References

BROWER, W. S., MINOR, D. B., PARKER, H. S., ROTH, R. S. & WARING, J. L. (1974). *Mater. Res. Bull.* **9**, 1045–1052.

CARS, P. Y. L., COMÈS, R., DESCHAMPS, L. & THERY, J. (1974). *Acta Cryst.* A**30**, 305–309.

COWLEY, J. M. & IIJIMA, S. (1973). *Z. Naturforsch. Teil A*, **27**, 445–451.

GOODENOUGH, J. B. & KAFALAS, J. A. (1973). *J. Solid State Chem.* **6**, 493–501.

IIJIMA, S. (1971). *J. Appl. Phys.* **42**, 5891–5893.

MCWHAN, D. B., ALLEN, S. J. JR, REMEIKA, J. R. & DERNIER, P. D. (1975). *Phys. Rev. Lett.* **35**, 953–956.

ROTH, W. L. (1972). *Proc. 5th Mater. Res. Symp. NBS Spec. Publ.* Vol. 364, pp. 129–136.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

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On the generation of 'magic integers'.

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The results of a new method of generating 'magic integers' are given. The integers are considerably smaller than those described by Main [*Acta Cryst.* (1977), A**33**, 750–757].

Main (1977) has detailed a method based on the Fibonacci series for generating 'magic integers' for use in the multisolution direct method as described by White & Woolfson (1975). Main's method has the disadvantage that the series are rapidly divergent. In the series with limiting ratio 1·618, the 30th term is 1 346 269 and the 100th approximately $5{\cdot}7315 \times 10^{20}$.

There is, however, another method for generating such integers, obeying Main's rules for efficient sequences, which consists in using a computer to list those series of integers which possess unique sums and differences which themselves are not members of the set. The process is rapid and there appear to be an infinite number of series starting with any given number. The divergence is considerably less than Main's series, for example, the 100th terms of the series starting with 1, 10, 100, 1000 and 1300 are 46 963, 48 493, 48 159, 48 227, and 48 487 respectively. All values less than 80 000 for the series starting with 1 are given in Table 1 (values for the series mentioned above and also for those starting with 2 through 9 may be obtained from the author).

Table 1. *The first* 120 *terms of the series of unique integers beginning with unity*

1	3	8	18	30	43	67	90	122	161
202	260	305	388	416	450	555	624	730	750
983	1059	1159	1330	1528	1645	1774	1921	2140	2289
2580	2632	2881	3158	3304	3510	3745	4086	4563	4741
4928	5052	5407	5864	6242	6528	6739	7253	7804	8609
8725	9244	9680	9745	10018	10972	11049	11717	12010	12666
13512	13666	14829	15624	16076	17695	17919	18683	18941	19320
20688	21256	22357	22996	23670	24209	24580	25527	25883	26382
27076	29594	30117	30809	31658	31854	33060	35072	37158	38037
39503	40211	40531	42251	42681	42912	44604	45505	46112	46963
47937	49690	52149	52939	54753	54992	56749	57699	59984	61499
62370	63981	68300	68830	70844	71305	72119	76877	78227	78909

Monte Carlo tests indicate that the first series leads to r.m.s. deviations comparable with the Fibonacci series of Main but the saving in the number of points needing calculation is large once the number of phases represented exceeds about 14. The results for a representation of 10 phases are given as a typical example. The complementation (Main, 1977) technique for n integers, as adopted in the present work, gives the 'magic integer', $I_i = S_m - S_i$, where S_m is the first member of the series $\geq 2S_n$ and S_i is the ith member of the series. With Main's integers from the Fibonacci series as given, the r.m.s. value of the best fits to the sets of randomly generated phases was 46° with a range of 35° to 56°, in good agreement with the values given by Main (1977). The unique integers in the present work gave an r.m.s. value of 44° with a range of 34° to 55°. It is however debatable whether a linear sampling of the variable is the most efficient since, in a multidimensional closed figure, points tend to lie close to the surface. For example, in a hypersphere of unit radius and dimension 10, 99% of the hypervolume occurs in the shell from 0·631 to 1. Non-linear approaches have not been tried as yet.

References

MAIN, P. (1977). *Acta Cryst.* A**33**, 750–757.

WHITE, P. S. & WOOLFSON, M. M. (1975). *Acta Cryst.* A**31**, 53–56.