

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_caznp6
_shelx_title ' CaZnSi2O6 data collection i n DAC by Xcaliber-I at VT'
_shelx_refl_list_code      4
_shelx_F_calc_maximum     200.40
_exptl_crystal_F_000      504.00
_reflns_d_resolution_high  0.7142
```

```
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  9.6418
_cell_length_b  8.7601
_cell_length_c  5.1572
_cell_angle_alpha 90.000
_cell_angle_beta  104.916
_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  5283.15  5761.50  306.73 o
  4  0  0  6345.61  5716.34  549.43 o
  6  0  0 18999.35 19888.74  420.84 o
  8  0  0 14485.63 14284.71  308.54 o
 10  0  0  7088.57  7343.57  668.03 o
  1  1  0  3141.53  3270.49  182.26 o
  3  1  0 16465.80 16565.92  457.33 o
  5  1  0   395.13   519.81   62.22 o
  7  1  0  5898.17  6207.23  185.70 o
  9  1  0   538.90   566.96  103.71 o
 11  1  0  2677.31  2874.97  206.96 o
  0  2  0  2284.20  2125.31   62.61 o
  2  2  0  1333.94  1357.74   65.48 o
  6  2  0    40.12   20.92   37.87 o
  1  3  0    35.13   14.31   11.84 o
```

3	3	0	3440.04	3799.03	122.09 o
5	3	0	1700.88	1641.06	110.37 o
7	3	0	162.76	256.45	31.96 o
9	3	0	855.60	915.19	58.42 o
11	3	0	331.51	360.77	69.38 o
0	4	0	3093.93	2671.53	143.20 o
2	4	0	529.23	595.32	79.98 o
4	4	0	9857.31	10400.19	286.40 o
6	4	0	18.46	90.87	43.27 o
10	4	0	4786.57	4643.42	306.56 o
1	5	0	21302.75	21464.23	690.88 o
3	5	0	14694.10	14553.73	621.38 o
5	5	0	1002.20	969.35	54.56 o
7	5	0	22405.92	23461.53	1237.73 o
9	5	0	1860.72	2094.87	123.93 o
11	5	0	4849.89	4662.07	337.52 o
0	6	0	20208.27	19789.59	559.43 o
2	6	0	32.80	93.31	43.25 o
4	6	0	2189.31	2197.81	130.74 o
6	6	0	734.97	654.64	94.66 o
8	6	0	1647.15	1760.11	100.88 o
10	6	0	2562.44	2757.62	463.62 o
1	7	0	750.41	768.57	72.54 o
5	7	0	495.35	504.80	114.54 o
7	7	0	2005.90	2127.00	197.49 o
0	8	0	102.84	170.39	52.84 o
2	8	0	1589.57	1662.70	100.17 o
4	8	0	2180.57	2234.57	156.71 o
6	8	0	229.12	238.99	46.75 o
8	8	0	286.22	334.02	62.45 o
1	9	0	375.47	359.50	131.15 o
3	9	0	1107.58	1100.64	122.03 o
5	9	0	66.01	187.30	62.96 o
7	9	0	1383.79	1530.53	291.39 o
0	10	0	10140.83	10206.44	317.29 o
2	10	0	1147.76	1236.48	94.95 o
4	10	0	6394.66	5671.41	2357.54 o
6	10	0	1557.42	1587.92	273.18 o
-13	1	1	133.38	248.46	84.11 o
-11	1	1	218.25	189.27	44.08 o
-7	1	1	354.05	422.97	50.15 o
-5	1	1	2216.14	2288.06	219.48 o
-3	1	1	3035.68	3202.90	96.03 o
1	1	1	223.19	212.35	13.04 o
3	1	1	2328.39	2556.31	93.00 o
5	1	1	975.15	1014.03	47.90 o
9	1	1	354.81	413.98	47.94 o
11	1	1	775.98	716.67	63.72 o
-12	2	1	9079.22	9269.34	326.44 o
