

RECREATIONAL SYMMETRY

SYMMETRICAL COMBINATION OF THE SUMS AND PRODUCTS OF TRIGONOMETRIC FUNCTIONS GIVING INTEGERS

Haruo Hosoya

Department of Chemistry, Ochanomizu University, Bunkyo-ku, Tokyo 112, Japan

1. INTRODUCTION

The purpose of the present paper is to disclose the secret receipt of deriving the fantastic identities, involving the symmetrical combination of trigonometric functions, such as,

$$\sum_{k=1}^{100} (2 \cos \frac{k\pi}{202})^6 = \sum_{k=1}^{100} (2 \sin \frac{k\pi}{202})^6 = 1988, \quad (1)$$

$$\begin{aligned} & 2(1 + 4 \cos^2 \frac{\pi}{7})(1 + 4 \cos^2 \frac{2\pi}{7})(1 + 4 \cos^2 \frac{3\pi}{7}) \\ & \times (1 + 4 \cos^2 \frac{\pi}{9})(1 + 4 \cos^2 \frac{2\pi}{9})(1 + 4 \cos^2 \frac{3\pi}{9})(1 + 4 \cos^2 \frac{4\pi}{9}) \\ & \times (\cos^2 \frac{\pi}{11} + \cos^2 \frac{2\pi}{11} + \cos^2 \frac{3\pi}{11} + \cos^2 \frac{4\pi}{11} + \cos^2 \frac{5\pi}{11}) \\ & = 1989 \end{aligned} \quad (2)$$

$$\sum_{k=1}^{332} (2 \cos \frac{k\pi}{666})^4 = \sum_{k=1}^{332} (2 \sin \frac{k\pi}{666})^4 = 1990, \quad (3)$$

$$\begin{aligned} & 2^{11} (\cos^2 \frac{\pi}{6} + \cos^2 \frac{2\pi}{6} + \cos^2 \frac{3\pi}{6}) \times (\cos^2 \frac{\pi}{7} + \cos^2 \frac{2\pi}{7} + \cos^2 \frac{3\pi}{7}) \\ & \times \{ (\cos^8 \frac{\pi}{6} + \cos^8 \frac{2\pi}{6} + \cos^8 \frac{3\pi}{6}) + (\cos^8 \frac{\pi}{7} + \cos^8 \frac{2\pi}{7} + \cos^8 \frac{3\pi}{7}) \} \\ & = 1990 \end{aligned} \quad (4)$$

and

$$\frac{1}{2} \sum_{k=1}^6 (2 \cos \frac{k\pi}{14})^8 \{ \sum_{k=1}^6 (2 \cos \frac{k\pi}{14})^4 - \sum_{k=1}^6 (2 \cos \frac{k\pi}{14})^2 \} = 1991. \quad (5)$$

These relations are examples of a more general relation,

$$F(\sum_{k=1}^m, \prod_{k=1}^m, 4 \sin^2 \frac{k\pi}{n}, 4 \cos^2 \frac{k\pi}{n}) \in \text{Integer} \quad (m = [(n-1)/2]). \quad (6)$$

Namely, any symmetrical combination of the sum and/or product operation on the square of $2 \sin (k\pi/n)$ or $2 \cos (k\pi/n)$ is shown to yield an integer. Although one can extend this idea into tangent functions, in this paper we will be concerned with only sines and cosines. These results are one of the by-products of the counting of the Kekulé structures, or perfect matching number, of molecular graphs, which represent the carbon atom skeletons of unsaturated hydrocarbon molecules (Hosoya, 1986).

2. FIBONACCI, LUCAS, AND CHEBYSHEV

The first and second kinds of Chebyshev polynomials are defined, respectively, as (Abramowitz and Stegun, 1965)

$$T_n(\cos \theta) = \cos n\theta \quad (7)$$

$$U_n(\cos \theta) = \sin(n+1)\theta/\sin \theta. \quad (8)$$

For convenience sake let us use the following alternative forms (Lyusternik et al., 1965; Hosoya, 1981),

$$C_n(x) = 2 T_n(x/2) = \sum_{k=0}^{[n/2]} (-1)^k \frac{n}{n-k} \binom{n-k}{k} x^{n-2k} \quad (9)$$

