

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_caznp1
_shelx_title ' CaZnSi2O6 data collection i n DAC by Xcaliber-I at VT'
_shelx_refln_list_code      4
_shelx_F_calc_maximum      204.48
_exptl_crystal_F_000       504.00
_reflns_d_resolution_high  0.7111
```

```
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    9.7738
_cell_length_b    8.9371
_cell_length_c    5.2335
_cell_angle_alpha 90.000
_cell_angle_beta  105.590
_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
  2  0  0   5262.20   5676.67   269.56 o
  4  0  0   6419.68   5778.02   142.28 o
  6  0  0  18935.78  20406.70   458.17 o
  8  0  0  14802.34  14667.83   374.95 o
 10  0  0   7211.54   7520.56   273.29 o
 12  0  0   337.04    291.12    82.93 o
  1  1  0   3202.19   3347.10    96.74 o
  3  1  0  17121.36  18235.76   589.45 o
  5  1  0   485.20    622.57   102.46 o
  7  1  0   6059.32   6382.67   419.25 o
  9  1  0   641.74    641.80    50.54 o
 11  1  0   2730.76   2778.86   168.89 o
  0  2  0   2278.16   2121.54    83.75 o
  2  2  0   1910.49   2074.94   149.58 o
  8  2  0    85.84    124.42    47.61 o
```

10	2	0	80.07	158.55	69.41 o
12	2	0	136.98	194.93	65.33 o
3	3	0	2957.19	3214.34	104.11 o
5	3	0	1088.97	1093.89	67.07 o
7	3	0	171.40	194.45	36.34 o
9	3	0	747.32	779.79	53.70 o
11	3	0	213.07	152.23	48.38 o
0	4	0	2420.36	2137.73	92.39 o
2	4	0	611.08	548.46	70.73 o
4	4	0	10176.75	10375.96	446.12 o
8	4	0	204.40	231.49	76.59 o
10	4	0	4749.01	4739.25	480.59 o
12	4	0	36.16	53.04	89.80 o
1	5	0	23300.38	23055.55	781.80 o
3	5	0	13835.98	13696.87	382.51 o
5	5	0	1143.02	1171.71	88.77 o
7	5	0	23833.27	24976.54	618.27 o
9	5	0	1812.84	1802.77	130.88 o
11	5	0	4935.97	4908.61	377.13 o
0	6	0	21431.10	20755.09	680.54 o
4	6	0	2552.13	2615.37	258.69 o
6	6	0	672.53	687.93	50.87 o
8	6	0	2053.10	2114.35	124.54 o
10	6	0	3042.42	3020.38	224.02 o
1	7	0	437.25	382.11	46.66 o
5	7	0	936.09	835.56	70.59 o
7	7	0	1832.39	2020.76	212.19 o
9	7	0	123.18	119.53	87.44 o
2	8	0	933.59	1012.43	75.16 o
4	8	0	1953.63	1999.41	142.95 o
10	8	0	1141.39	1298.71	110.75 o
1	9	0	239.31	334.61	111.57 o
3	9	0	1428.04	1334.74	80.75 o
7	9	0	885.29	966.67	89.23 o
0	10	0	11180.20	11162.20	517.10 o
2	10	0	1374.31	1520.32	183.33 o
4	10	0	6695.05	7503.89	278.87 o
6	10	0	1988.07	1952.53	212.49 o
8	10	0	2013.44	2050.65	298.98 o
1	11	0	962.19	985.93	80.97 o
3	11	0	2072.23	1975.92	142.46 o
5	11	0	167.97	163.97	74.38 o
-13	1	1	164.32	136.68	78.31 o
-11	1	1	252.20	226.43	44.57 o
-9	1	1	113.53	135.55	53.83 o
-7	1	1	271.14	308.80	52.06 o
-5	1	1	2082.16	2037.22	160.03 o
-3	1	1	3075.74	3306.13	227.52 o
3	1	1	2239.82	2446.47	147.81 o
