SPREADSHEET-BASED MOLECULAR
POTENTIAL FUNCTION CONVERTER

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Abstract

Recently mathematical relationships among potential functions within the categories of bond-stretching, bond-bending, bond-twisting and van der Waals interactions have been reviewed and summarized [26] in preparation for the development of a molecular potential function converter. Such parametric conversion is of importance when available parameters (from handbook) and required parameters (in software) correspond to different potential functions for the same category of interatomic interaction. Based on [26], the present paper proposes a spreadsheet-based converter that can be easily set up using the Microsoft Excel® platform. A sample illustration is demonstrated and shown to be workable. The present parametric converter reported herein is a prototype of a more user-friendly and aesthetic version, which is currently in the planning stage.

1. Introduction

Relationships between parameters of molecular potential functions, within the same category of n-body (n=2,3,4) or non-bonded interatomic interaction, is of importance due to the following reasons. First of all these relationships allow non-

dimensionalized potential energy functions to be plotted against non-dimensionalized interatomic distance, bending angle or twisting angle – thereby allowing a graphical display of discrepancies among similar class of interatomic potentials. Secondly such parametric relationships enable available atomic and molecular data based on a specific potential function to be converted to parameters of another specific potential function adopted in certain computational chemistry software. As such, a spreadsheet-based potential function converter is proposed herein for the convenient designing of drugs, analysis of nano-scale and nano-structured devices, or any other molecular modeling tasks, when problems of mismatch between parametric data and adopted potential function in software are encountered. In development of a molecular potential function converter, commonly-used potential functions are taken into consideration. Hence the potential functions connected for 2-body interaction are the harmonic potential, polynomial series potential and Morse potential. The potential functions being related for 3-body interaction are the harmonic angle potential, polynomial angle series potential, harmonic cosine angle potential and the Fourier series potential. For 4-body interaction, the trigonometric series potential is converted to cosine power series potential and vice versa. Finally, relationships among Lennard-Jones (12-6) potential, Lennard-Jones (9-6) potential and Exponential-6 potential are related for the category of van der Waals interaction. These 12 potential functions are chosen due to their high utilization as can be inferred from the fact that at least one of these potentials functions from each category is adopted in typical computational chemistry softwares such as EAS [1], CVFF [2], CHARMM [3], GROMOS [4], TRIPOS [5], DREIDING [6], COSMIC [7], SHAPES [8], UFF [9], AMBER [10], MOMEC [11], OPLS [12], MM2 [13], MM3 [14], CFF91/93/95 [15], EFF [16], MMFF [17], MM4 [18], ESFF [19] and ECEPP [20], among others.

Functional forms of the four categories of molecular functions are furnished in the appendix. The symbols and nomenclature follow the usual meaning given in earlier papers [21-26]. The objective of this paper is to provide an easy-to-make and easy-to-use potential function converter right from the beginning with a suggested

spreadsheet layout to the conversion computation in the Microsoft Excel® software. This software is selected due to its ease of usage as well as its widespread use.

2. Spreadsheet Layout

Based on Microsoft Excel®, the layout of the potential function converter spreadsheet is set up such that each category of interatomic interaction fits into one page-width of A4-sized or Letter-sized paper for the convenience of printing. The layout is based on these two paper sizes as they are the paper size mostly used for personal computer printout. For a category of interatomic interaction that considers x number of potential functions, we set $(x +2)$ number of columns such that the first column identifies the parameter symbols with the corresponding SI units in parentheses. The second column caters for numerical input corresponding to the first column. The third to the $(x +2)^{th}$ columns are the output columns. As a generalized illustration, Figure 1 depicts how the input for potential function Q gives output results for potential functions P, R and S. For example, typing the input qq1 and qq2, the spreadsheet calculates pp1 to pp3, rr1 & rr2, and ss1 to ss4.

Parameter [Unit]	Input	Output			
		Potential P	Potential Q	Potential R	Potential S
	Potential P				
xxx [ ]		-	pp1		
xxx [ ]		-	pp2		
xxx [ ]		-	pp3		
	Potential Q				
xxx [ ]	qq1		-		
xxx [ ]	qq2		-		
	Potential R				
xxx [ ]			rr1	-	
xxx [ ]			rr2	-	
	Potential S				
xxx [ ]			ss1		-
xxx [ ]			ss2		-
xxx [ ]			ss3		-
xxx [ ]			ss4		-

Figure 1. Example of input for Potential Q gives output for Potentials P, R and S.

