60	36.95 o
4	4	2	5142.58	5019.12	211.65 o
6	4	2	479.04	266.33	85.74 o
8	4	2	165.36	62.24	68.92 o
-11	5	2	4635.68	4891.19	484.06 o
-9	5	2	2264.01	2337.70	216.46 o
-7	5	2	17772.23	16148.99	2321.62 o
-5	5	2	2943.61	3194.28	147.56 o

-3	5	2	22928.05	22543.23	868.92 o
-1	5	2	3358.61	3196.91	130.94 o
1	5	2	14646.16	15145.52	399.29 o
3	5	2	22859.15	20764.92	1106.57 o
5	5	2	1382.85	1689.55	211.86 o
7	5	2	8162.17	8322.03	274.32 o
9	5	2	1519.39	1757.99	80.32 o
-10	6	2	816.59	925.85	66.82 o
-8	6	2	687.79	598.42	154.61 o
-6	6	2	6847.22	6612.41	550.52 o
-4	6	2	1277.06	1425.27	86.09 o
-2	6	2	1110.79	1182.53	61.04 o
0	6	2	17023.61	16035.69	740.75 o
2	6	2	604.42	673.37	53.05 o
4	6	2	2575.73	2614.12	151.68 o
8	6	2	1555.52	1561.12	82.56 o
-9	7	2	46.52	82.15	71.43 o
-7	7	2	1023.03	1058.30	172.03 o
-3	7	2	846.52	884.62	189.13 o
-1	7	2	301.58	349.03	60.49 o
1	7	2	352.84	229.81	54.64 o
3	7	2	1378.66	1242.34	134.45 o
5	7	2	342.49	327.44	68.54 o
7	7	2	143.51	158.51	83.83 o
-10	8	2	539.12	589.73	105.33 o
-8	8	2	919.91	713.25	249.21 o
-4	8	2	508.34	452.66	46.76 o
-2	8	2	1560.84	1580.45	91.51 o
0	8	2	721.26	649.83	64.79 o
2	8	2	330.05	453.59	68.96 o
4	8	2	1021.20	1030.94	88.27 o
6	8	2	848.60	878.12	156.75 o
-7	9	2	1899.63	1774.48	248.47 o
-3	9	2	782.03	682.53	86.19 o
1	9	2	764.03	711.81	81.50 o
7	9	2	977.88	1187.31	74.39 o
-6	10	2	2868.68	2391.91	586.96 o
-4	10	2	5198.24	5386.60	352.14 o
-2	10	2	1422.27	1247.18	151.03 o
0	10	2	7729.63	7608.03	285.59 o
2	10	2	925.96	959.53	102.19 o
4	10	2	8334.93	8725.99	322.33 o
-3	11	2	1710.16	1671.83	194.10 o
-1	11	2	46.79	128.83	82.51 o
1	11	2	1298.37	1257.48	78.98 o
3	11	2	1871.15	1778.60	98.01 o
-4	8	3	2622.10	2828.51	230.71 o
-1	9	3	3471.59	2824.61	207.61 o
-2	10	3	633.23	681.02	62.09 o
1	11	3	198.81	452.06	96.11 o