5	1	1	879.62	955.21	104.76 o
9	1	1	438.63	448.35	57.38 o
11	1	1	784.61	749.72	94.84 o
-12	2	1	9026.76	9260.27	338.04 o
-10	2	1	1092.24	949.57	102.94 o

-8	2	1	5318.44	5134.40	300.46 o
-6	2	1	8892.68	8389.75	595.33 o
-4	2	1	14310.74	14261.24	389.63 o
-2	2	1	41811.07	41921.70	1124.88 o
0	2	1	418.97	331.17	29.41 o
2	2	1	29697.82	28532.62	1603.67 o
4	2	1	5705.29	5867.56	492.75 o
6	2	1	14083.19	13786.81	382.39 o
8	2	1	5052.17	5294.36	204.51 o
10	2	1	576.41	420.12	110.33 o
12	2	1	4761.12	4822.21	349.05 o
-13	3	1	1953.53	2112.99	111.67 o
-11	3	1	2973.11	2920.68	182.70 o
-9	3	1	12010.00	11700.05	500.01 o
-7	3	1	79.96	114.39	31.89 o
-5	3	1	25238.68	25421.56	690.99 o
-3	3	1	22269.26	24196.96	595.28 o
-1	3	1	22801.34	21684.37	779.53 o
1	3	1	1331.66	1071.18	109.83 o
3	3	1	8442.58	8724.45	281.31 o
5	3	1	38754.29	37414.86	950.68 o
7	3	1	210.67	177.64	37.15 o
9	3	1	5949.98	5962.57	246.13 o
11	3	1	1297.64	1158.13	127.42 o
-12	4	1	1806.88	1994.38	110.00 o
-10	4	1	214.86	242.30	68.28 o
-6	4	1	257.12	276.45	34.46 o
-4	4	1	421.10	406.13	28.16 o
-2	4	1	2814.43	3021.53	344.16 o
0	4	1	3467.55	3360.76	232.23 o
2	4	1	3124.88	3248.63	287.76 o
4	4	1	184.95	182.00	27.40 o
6	4	1	1074.34	954.18	115.59 o
8	4	1	211.09	297.26	46.16 o
10	4	1	355.89	347.01	78.80 o
-9	5	1	201.64	268.93	63.19 o
-5	5	1	374.86	395.77	47.15 o
-3	5	1	61.06	126.45	39.99 o
-1	5	1	1725.27	1596.95	185.24 o
1	5	1	409.77	427.07	34.78 o
3	5	1	128.71	124.31	28.07 o
5	5	1	768.63	760.35	46.44 o
7	5	1	155.72	68.10	58.70 o
9	5	1	143.94	141.02	65.46 o
11	5	1	26.95	101.28	83.52 o
-10	6	1	251.35	226.82	78.56 o
-4	6	1	493.33	573.15	89.26 o
-2	6	1	704.27	701.79	79.01 o
0	6	1	1210.45	1197.29	119.27 o
8	6	1	231.83	219.95	50.27 o
-11	7	1	1141.50	1041.51	245.39 o
-9	7	1	2794.99	2788.65	157.76 o
-7	7	1	629.32	526.80	52.59 o
-5	7	1	15444.53	15316.04	395.53 o

-3	7	1	845.34	843.20	102.72 o
-1	7	1	6508.66	6328.70	218.58 o
1	7	1	9250.40	9316.21	314.24 o
3	7	1	1618.70	1628.30	181.82 o
5	7	1	6401.20	6308.20	221.76 o
7	7	1	1530.94	1400.54	139.77 o
9	7	1	5479.88	5688.84	290.62 o
-10	8	1	613.91	559.56	119.22 o
-8	8	1	4306.07	4223.50	219.76 o
-6	8	1	2639.33	2918.07	283.21 o
-4	8	1	2927.59	2969.06	365.68 o
-2	8	1	19101.06	18692.54	542.29 o
0	8	1	122.54	208.10	53.87 o
2	8	1	8258.31	7846.17	279.89 o
4	8	1	2760.25	2549.56	171.68 o
6	8	1	7903.83	7754.80	313.77 o
8	8	1	1521.48	1545.51	205.26 o
-9	9	1	447.97	458.98	92.71 o
-7	9	1	2070.59	2168.89	165.66 o
-5	9	1	3743.05	3757.97	206.61 o
-3	9	1	129.18	60.70	60.04 o
-1	9	1	139.38	254.13	61.42 o
3	9	1	38.21	31.74	61.45 o
5	9	1	2442.46	2161.07	608.28 o
7	9	1	502.71	467.72	202.91 o