$$S_n(x) = U_n(x/2) = \sum_{k=0}^{[n/2]} (-1)^k \binom{n-k}{k} x^{n-2k}, \quad (10)$$

which are nothing else but the matching polynomials (Aihara, 1976; Gutman et al., 1977; Farrel, 1979). $M_G(x)$, of cycle graph C_n and path graph S_n , respectively.*² The matching polynomial is essentially the same as the Z-counting polynomial, $Q_G(x)$, proposed by the present author (Hosoya, 1971, 1972, 1973; see also Heilman and Lieb, 1970, 1972), since both of them are expressed in terms of the non-adjacent number, $p(G,k)$, as

$$Q_G(x) = \sum_{k=0}^{[n/2]} p(G,k) x^k \quad (11)$$

$$M_G(x) = \sum_{k=0}^{[n/2]} (-1)^k p(G,k) x^{n-2k}. \quad (12)$$

It has been known that these polynomials, S_n and C_n , are closely related, respectively, to the Fibonacci (F_n) and Lucas (L_n) numbers (Hoggatt, 1969). Namely,

$$F_n = i^{-n} S_n(i) \quad (13)$$

$$L_n = i^{-n} C_n(i), \quad (14)$$

where

$$F_n = F_{n-1} + F_{n-2}^{*3} \quad (15)$$

$$F_0 = F_1 = 1$$

$$L_n = L_{n-1} + L_{n-2} \quad (16)$$

$$L_0 = 2, L_1 = 1.$$

The zeroes of $S_n(x)$ and $C_n(x)$ can readily be obtained by the substitution of $x = t + 1/t$. Namely, for S_n

$$S_n(t+1/t) = \sum_{k=0}^n t^{n-2k} = \frac{t^{2(n+1)} - 1}{t^n(t^2 - 1)} = 0 \quad (17)$$

giving $t = \exp(i\pi/(n+1))$. Then we get

$$x_k = 2 \cos \frac{k\pi}{n+1} \quad (k = 1, 2, \dots, n) \quad (18)$$

For C_n we have

$$C_n(t+1/t) = t^n + 1/t^n = 0 \quad (19)$$

giving $t = \exp(i\pi/2n)$. Then we get

$$x_k = 2 \cos \frac{(2k-1)\pi}{2n}. \quad (k = 1, 2, \dots, n) \quad (20)$$

In both the cases x_k is numbered in the decreasing order. Unless otherwise stated we will adopt this ordering for x_k .

These rigorous solutions (18) and (20) enable one to factorize these polynomials as

$$S_n(x) = \prod_{k=1}^n (x - 2 \cos \frac{k\pi}{n+1}) \quad (21)$$

$$C_n(x) = \prod_{k=1}^n (x - 2 \cos \frac{(2k-1)\pi}{2n}). \quad (22)$$

Since

$$\cos \frac{(n-k+1)\pi}{n+1} = -\cos \frac{k\pi}{n+1}$$

and

$$\cos \frac{[2(n-k+1)-1]\pi}{2n} = -\cos \frac{(2k-1)\pi}{2n},$$

both the products can be 'folded' into a half as,

$$S_n(x) = Y \prod_{k=1}^{[n/2]} (x^2 - 4 \cos^2 \frac{k\pi}{n+1}) \quad (23)$$

$$C_n(x) = Y \prod_{k=1}^{[n/2]} (x^2 - 4 \cos^2 \frac{(2k-1)\pi}{2n}) \quad (24)$$

with

$$Y = \begin{cases} 1 & \text{for even } n \\ x & \text{for odd } n. \end{cases} \quad (25)$$

Respective substitutions of Eqs. (23) and (24) with $x = i$ into Eqs. (13) and (14) give the following results,

$$F_n = \prod_{k=1}^{[n/2]} (1 + 4 \cos^2 \frac{k\pi}{n+1}) \quad (26)$$

$$L_n = \prod_{k=1}^{[n/2]} (1 + 4 \cos^2 \frac{(2k-1)\pi}{2n}). \quad (27)$$

Note that Eqs. (26) and (27) hold irrespective of the parity of n . Now all the Fibonacci and Lucas numbers are shown to be expressed in terms of the symmetrical product of cosine functions.*⁴

For a tree graph G as S_n the matching polynomial is identical to the characteristic polynomial, $P_G(x)$, which is defined as

$$P_G(x) = (-1)^n \det(A - xE) \quad (28)$$

with the adjacency matrix A of G and the unit matrix E of $n \times n$ (Hosoya, 1971). For a non-tree graph, the difference between the characteristic and matching polynomials has thoroughly been analyzed (Hosoya, 1972; Trinajstić, 1983).

