Matrix-Product Periodic Systems of Molecules

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Direct products of the periodic chart of the elements, considered as a matrix, with itself produce $2N$-dimensional periodic systems of N-atomic molecules. It is shown that these periodic systems subsume a large number of published molecular periodic systems.

Consider any two-dimensional form of the periodic chart of the elements, surrounded with zeros such that it is bounded by a square. Let it be a two-subscript matrix with subscripts R (the row or period number) and C (the column or group number). Perform the direct product of this matrix with itself $N - 1$ times to obtain the periodic system of N-atomic molecules, a $2N$-dimensional matrix with subscripts R_1, R_2, ..., C_1, C_2, ... The elements of the original matrix include symbols of the chemical elements, and those of the product matrix include molecular symbols (amid zeros).[1] Heteronuclear molecules appear more than once. These architectures fulfill all of Dias' definitions of a periodic table set,[2] generalized to apply to more than two dimensions. The independent variables R_1, C_1, R_2, and C_2 have proven very useful for making approximate predictions of erroneous or as-yet-unknown values of diatomic-molecular properties, to more precision than has been achieved using Z_1 and Z_2.[3]

It is the purpose of this paper to show how various cuts and projections of these product matrices produce previously published (or communicated) molecular periodic systems, which are useful representations of molecular behavior just as the chart of the elements provides an easily-grasped representation of atomic behavior. If it is not explicitly stated that $N > 2$, then the systems being described relate to diatomic molecules.

1. Several tesselated molecular periodic systems of diatomic molecules have been proposed. They consist of two-dimensional charts, each produced by a slice through the four-dimensional periodic system of diatomic molecules. Each is similar to the chart of the elements but with a different atomic symbol in the first (or second) place of the molecular symbol; they can be tiled[4] or presented separately.[5,6]

2. Kong's elegant two-dimensional periodic chart consists of a complete series of slices like those just described, but overlapped in such a way that the center of each chart (R_1, C_1), lies at (R_2,C_2).[7] More succinctly, it is a *projection* [and reduction] of the four-dimensional architecture defined by

$$x = R_1 + R_2 \quad \text{(the molecular period number)}$$

$$y = C_1 + C_2 \quad \text{(the molecular group number)}$$

$$p = R_1 - R_2 \quad \text{[into the plane of the chart]}$$

$$q = C_1 - C_2 \quad \text{[into the plane of the chart]}$$

(Figures 1 and 2). Kong gives tables of (p,q). Kong's system (x,y) can be extended to triatomic,[8] tetraatomic (being prepared for publication), and larger molecules without limit, but the tables for $p, q, r, \ldots$ become too lengthy for publication.

3. Cut-and-stack molecular periodic systems require serpentine cuts and result in a stacked series of charts like those described in ref 11. Cut (a),

$$R_1 = 1, 2, \ldots$$

$$R_2 = R_1, R_1 + 1, \ldots$$

was presented in 1979[9] but then replaced by another which much better fits the data, i.e., (b) a monotonic increase in the quantity R_1R_2.[10] Each plane in these three-dimensional structures has coordinates (C_1,C_2) and contains molecules which are isovalent (homologous) to molecules having the same coordinates on the other planes (Figure 3). There may be several blocks if the atomic chart on which they are based was formed of separate blocks (e.g., molecules formed from p atoms, Figure 3). Cut (c),

$$C_1 + C_2 = 1, 2, \ldots$$

(each one defining a block of the system)

$$C_1 - C_2 = \mathrm{n}, \mathrm{n} - 2, \ldots$$

(defining the stacking order; n is an integer)

was proposed by Monyakin in 1980 (Figure 4).[11] The planes stacked in this manner in each block contain isovalent molecules addressed by coordinates (R_1,R_2). Isoelectronic molecules are found on lines perpendicular to the planes.

The procedure is not restricted to commencing with two-dimensional atomic periodic charts bounded by straight lines. Consider, for example, a polar-coordinate chart containing only representative-group elements from periods 2 through 6 (Figure 5). The elements lie at (R,θ), where R is the period number and the integer n, in $\theta = n\pi/8$, is the group number. The direct product produces a kind of hypersphere in the space (R_1,θ_1,R_2,θ_2). Cuts (θ_1,θ_2) produce planes (R_1,R_2) such as which make up the volume in Figure 4. Cuts (R_1,R_2) produce tori upon which fixed-row molecules are addressed by (θ_1,θ_2).[12] Cuts (R_1,θ_1) produce circles resembling the