-8	10	1	463.12	333.53	90.94 o
-2	10	1	2412.77	2350.34	115.77 o
2	10	1	257.02	258.75	48.95 o
6	10	1	999.77	949.33	72.14 o
-5	11	1	494.06	430.76	77.52 o
1	11	1	1065.47	853.48	88.32 o
3	11	1	133.91	180.60	78.07 o
-4	12	1	1311.02	1021.13	225.81 o
-2	12	1	2140.51	2331.17	150.38 o
0	12	1	239.08	230.09	78.22 o
2	12	1	3936.38	4222.86	260.18 o
7	1	2	6276.45	6440.67	533.65 o
9	1	2	60.55	118.27	75.42 o
6	2	2	984.50	1041.21	66.35 o
8	2	2	510.25	507.28	51.30 o
10	2	2	371.92	439.24	61.70 o
-9	3	2	133.92	229.95	62.02 o
-7	3	2	597.44	571.29	43.33 o
5	3	2	709.76	782.09	48.58 o
7	3	2	450.15	415.82	74.94 o
9	3	2	92.58	100.85	69.65 o
-10	4	2	1861.00	1712.96	84.41 o
-8	4	2	817.55	829.73	97.69 o
-6	4	2	1888.81	2048.14	303.61 o
-4	4	2	1205.67	1441.99	94.10 o
-2	4	2	250.33	389.36	32.24 o
0	4	2	9866.13	9159.31	1536.75 o
2	4	2	147.07	136.01	36.64 o
4	4	2	5072.72	4544.08	304.49 o

6	4	2	552.76	527.74	54.79 o
10	4	2	699.36	685.48	151.36 o
-11	5	2	4461.16	4252.75	251.96 o
-9	5	2	2369.55	2557.34	186.22 o
-7	5	2	18078.87	17237.52	606.13 o
-5	5	2	2999.14	3500.76	773.45 o
-3	5	2	23366.61	22393.09	869.21 o
-1	5	2	3328.81	3337.62	151.78 o
1	5	2	15215.42	15567.54	1451.20 o
3	5	2	22952.02	22656.79	1376.95 o
5	5	2	1361.23	1871.02	104.83 o
7	5	2	8132.52	7879.62	281.95 o
9	5	2	1602.72	1637.95	221.26 o
-10	6	2	782.37	827.51	62.64 o
-8	6	2	705.68	763.29	99.08 o
-6	6	2	7704.51	7473.59	298.23 o
-4	6	2	1336.27	1532.31	172.72 o
-2	6	2	1229.51	1474.69	91.85 o
0	6	2	18063.62	17611.32	644.41 o
2	6	2	673.49	657.39	58.34 o
4	6	2	2801.80	2868.92	158.92 o
8	6	2	1715.17	1872.85	112.09 o
10	6	2	1435.05	1416.79	94.41 o
-11	7	2	28.85	164.51	76.79 o
-7	7	2	913.75	817.48	55.27 o
-5	7	2	293.53	254.43	65.24 o
-3	7	2	924.46	941.61	46.25 o
3	7	2	1310.54	1161.73	333.03 o
5	7	2	475.27	439.20	72.05 o
7	7	2	94.64	88.56	70.29 o
9	7	2	52.98	170.41	92.08 o
-10	8	2	458.63	471.20	61.71 o
-8	8	2	610.35	469.74	210.47 o
-4	8	2	365.16	368.26	94.42 o
-2	8	2	1029.41	1031.40	52.25 o
0	8	2	698.62	700.41	48.48 o
4	8	2	884.80	891.42	72.39 o
6	8	2	666.93	693.61	93.67 o
-7	9	2	1717.37	1540.77	196.12 o
-3	9	2	728.03	700.81	88.84 o
1	9	2	710.07	636.52	82.26 o
3	9	2	517.59	449.39	104.44 o
7	9	2	889.47	978.68	102.95 o
-8	10	2	1808.83	1845.64	166.90 o
-6	10	2	2784.93	3010.07	242.17 o
-4	10	2	5596.34	5382.83	265.40 o
-2	10	2	1697.93	1785.74	126.80 o
0	10	2	7445.45	7370.39	324.59 o
2	10	2	1016.87	1108.69	72.50 o
4	10	2	8746.49	8287.99	398.22 o
6	10	2	967.80	1009.20	161.56 o
-3	11	2	1742.97	1528.09	113.03 o
1	11	2	1713.00	1694.07	83.69 o
3	11	2	1931.68	1819.01	206.04 o

-2	12	2	795.65	734.96	74.88 o
0	12	2	1391.26	1482.45	141.05 o