Recently it was shown that for a graph G with one cycle the characteristic polynomial of such an edge-weighted graph of G is equal to the matching polynomial of G that one edge rs in the cycle has the following elements (Aihara, 1979; Schaad et al., 1979; Graovac, 1981; Mizoguchi, 1985; Hosoya and Balasubramanian, 1989)

$$A_{rs} = i \quad \text{and} \quad A_{sr} = -i \quad (i^2 = -1). \quad (29)$$

An example is shown for a square graph G in Fig. 1. Choose one edge in the cycle, say, 12, assign the weights as

$$A_{12} = e^{i\theta} \quad \text{and} \quad A_{21} = e^{-i\theta} \quad (30)$$

to keep the matrix $A - xE$ Hermitian, and we get the determinant as

$$x^4 - 4x^2 + 2(1 - \cos \theta),$$

whose zeroes are obtained to be

$$x = \pm 2 \cos(\theta/4), \pm 2 \sin(\theta/4). \quad (31)$$

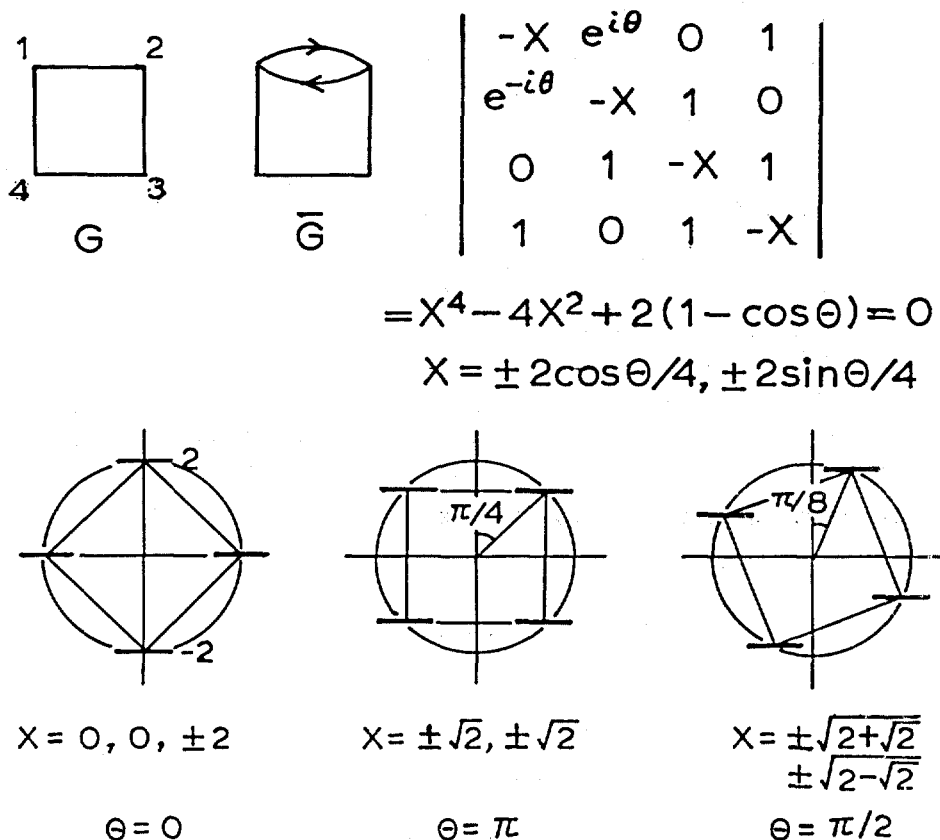


Figure 1

Symmetrical solutions are obtained for $\theta = 0$ and π , respectively, corresponding to the characteristic $(x^4 - 4x^2)$ and matching $(x^4 - 4x^2 + 4)$ polynomials. However, we can find several unsymmetrical solutions of interest, e.g., with $\theta = \pi/2$ (See Fig. 1).

