

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_caznp0
_shelx_title ' CaZnSi2O6 data collection i n DAC by Xcaliber-I at VT'
_shelx_refl_list_code      4
_shelx_F_calc_maximum     205.44
_exptl_crystal_F_000      504.00
_reflns_d_resolution_high 0.7143
```

```
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  9.8055
_cell_length_b  8.9778
_cell_length_c  5.2499
_cell_angle_alpha 90.000
_cell_angle_beta 105.761
_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 5332.27 5621.38 120.93 o
 4 0 0 6353.26 5472.28 180.03 o
 6 0 0 18495.93 19050.10 1373.36 o
 8 0 0 15108.14 14888.10 512.10 o
10 0 0 7173.27 7226.51 260.90 o
 1 1 0 3189.14 3374.34 100.02 o
 3 1 0 17138.13 17491.00 722.39 o
 5 1 0 466.92 663.34 111.49 o
 7 1 0 6063.63 6329.09 184.33 o
 9 1 0 608.29 669.69 105.09 o
11 1 0 2757.05 2946.33 185.52 o
13 1 0 22.99 161.71 75.30 o
 0 2 0 2257.35 2078.08 191.54 o
 2 2 0 2087.07 2231.31 98.36 o
 6 2 0 42.31 78.45 32.40 o
```

8	2	0	92.05	97.26	46.95 o
10	2	0	50.34	96.48	58.17 o
12	2	0	144.69	266.04	78.60 o
3	3	0	2815.48	3059.67	116.82 o
5	3	0	1003.78	995.91	74.51 o
7	3	0	181.80	241.62	49.64 o
9	3	0	710.14	828.89	55.83 o
11	3	0	202.32	116.57	66.44 o
0	4	0	2295.13	1959.35	79.82 o
2	4	0	561.62	696.51	96.90 o
4	4	0	10159.76	10472.12	481.42 o
6	4	0	28.27	81.91	41.51 o
8	4	0	188.21	245.60	55.50 o
10	4	0	4510.74	4263.64	232.63 o
1	5	0	23774.13	24278.75	740.15 o
3	5	0	13422.12	13442.87	376.63 o
5	5	0	1115.57	1119.43	60.35 o
7	5	0	24246.94	24911.13	935.74 o
9	5	0	1751.58	1682.05	117.39 o
11	5	0	4788.16	4518.31	348.90 o
0	6	0	21556.02	20843.93	698.41 o
2	6	0	80.08	69.32	53.76 o
4	6	0	2701.72	2589.34	233.10 o
6	6	0	617.07	751.00	91.28 o
8	6	0	2123.19	2226.68	277.10 o
10	6	0	3174.56	3262.47	420.45 o
1	7	0	353.17	355.81	34.49 o
5	7	0	1068.40	875.18	95.78 o
7	7	0	1762.28	1845.79	105.66 o
2	8	0	778.67	817.54	62.81 o
4	8	0	1844.72	1841.03	108.39 o
10	8	0	1048.27	1122.15	76.21 o
1	9	0	189.18	193.47	48.24 o
3	9	0	1461.82	1416.47	87.88 o
7	9	0	752.65	884.78	145.76 o
0	10	0	11485.54	11034.72	423.98 o
2	10	0	1338.48	1389.33	159.32 o
4	10	0	6532.87	7116.32	393.77 o
6	10	0	2072.72	2238.01	145.69 o
8	10	0	2065.13	2172.98	135.82 o
1	11	0	1028.08	1083.69	71.79 o
3	11	0	2121.19	2475.69	386.38 o
-13	1	1	138.13	32.07	99.29 o
-11	1	1	267.24	251.19	44.50 o
-9	1	1	144.09	183.36	58.18 o
-7	1	1	280.61	433.74	72.41 o
-5	1	1	1947.97	1908.68	100.96 o
-3	1	1	3050.55	3351.34	105.35 o
1	1	1	298.24	291.41	16.72 o
3	1	1	2141.49	2339.84	146.54 o
5	1	1	836.64	862.01	55.09 o