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TABLE 1

THE PERIODIC TABLE OF THE DIATOMIC MOLECULES

Periodic Number		Group Number 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1		1 (H H)	2 (H⁻ H)											Diatom Molecular Number N; 26; 14; Total Nuclear Charge z; N_2; Molecular Formula			
2		3	4 H_2^2	5 HHe^3	6 He_2^4												
3		7	8 (LiH)	9 (BeH)	10 (BH)	11 (CH)	12 (NH)	13 (OH)	14 (HF)	15 (HNe)	16 (HeNe)						
4		17 $LiNe^{13}$	18 Li_2^6	19 $LiBe^7$	20 Be_2^8	21 BeB^9	22 B_2^{10}	23 BC^{11}	24 C_2^{12}	25 CN^{13}	26 N_2^{14}	27 NO^{15}	28 O_2^{16}	29 OF^{17}	30 F_2^{18}	31 NeF^{19}	32 Ne_2^{20}
5		33 $NaNe^{21}$	34 $NaLi^{14}$	35 $NaBe^{15}$	36 $MgBe^{16}$	37 MgB^{17}	38 AlB^{18}	39 AlC^{19}	40 SiC^{20}	41 SiN^{21}	42 PN^{22}	43 PO^{23}	44 SO^{24}	45 SF^{25}	46 ClF^{26}	47 $NaCl^{27}$	48 $NeAr^{28}$
6		49 KNe^{29} $NaAr^{39}$	50 Na_2^{22} KLi^{22}	51 $NaMg^{23}$ $LiCa^{23}$	52 Mg_2^{24} $BeGa^{24}$	53 $MgAr^{25}$ $BeGe^{25}$	64 Al_2^{26} GaB^{26}	65 $AlSi^{27}$ GeB^{27}	66 Si_2^{28} GeC^{28}	67 SiP^{29} AsC^{29}	68 P_2^{30} AsN^{30}	69 PS^{31} SeN^{41}	70 S_2^{32} SeO^{42}	71 SCl^{33} BrO^{43}	72 Cl_2^{34} BrF^{44}	73 $ArCl^{35}$ KrF^{45}	74 Ar_2^{36} $NcKr^{46}$
7		75 $RbNe^{47}$ KAr^{55}	76 KNa^{30} $RbLi^{40}$	77 KMg^{31} $RbBe^{41}$	78 $CaMg^{32}$ $SrBe^{42}$	89 $AlCa^{33}$ SrB^{43}	90 $AlGa^{34}$ InB^{43}	91 $SiGa^{35}$ InC^{45}	92 $GeSi^{36}$ SnC^{46}	93 GeP^{37} SnN^{47}	94 AsP^{48} SbN^{58}	95 AsS^{49} SbO^{59}	96 SeS^{50} TeO^{60}	97 $SeCl^{51}$ TeF^{61}	98 $BrCl^{52}$ IF^{62}	99 $BrAr^{53}$ NeI^{63}	100 $ArKr^{54}$ $XeNe^{64}$
8		101 $RbAr^{55}$ $NaXe^{65}$	102 K_2^{38} $RbNa^{48}$	103 KCa^{39} $RbMg^{49}$	104 Ca_2^{40} $SrMg^{50}$	115 $CaGa^{51}$ $SrAl^{51}$	116 Ga_2^{52} $InAl^{52}$	127 $GaGe^{53}$ $InSi^{53}$	128 Ge_2^{54} $SnSi^{54}$	129 $GeAs^{55}$ SnP^{55}	130 As_2^{56} SbP^{56}	131 $AsSe^{67}$ SbS^{67}	132 Se_2^{68} TeS^{68}	133 $SeBr^{69}$ $TeCl^{69}$	134 Br_2^{70} ICl^{70}	135 $KrBr^{71}$ ArI^{71}	136 Kr_2^{72} $ArXe^{72}$
9		137 $RbKr^{73}$	138 RbK^{56}	139 $RbCa^{57}$	140 $SrCa^{58}$	151 $SrGa^{69}$	162 $InGa^{70}$	163 $InGe^{71}$	164 $GeSn^{72}$	165 $SnAs^{73}$	166 $AsTe^{74}$	167 $SbSe^{85}$	168 $TeSe^{86}$	169 $TeBr^{87}$	170 IBr^{88}	171 KrI^{89}	172 $KrXe^{90}$
10		173 $RbXe^{91}$	174 Rb_2^{74}	175 $RbSr^{75}$	176 Sr_2^{76}	187 $SrIn^{87}$	198 In_2^{88}	199 $InSn^{89}$	200 Sn_2^{90}	201 $SnSb^{91}$	202 Sb_2^{92}	203 $SbTe^{103}$	204 Te_2^{104}	205 TeI^{105}	206 I_2^{106}	207 XeI^{107}	208 Xe_2^{108}
Ground State	Configuration	σ^1	σ^2	σ^1	σ^2	π^1	π^2	π^3	π^4	σ^1	σ^2	π^1	π^2	π^3	π^4	σ^1	σ^2
	Spectral Term	$^2\Sigma^+$	$^1\Sigma^+$	$^2\Sigma^+$	$^1\Sigma^+$	$^2\Pi$	$^3\Sigma^-$	$^2\Pi$	$^1\Sigma^+$	$^2\Sigma^+$	$^2\Sigma^+$	$^2\Pi$	$^3\Sigma^-$	$^2\Pi$	$^1\Sigma^+$	$^2\Sigma^+$	$^1\Sigma^+$
1st Excited State	Configuration	σ^1	$\sigma^1\sigma^1$		$\sigma^1\pi^1$				$\pi^3\sigma^1$	$\pi^3\sigma^2$	$\sigma^1\pi^1$	$\sigma^1\pi^2$		$\pi^3\sigma^2$	$\pi^3\sigma^1$	$\pi^3\sigma^2$	
	Spectral Term	$^2\Pi$	$^1\Pi$		$^3\Pi$				$^3\Pi$	$^2\Pi$	$^1\Pi^3\Pi$	$^2\Delta^2\Sigma$		$^2\Pi$		$^2\Pi$	
Multiplicity		2	1	2	1	2	3	2	1	2	1	2	3	2	1	2	1
Free Radical		mono	non	mono	non	mono	bi	mono	non	mono	non	mono	bi	mono	non	mono	non
Magnetic Susceptibility		para	anti	para	anti	para	para	para	anti	para	anti	para	para	para	anti	para	anti
Frontier Orbitals	HOMO	$z\sigma$	$z\sigma$	$y\sigma$	$y\sigma$	$w\pi$	$w\pi$	$w\pi$	$w\pi$	$x\sigma$	$x\sigma$	$v\pi$	$v\pi$	$v\pi$	$v\pi$	$u\sigma$	$u\sigma$
	LUMO	$y\sigma$	$y\sigma$	$w\pi$	$w\pi$	$x\sigma$	$x\sigma$	$x\sigma$	$x\sigma$	$v\pi$	$v\pi$	$u\sigma$	$u\sigma$	$u\sigma$	$u\sigma$	$z^*\sigma$	$z^*\sigma$