-10	2	1	966.34	1018.81	123.08 o
-8	2	1	5414.50	5308.67	330.96 o
-6	2	1	9256.03	9223.66	401.62 o
-4	2	1	14167.83	14337.31	473.97 o
-2	2	1	40159.66	40305.53	1040.35 o

0	2	1	526.71	458.56	33.61 o
2	2	1	30951.47	30000.87	978.33 o
4	2	1	5442.01	6222.13	348.07 o
6	2	1	13790.77	13872.75	373.31 o
8	2	1	5312.14	5314.14	205.57 o
10	2	1	586.50	566.38	86.30 o
12	2	1	4719.39	4695.10	270.02 o
-13	3	1	1635.32	1578.55	99.97 o
-11	3	1	2713.59	2701.89	404.36 o
-9	3	1	12029.03	12599.39	361.72 o
-7	3	1	76.80	36.54	42.27 o
-5	3	1	23130.19	23650.90	977.97 o
-3	3	1	21606.94	23366.71	562.65 o
-1	3	1	22699.36	21677.94	702.96 o
1	3	1	1056.47	818.59	64.82 o
3	3	1	8088.96	7870.81	517.05 o
5	3	1	37886.13	37204.42	1344.34 o
7	3	1	165.03	288.58	61.11 o
9	3	1	5733.26	5992.48	314.57 o
11	3	1	1323.90	1325.53	134.64 o
-12	4	1	1730.51	1892.18	111.41 o
-8	4	1	11.70	64.39	55.61 o
-6	4	1	294.15	337.83	32.86 o
-4	4	1	562.21	542.96	27.92 o
-2	4	1	2550.44	2633.19	291.29 o
0	4	1	3138.12	3386.35	313.68 o
2	4	1	3373.99	3332.59	225.40 o
4	4	1	106.50	95.29	53.89 o
6	4	1	918.17	992.28	97.05 o
8	4	1	225.89	211.27	65.97 o
10	4	1	267.87	228.43	103.83 o
-7	5	1	511.70	495.78	41.36 o
-5	5	1	507.35	562.20	74.65 o
-3	5	1	14.99	91.31	35.75 o
-1	5	1	2411.79	2207.57	114.56 o
1	5	1	711.13	634.16	61.37 o
5	5	1	1115.29	995.51	105.79 o
7	5	1	383.85	466.87	98.41 o
9	5	1	168.07	226.18	83.02 o
-10	6	1	253.88	291.93	82.79 o
-6	6	1	507.43	524.83	70.62 o
-4	6	1	519.38	602.14	79.24 o
-2	6	1	986.23	984.98	51.92 o
0	6	1	2075.64	1894.49	109.87 o
6	6	1	57.52	148.12	60.46 o
8	6	1	397.90	383.37	78.06 o
-11	7	1	1248.15	1247.66	210.18 o
-9	7	1	2572.63	2877.51	196.89 o
-7	7	1	556.92	520.69	48.21 o
-5	7	1	16352.09	16189.22	402.65 o
-3	7	1	720.20	616.06	102.36 o
-1	7	1	6258.46	6471.12	220.85 o
1	7	1	9266.79	8827.92	317.21 o
3	7	1	1601.98	1657.60	134.65 o

5	7	1	6547.06	6149.20	640.68 o
7	7	1	1414.95	1353.80	173.08 o
9	7	1	5639.61	5991.08	273.87 o
-10	8	1	445.30	474.54	172.17 o
-8	8	1	4003.41	3534.04	885.60 o
-6	8	1	2210.50	2121.33	145.47 o
-4	8	1	2307.27	2456.06	408.95 o
-2	8	1	17199.81	17119.61	539.98 o
2	8	1	7291.54	7113.42	229.36 o
4	8	1	2144.04	2113.17	123.61 o
6	8	1	7242.27	7170.10	274.30 o
8	8	1	1353.54	1322.08	111.02 o
-9	9	1	373.56	388.84	91.92 o
-7	9	1	1551.72	1584.68	71.56 o
-5	9	1	3482.23	3356.91	202.95 o
-3	9	1	114.62	164.50	61.36 o
-1	9	1	150.66	188.00	59.71 o
5	9	1	2057.01	1993.46	129.37 o
7	9	1	412.49	387.99	61.93 o
-4	10	1	432.61	486.30	83.86 o
-2	10	1	3126.29	3051.47	197.41 o
2	10	1	430.33	674.81	84.45 o
4	10	1	869.95	935.83	124.94 o