9	1	1	458.59	361.85	47.77 o
11	1	1	765.06	660.38	74.83 o
-12	2	1	8935.66	9234.12	758.49 o

-10	2	1	1110.19	958.53	57.62 o
-8	2	1	5181.91	5088.19	263.02 o
-6	2	1	8703.80	8387.29	237.82 o
-4	2	1	14222.85	14417.83	375.23 o
-2	2	1	42205.32	43863.04	1144.61 o
0	2	1	371.20	319.76	31.52 o
2	2	1	29414.53	28234.03	900.12 o
4	2	1	5748.08	5985.87	291.29 o
6	2	1	14059.68	14292.88	383.41 o
8	2	1	4788.06	4822.37	305.40 o
10	2	1	568.93	487.09	73.68 o
12	2	1	4703.00	4711.34	273.01 o
-13	3	1	2059.21	2171.71	118.91 o
-11	3	1	2963.20	2775.58	183.42 o
-9	3	1	11881.02	11502.09	387.82 o
-5	3	1	25764.48	25925.83	637.32 o
-3	3	1	22367.28	23862.38	765.02 o
-1	3	1	22903.68	21719.80	829.65 o
1	3	1	1399.17	1099.92	61.57 o
3	3	1	8436.85	8903.37	294.27 o
5	3	1	38887.73	38296.48	1039.18 o
7	3	1	231.17	265.94	37.26 o
9	3	1	5850.22	6115.53	239.12 o
11	3	1	1177.37	1221.94	139.90 o
-12	4	1	1799.39	2266.39	127.84 o
-10	4	1	228.00	300.00	62.35 o
-6	4	1	250.90	282.46	94.25 o
-4	4	1	366.57	299.35	34.15 o
-2	4	1	2851.41	2803.51	123.01 o
0	4	1	3506.49	3496.40	386.67 o
2	4	1	3112.83	3490.70	445.78 o
4	4	1	210.37	213.86	26.63 o
6	4	1	1080.82	1025.14	57.74 o
8	4	1	186.09	277.57	73.51 o
10	4	1	365.65	396.46	52.67 o
-9	5	1	199.23	170.73	59.17 o
-7	5	1	173.22	219.32	49.87 o
-5	5	1	302.07	302.24	51.48 o
-3	5	1	102.41	145.50	32.91 o
-1	5	1	1560.14	1480.22	149.44 o
1	5	1	331.01	343.95	50.34 o
3	5	1	173.46	205.34	42.43 o
5	5	1	677.58	679.23	47.69 o
-6	6	1	203.85	127.61	33.39 o
-4	6	1	504.91	563.68	40.90 o
-2	6	1	642.60	727.41	39.72 o
0	6	1	1052.40	1113.86	88.81 o
4	6	1	118.67	193.05	55.66 o
8	6	1	210.20	203.04	62.87 o
10	6	1	222.10	290.68	79.19 o
-11	7	1	1075.14	860.41	92.30 o
-9	7	1	2858.17	2922.50	190.45 o
-7	7	1	572.83	615.83	79.25 o
-5	7	1	14949.88	14393.94	353.12 o

-3	7	1	866.34	892.87	46.58 o
-1	7	1	6423.81	6097.74	232.39 o
1	7	1	8930.04	8323.57	262.46 o
3	7	1	1652.34	1807.12	165.82 o
5	7	1	6274.18	5993.77	544.59 o
7	7	1	1381.04	1405.24	77.96 o
9	7	1	5407.75	5172.94	890.31 o
-10	8	1	672.42	611.44	134.09 o
-8	8	1	4265.31	4141.86	230.68 o
-6	8	1	2651.19	2675.95	175.61 o
-4	8	1	3060.50	2853.76	159.09 o
-2	8	1	19574.31	18754.09	805.22 o
2	8	1	8403.09	8190.95	254.11 o
4	8	1	2867.55	2573.40	505.77 o
6	8	1	8109.40	8044.22	267.31 o
8	8	1	1456.18	1496.56	101.50 o
-9	9	1	420.36	527.80	170.93 o
-7	9	1	2168.67	1879.80	122.83 o
-5	9	1	3797.41	3687.25	212.79 o
-3	9	1	110.35	41.92	54.12 o
5	9	1	2447.58	2396.68	143.74 o
7	9	1	525.56	473.10	85.87 o
-8	10	1	387.13	561.76	97.70 o
-2	10	1	2189.07	2061.87	448.09 o
2	10	1	203.88	181.29	45.12 o