Figure 1. Kong's periodic system of main-group diatomic molecules. The group number (increasing horizontaly) is the sum of the atomic group numbers; the period number (increasing down) is the sum of the atomic period numbers. The "diatomic molecular number" at the top left of each compartment is serial (except where jumps of 10 allow for transition-metal molecules), so as to play the same role as the atomic number in the atomic chart. Some separated atoms (H H and H⁻ H) and some molecules with row-1 atoms are included in the first three periods; rare-gas atoms are counted as being in both atomic groups 0 and 8. The values of some molecular properties are shown at the bottom. Reprinted by permission from ref 3. Copyright 1989 The Edwin Mellen Press.

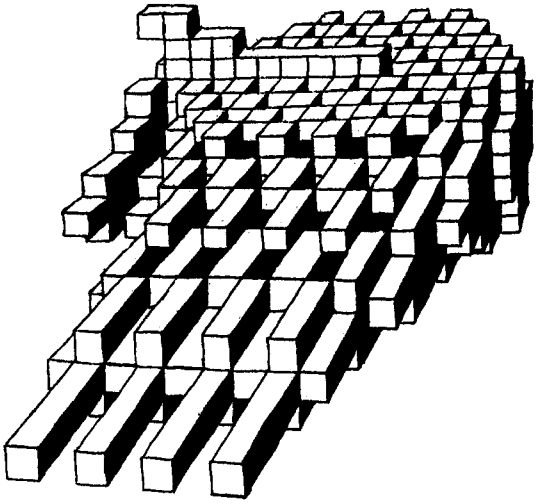

Figure 2. Kong's periodic chart for diatomic molecules, redrawn as a three-architecture by using his Table 2, giving the molecules in various compartments. The system is symmetric front-to-back across a plane passing through homonuclear molecules. Only right-hand sides are shaded. Vacant portions of Kong's Table 2 account for the alternate vacant volumes in the figure. The main portion of the architecture would continue more toward points at the front and rear if highly ionically-bonded molecules had been included in Kong's tables.