In quantum chemistry the eigenvalues, spectra, or zeroes of $P_G(x)$ play an important role for describing the electronic states of a conjugated hydrocarbon molecule whose carbon atom skeleton is represented by G (Hückel, 1931). The interested readers may refer to the standard textbooks (Streitwieser, 1961; Salem, 1966; Heilbronner and Bock, 1976; Coulson et al., 1978).

3. SYMMETRICAL SUMS AND PRODUCTS

Encouraged by the finding of Eqs. (26) and (27), let us try to find out symmetrical sums and products of trigonometric functions to give integers as Eqs. (26) and (27). From the standard compilations of mathematical formulas we can select the following sets of relations (Moriguchi et al., 1960; Gradshteyn and Ryzhik, 1980);

$$\begin{aligned}
 \sum_{k=1}^{n-1} \left(2 \sin \frac{k\pi}{2n}\right)^2 &= 2n - 2 & \prod_{k=1}^{n-1} \left(2 \sin \frac{k\pi}{2n}\right)^2 &= n \\
 \sum_{k=1}^n \left(2 \sin \frac{k\pi}{2n+1}\right)^2 &= 2n + 1 & \prod_{k=1}^n \left(2 \sin \frac{k\pi}{2n+1}\right)^2 &= 2n + 1 \\
 \sum_{k=1}^{n-1} \left(2 \cos \frac{k\pi}{2n}\right)^2 &= 2n - 2 & \prod_{k=1}^{n-1} \left(2 \cos \frac{k\pi}{2n}\right)^2 &= n \\
 \sum_{k=1}^n \left(2 \cos \frac{k\pi}{2n+1}\right)^2 &= 2n + 1 & \prod_{k=1}^n \left(2 \cos \frac{k\pi}{2n+1}\right)^2 &= 1 \\
 \sum_{k=1}^{n-1} \left(2 \tan \frac{k\pi}{2n}\right)^2 &= \frac{1}{3}(n-1)(2n-1) & \prod_{k=1}^{n-1} \left(2 \tan \frac{k\pi}{2n}\right)^2 &= 1 \\
 \sum_{k=1}^n \left(2 \tan \frac{k\pi}{2n+1}\right)^2 &= n(2n+1) & \prod_{k=1}^n \left(2 \tan \frac{k\pi}{2n+1}\right)^2 &= 2n + 1
 \end{aligned} \tag{32}$$

Similar formulas can be found for the fourth power of the trigonometric functions (Moriguchi, 1960). However, no explicit formulas for higher powers seem to have been documented.

The $2l$ -th power of cosine can be converted as follows:

$$\begin{aligned}
 2^{2l} \cos^{2l} \theta &= (e^{i\theta} + e^{-i\theta})^{2l} \\
 &= \sum_{j=0}^{2l} \binom{2l}{j} e^{ij\theta} e^{-i(2l-j)\theta} \\
 &= \binom{2l}{1} + \sum_{j=0}^{l-1} \binom{2l}{j} (e^{2i(l-j)\theta} + e^{-2i(l-j)\theta}) \\
 &= \binom{2l}{1} + 2 \sum_{j=1}^l \binom{2l}{1-j} \cos 2j\theta
 \end{aligned} \tag{33}$$

By using the known formula for the summation of the series of successive cosine functions we get the sum of $\cos^2 k\theta$ as follows:

$$\sum_{k=1}^r \cos^{2l} k\theta = \frac{1}{2^{2l}} \left[\binom{2l}{1} r + 2 \sum_{j=1}^l \binom{2l}{1-j} \frac{\cos(jr+1)\theta \sin jr\theta}{\sin j\theta} \right] \tag{34}$$

If we put $\theta = \pi/n = \pi/2m$ and $r = [(n-1)/2] = m-1$, we have

$$\begin{aligned}
 S &= \sum_{k=1}^{m-1} \left(2 \cos \frac{k\pi}{2m}\right)^{2l} = \binom{2l}{1} (m-1) \\
 &\quad + 2 \sum_{j=1}^l \binom{2l}{1-j} \frac{\cos(j\pi/2) \sin[j(n-1)\pi/2m]}{\sin(j\pi/2m)}
 \end{aligned}$$

However, it turns out that

$$\frac{\cos(j\pi/2) \sin[j(n-1)\pi/2m]}{\sin(j\pi/2m)} = \begin{cases} 0 & \text{for } j = \text{odd} \\ 1 & \text{for } j = \text{even} \end{cases}.$$