6	10	1	1344.35	1181.75	187.41 o
-5	11	1	459.12	330.54	92.56 o
1	11	1	1285.48	1129.47	122.56 o
3	11	1	265.95	321.39	85.77 o
-2	12	1	2464.94	2795.60	197.50 o
8	0	2	7754.22	7150.15	253.20 o
7	1	2	6289.01	6248.03	271.88 o
4	2	2	3118.38	2931.00	132.02 o
6	2	2	834.64	857.59	48.50 o
10	2	2	412.70	409.51	125.12 o
-7	3	2	585.81	648.98	67.75 o
5	3	2	1097.58	1091.09	60.69 o
7	3	2	487.25	505.82	81.39 o
-10	4	2	1932.90	1941.19	271.47 o
-8	4	2	967.06	928.54	60.69 o
-6	4	2	1762.84	1765.91	106.39 o
-4	4	2	1050.62	1123.33	134.59 o
-2	4	2	313.57	312.58	46.38 o
0	4	2	10177.41	10824.20	329.81 o
2	4	2	171.71	178.05	37.65 o
4	4	2	5293.13	5099.12	331.63 o
6	4	2	467.05	353.49	78.42 o
8	4	2	168.75	215.17	74.67 o
10	4	2	804.28	873.01	108.74 o
-11	5	2	4367.99	4441.44	276.78 o
-9	5	2	2234.45	2275.30	119.40 o
-7	5	2	17372.75	16783.00	575.44 o
-5	5	2	2728.42	2887.69	388.09 o
-3	5	2	22645.45	20900.60	1284.54 o
-1	5	2	3244.35	3065.36	126.19 o
1	5	2	14632.52	13850.67	382.09 o

3	5	2	21803.93	21140.36	642.72 o
5	5	2	1366.44	1559.47	153.75 o
7	5	2	8103.28	8251.77	513.96 o
9	5	2	1433.28	1571.71	90.57 o
-10	6	2	811.18	871.88	93.52 o
-8	6	2	529.24	717.83	123.68 o
-6	6	2	6570.11	5467.28	1621.29 o
-4	6	2	1275.03	1351.31	269.24 o
-2	6	2	1080.37	1076.22	54.76 o
0	6	2	15871.24	15481.37	514.77 o
4	6	2	2590.51	2599.44	142.80 o
8	6	2	1530.38	1669.98	262.88 o
-11	7	2	63.26	100.13	84.08 o
-9	7	2	32.37	589.96	160.89 o
-7	7	2	1168.52	1294.40	238.74 o
-3	7	2	870.72	870.34	53.57 o
-1	7	2	194.49	205.67	51.02 o
1	7	2	541.09	532.67	49.30 o
3	7	2	1335.12	1388.20	191.19 o
5	7	2	273.08	296.67	69.73 o
7	7	2	229.41	333.48	81.77 o
-10	8	2	649.23	783.12	102.99 o
-8	8	2	1008.47	899.85	65.09 o
-6	8	2	353.69	214.77	99.78 o
-4	8	2	650.52	659.75	48.74 o
-2	8	2	1902.25	2013.24	101.90 o
0	8	2	737.53	802.73	118.63 o
2	8	2	412.70	379.14	49.40 o
4	8	2	1172.39	964.38	208.17 o
6	8	2	980.03	1021.58	83.78 o
8	8	2	152.31	161.97	89.77 o
-7	9	2	1886.69	1633.71	109.68 o
-3	9	2	822.59	826.46	56.71 o
1	9	2	840.02	860.01	87.44 o
3	9	2	708.07	731.85	117.70 o
7	9	2	938.88	995.47	112.25 o
-6	10	2	2834.91	2538.95	321.08 o
-4	10	2	4547.82	4420.24	229.88 o
-2	10	2	1303.54	1447.26	78.63 o
0	10	2	7717.56	7515.20	283.57 o
2	10	2	752.01	559.69	100.13 o
4	10	2	7782.71	7805.19	352.52 o
-3	11	2	1765.37	1762.48	94.28 o
1	11	2	1069.00	916.95	74.58 o
3	11	2	1749.99	1730.76	93.52 o
0	8	3	898.56	768.14	171.85 o
2	8	3	9118.30	8614.12	335.56 o
-1	9	3	3523.81	3073.11	279.48 o
-2	10	3	754.91	817.35	204.74 o
0	10	3	325.54	282.68	86.63 o
2	10	3	1271.44	1271.09	106.86 o
-1	11	3	103.14	190.54	57.57 o