6	10	1	912.26	717.69	226.86 o
-5	11	1	487.10	295.93	82.90 o
1	11	1	990.01	1068.69	205.92 o
-4	12	1	1224.02	1178.95	159.57 o
-2	12	1	1988.23	1948.76	118.08 o
2	12	1	3863.04	3720.65	260.88 o
7	1	2	6302.69	6184.99	226.91 o
4	2	2	3129.25	3256.95	140.11 o
6	2	2	1000.12	1125.02	353.15 o
8	2	2	523.18	487.43	51.86 o
10	2	2	334.86	451.60	88.84 o
-7	3	2	603.06	686.86	85.26 o
3	3	2	169.18	128.86	39.54 o
5	3	2	590.84	590.39	44.64 o
7	3	2	460.70	450.69	62.86 o
-10	4	2	1728.28	1657.27	91.50 o
-8	4	2	725.44	805.66	90.42 o
-6	4	2	1939.74	2097.46	125.05 o
-4	4	2	1234.95	1333.31	88.20 o
-2	4	2	192.84	374.49	66.35 o
0	4	2	9808.01	9439.19	275.44 o
2	4	2	138.47	200.18	39.43 o
4	4	2	4782.65	4527.76	179.24 o
6	4	2	524.75	506.77	177.82 o
8	4	2	180.87	176.06	47.14 o
10	4	2	602.85	630.83	71.43 o
-11	5	2	4425.35	4332.95	241.56 o
-9	5	2	2266.00	2124.41	444.92 o
-7	5	2	18175.77	18753.92	870.76 o

-5	5	2	3032.46	3440.54	148.55 o
-3	5	2	23359.50	23024.48	654.74 o
-1	5	2	3293.53	3353.19	145.34 o
1	5	2	15292.51	15539.42	472.61 o
3	5	2	22894.93	21455.65	692.76 o
5	5	2	1344.90	1775.50	127.19 o
7	5	2	7987.08	8659.24	315.48 o
9	5	2	1575.15	1911.60	242.45 o
-10	6	2	766.97	886.60	68.65 o
-8	6	2	762.10	806.16	51.16 o
-6	6	2	7834.61	7093.65	801.95 o
-4	6	2	1350.90	1488.23	83.65 o
-2	6	2	1242.96	1635.75	85.99 o
0	6	2	18442.43	17979.47	949.34 o
2	6	2	700.11	664.88	43.29 o
4	6	2	2874.24	2595.98	246.33 o
8	6	2	1758.90	1807.03	98.83 o
10	6	2	1449.97	1514.69	86.04 o
-11	7	2	22.46	94.91	71.26 o
-9	7	2	87.73	29.78	77.63 o
-7	7	2	814.82	850.10	52.50 o
-5	7	2	391.65	504.06	76.40 o
-3	7	2	937.16	959.77	211.57 o
-1	7	2	637.75	724.33	65.63 o
1	7	2	113.44	94.21	47.90 o
3	7	2	1246.27	1112.51	81.49 o
5	7	2	515.04	521.94	84.84 o
-8	8	2	500.91	443.28	55.68 o
-6	8	2	253.09	245.22	127.71 o
-4	8	2	307.65	330.22	64.36 o
-2	8	2	817.26	871.03	52.92 o
0	8	2	691.74	706.41	47.26 o
4	8	2	747.42	739.90	55.59 o
6	8	2	597.89	667.54	81.00 o
-7	9	2	1630.77	1789.13	92.52 o
-3	9	2	682.96	705.44	151.25 o
1	9	2	655.39	604.15	53.11 o
3	9	2	451.07	413.49	70.84 o
7	9	2	846.95	954.35	69.39 o
-8	10	2	1730.55	1737.45	255.66 o
-6	10	2	2791.73	3095.82	199.71 o
-4	10	2	5726.02	5677.31	570.80 o
-2	10	2	1662.69	1774.82	244.33 o
0	10	2	7363.72	7261.20	317.73 o
2	10	2	1045.50	1155.22	113.53 o
4	10	2	8715.87	8573.08	370.03 o
6	10	2	910.53	869.88	402.02 o
-3	11	2	1693.30	1694.56	115.81 o
1	11	2	1906.67	1748.17	103.30 o
3	11	2	1928.67	1815.13	160.81 o
-2	12	2	895.90	871.41	68.13 o
0	12	2	1228.62	1244.67	86.52 o
2	10	3	1038.89	918.92	80.77 o