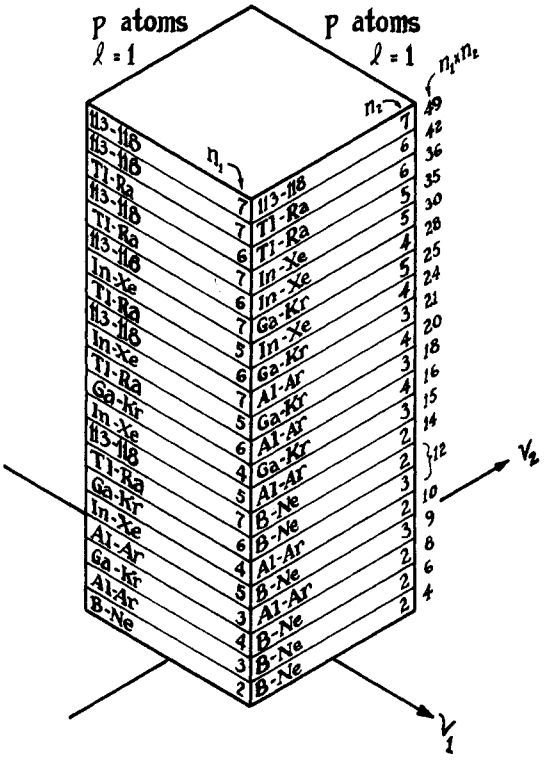

Figure 3. One block of a period system of molecules, formed from an atomic periodic chart in which s, p, d, and f atoms are in separate blocks. The molecule BB is at the bottom left; BNe is at the bottom front and back corners; NeNe is at the bottom right; and 118118 (presumably the next rare-gas homonuclear diatomic molecule) is at the top right. The stacking order is n_1n_2. Reprinted by permission from ref 13. Copyright 1987 Southern College.

original polar-coordinate chart; on each circle the hydrides, ..., borides, carbides, ... are addressed by (R_2,θ_2).

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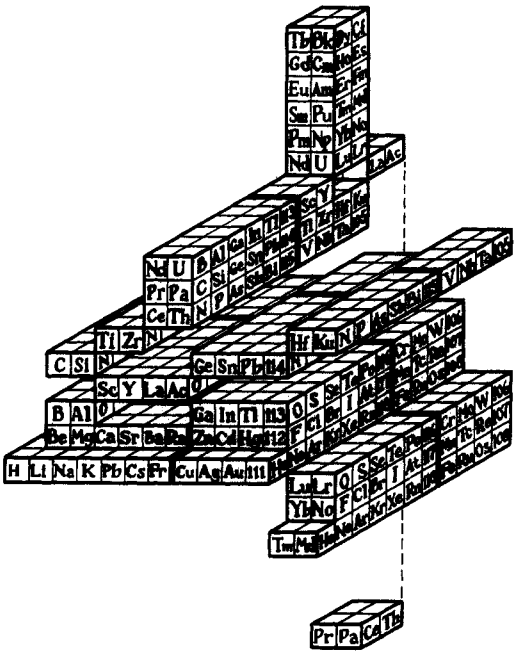

Figure 4. $C_1 + C_2 = 9$ block of Monyakin's periodic system. The bottom area of this system has $C_1 - C_2 = 7$ (the group numbers of regal metals and of the iron family being set to 1 and 8); the next area up has $C_1 - C_2 = 5$. The structures at the top of the chart can be related to a very strange chart of the atoms. Reprinted by permission from ref 3. Copyright 1989 The Edwin Mellen Press.

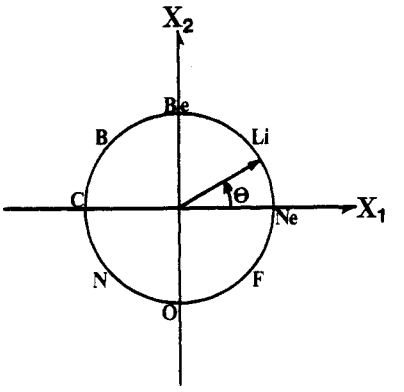

Figure 5. One main-group cycle of a polar coordinate chart of the elements. Reprinted by permission from ref 3. Copyright 1989 The Edwin Mellen Press.

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