Then the expression of S can be simplified as

$$\begin{aligned} S &= \binom{2l}{1} (m-1) - 2 \sum_{j=1}^{[l/2]} \binom{2l}{1-2j} \\ &= \binom{2l}{1} m - \sum_{j=-[l/2]}^{[l/2]} \binom{2l}{1+2j} \end{aligned}$$

It is easy to verify

$$\sum_{j=-[l/2]}^{[l/2]} \binom{2l}{1+2j} = \frac{1}{2} \sum_{j=0}^{2l} \binom{2l}{j} = 2^{2l-1}.$$

Finally we get

$$S = \binom{2l}{1} m - 2^{2l-1} \quad (35)$$

or

$$\sum_{k=1}^{[(n-1)/2]} (2 \cos \frac{k\pi}{n})^{2l} = \binom{2l-1}{1-1} n - 2^{2l-1} \quad (n \geq l+1) \quad (36)$$

For the case of odd n we get exactly the same expression as Eq. (36) by putting $\theta = \pi/(2m+1)$ and $r = m$. Thus Eq. (36) is proven to be valid for all n .

Quite similarly to the cosine function, we can prove the results for the sine function as

$$2^{2l} \sin^{2l} \theta = \binom{2l}{1} + 2 \sum_{j=1}^l (-1)^j \binom{2l}{1-j} \cos 2j\theta \quad (37)$$

$$\sum_{k=1}^r \sin^{2l} k\theta = \frac{1}{2^{2l}} \left[\binom{2l}{1} r + 2 \sum_{j=1}^l (-1)^j \binom{2l}{1-j} \frac{\cos j(r+1)\theta \sin jr\theta}{\sin j\theta} \right] \quad (38)$$

and

$$\sum_{k=1}^{[(n-1)/2]} (2 \sin \frac{k\pi}{n})^{2l} = \binom{2l-1}{1-1} n - 2^{2l-2} [1 + (-1)^n] \quad (n \geq l+1). \quad (39)$$

Though simple, Eqs. (33)-(39) have not yet been documented before.

The trial-and-error substitution of integer 1 and n into Eqs. (36) and (39) together with the set of Eq. (32) gives us fantastic relations as Eqs. (1), (3), and also the following ones,

$$\sum_{k=1}^5 (2\cos \frac{k\pi}{12})^{10} = \sum_{k=1}^5 (2\sin \frac{k\pi}{12})^{10} = 1000 \quad (40)$$

and so on. Equations (2), (4), and (5) can be obtained by combining the identities, (26), (27), and (32). Since any of the symmetrical sums and products of sines and cosines in the types of Eq. (32) is found to be an integer, the statement given under Eq. (6) is approved.

Relations for the tangent functions have not thoroughly been explored yet, but we could obtain several interesting relations as

$$\sum_{k=1}^{12} (\tan \frac{k\pi}{26})^2 = \sum_{k=1}^{12} (\cot \frac{k\pi}{26})^2 = 100 \quad (41)$$

and

$$\sum_{k=1}^{[(n-1)/2]} (\tan \frac{k\pi}{n})^4 = \begin{cases} \frac{1}{96}(n-1)(n-2)(n^2+3n-13) & n = \text{even} \\ \frac{n}{6}(n-1)(n^2+n-3) & n = \text{odd} \end{cases} \quad (42)$$

REMARKS

- *1 For the sake of aesthetics the last term of k for the cosine sum is rather to be chosen as 333.
- *2 Interestingly enough, in the graph theory the pair of symbols S_n and C_n have been used, respectively, for the path and cycle graphs long before the relations (9) and (10) came to be known (Harary, 1969).
- *3 Alternative definition of the Fibonacci numbers is $F_1 = F_2 = 1$.
- *4 Equation (26) can also be derived from the diagonalization of the skew-symmetric matrix representing the $2 \times n$ rectangular lattice (Kasteleyn, 1961; Temperley and Fisher, 1961).

REFERENCES

- Abramowitz, M. and Stegun, I. A. eds. (1972) *Handbook of Mathematical Functions*, New York: Dover.
- Aihara, J. (1976) A new definition of Dewar-type resonance energy, *Journal of the American Chemical Society*, 98, 2750-2758.
- Aihara, J. (1979) Matrix representation of an olefinic reference structure for monocyclic conjugated compounds, *Bulletin of the Chemical Society of Japan*, 52, 1529-1530.
- Coulson, C. A., O'Leary, B., and Mallion, R. B. (1978) *Hückel Theory for Organic Chemists*, London: Academic Press.
- Farrell, E. J. (1979) An introduction to matching polynomials, *Journal of combinatorial Theory*, Series B, 27, 75-86.
- Gradshteyn, I. S. and Ryzhik, I. M. (1980) *Table of Integrals, Series, and Products*, New York: Academic Press.
- Graovac, A. (1981) On the construction of a Hermitian matrix associated with the acyclic polynomial of a conjugated hydrocarbon, *Chemical Physics Letters*, 82, 248-251.

- Gutman, I., Milun, M., and Trinajstić, N. (1977) Non-parametric resonance energies of arbitrary conjugated systems, *Journal of the American Chemical Society*, 99, 1692-1704.
- Harary, F. (1969) *The Graph Theory*, Reading, Mass.: Addison-Wesley.
- Heilbronner, E. and Bock, H. (1966) *The HMO Model and Its Application*, London: John Wiley.
- Heilman, O. J. and Lieb, E. H. (1970) Monomers and dimers, *Physical Review Letters*, 24, 1412-1414.
- Heilman, O. J. and Lieb, E. H. (1972) Theory of monomer-dimer systems, *Communication in Mathematical Physics*, 25, 190-232.
- Hoggatt, V. E., Jr. (1969) *Fibonacci and Lucas Numbers*, Boston: Houghton Mifflin.
- Hosoya, H. (1971) Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bulletin of the Chemical Society of Japan*, 44, 2332-2339.
- Hosoya, H. (1972) Graphical enumeration of the coefficients of the secular polynomials of the Hückel molecular orbitals, *Theoretica Chimica Acta*, 25, 215-222.
- Hosoya, H. (1973) Topological index and Fibonacci numbers with relation to chemistry, *Fibonacci Quarterly*, 11, 255-266.
- Hosoya, H. (1981) Graphical and combinatorial aspects of some orthogonal polynomials, *Natural Science Report of Ochanomizu University*, 32, 127-138.
- Hosoya, H. (1986) Matching and symmetry, *Computers and Mathematics with Applications*, 12B, 271-290.
- Hosoya, H. and Balasubramanian, K. (1989) Computational algorithms for matching polynomials of graphs from the characteristic polynomials of edge-weighted graphs, *Journal of Computational Chemistry*, 10, 698-710.
- Hückel, E. (1931) Quanten theoretische Beiträge zum Benzol-problem, *Zeitschrift für Physik*, 60, 204-272.
- Kasteleyn, P. W. (1961) The statistics of dimers on a lattice, *Physica*, 27, 1209-1225.
- Lyusternik, L. A., Chervonenkis, O. A., and Yanpol'skii, A. R. (1965) *Handbook of Computing Elementary Functions*, Oxford: Pergamon.
- Mizoguchi, N. (1985) The structure corresponding to the reference polynomial of [N]annulene in the topological resonance energy theory, *Journal of the American Chemical Society*, 107, 4419-4421.
- Moriguchi, S., Udagawa, K., and Hitotsumatsu, S. (1960) *Handbook of Mathematical Functions and Formulas*, [Suugaku Kooshikishuh, in Japanese], Tokyo: Iwanami.
- Salem, L. (1966) *The Molecular Orbital Theory of Conjugated Systems*, New York: Benjamin.
- Schaad, L. J., Hess, B. A., Jr., Nation, J. B., Trinajstić, N., and Gutman, I. (1979) On the reference structure for the resonance energy of aromatic hydrocarbons, *Croatica Chemica Acta*, 52, 233-248.
- Streitwieser, A., Jr., (1961) *Molecular Orbital Theory for Organic Chemists*, New York: John Wiley.
- Temperley, H. N. V. and Fisher, M. E. (1961) Dimer problems in statistical mechanics. An exact result, *Philosophical Magazine*, 6, 1061-1063.
- Trinajstić, N. (1983) *Chemical Graph Theory*, Boca Raton, Florida: CRC Press.