As there are 3, 4, 2 and 3 potential functions considered herein for 2-body, 3-body, 4-body and van der Waals interactions respectively, suitable column widths are 15.71, 12.57, 19.86 and 15.71 points respectively. By formatting the widths according to the 5, 6, 4 and 5 required columns for the 2-body, 3-body, 4-body and van der Waals pages respectively, each of these categories fit exactly into the chosen paper size as displayed in Figures 2 to 5, in spite of both A4- and Letter-sized papers possessing slightly different page widths. In the input columns, blocks corresponding to parametric input are bolded on their boundaries for the user's ease of identification.

3. Spreadsheet Computation

With reference to Eqs.(A1) to (A3) of the Appendix, the parametric conversion for 2-body potentials are [21]

$$k_H = k_{S2} = 2D_M \alpha^2 \tag{1}$$

$$\begin{Bmatrix} k_{S2} \\ k_{S3} \\ k_{S4} \\ k_{S5} \\ k_{S6} \end{Bmatrix} = 2D_M \alpha^2 \begin{Bmatrix} 1 \\ -\alpha \\ \dfrac{7}{12}\alpha^2 \\ -\dfrac{1}{4}\alpha^3 \\ \dfrac{31}{360}\alpha^4 \end{Bmatrix} \tag{2}$$

and [26]

$$D_M = \frac{k_{S2}{}^3}{2k_{S3}{}^2} \tag{3}$$

$$\alpha = -\frac{k_{S3}}{k_{S2}}. \tag{4}$$

Equations (3) and (4) are of functions $D_M = D_M(k_{S2}, k_{S3})$ and $\alpha = \alpha(k_{S2}, k_{S3})$. The alternative functions $D_M = D_M(k_{S2}, k_{S4})$ and $\alpha = \alpha(k_{S2}, k_{S4})$, also in [26], are not adopted in the proposed converter in order to allow the possibility of converting the polynomial series function of order $m = 3$ (see Eq.(A2)) – that is used in MM2 [13] – into Morse potential function.

	A	B	C	D	E
1	Parametric Conversion for 2-Body Potential Functions				
2					
3	Parameter [Unit]	Input	Output		
4			Harmonic	Polynomial Series	Morse
5		Harmonic			
6	kH [kJ/mol/m2]		-		
7					
8		Polynomial Series			
9	kS2 [kJ/mol/m2]			-	
10	kS3 [kJ/mol/m3]			-	
11	kS4 [kJ/mol/m4]			-	
12	kS5 [kJ/mol/m5]			-	
13	kS6 [kJ/mol/m6]			-	
14					
15		Morse			
16	DM [kJ/mol]		-		-
17	α [/m]		-		-

Figure 2. Spreadsheet layout for 2-body potential function converter

To implement Eqs.(1) to (4), we program the 2-body potential function converter (Fig.2) as

```
C9 = B6
C10 = 0
C11 = 0
C12 = 0
C13 = 0
D6 = B9
D16 = (B9^3)/2/(B10^2)
D17 = - B10/B9
E6 = 2*B16*B17^2
E9 = 2*B16*B17^2
E10 = - 2*B16*B17^3
E11 = (7/6)*B16*B17^4
E12 = - 0.5*B16*B17^5
E13 = (31/180)*B16*B17^6
```

where the input elements are (i) B6, (ii) B9 to B13, or (iii) B16 and B17. The parametric conversions for 3-body potentials, corresponding to Eqs.(A4) to (A7) of the Appendix, are given as [22,26]

$$k_\theta = k_{\theta 2}. \tag{5}$$

$$\begin{Bmatrix} k_{\theta 2} \\ k_{\theta 3} \\ k_{\theta 4} \\ k_{\theta 5} \\ k_{\theta 6} \end{Bmatrix} = k_{C\theta} \begin{Bmatrix} \sin^2 \theta_0 \\ \sin \theta_0 \cos \theta_0 \\ -\dfrac{1}{3}\sin^2 \theta_0 + \dfrac{1}{4}\cos^2 \theta_0 \\ -\dfrac{1}{4}\sin \theta_0 \cos \theta_0 \\ \dfrac{2}{45}\sin^2 \theta_0 - \dfrac{1}{24}\cos^2 \theta_0 \end{Bmatrix}, \tag{6}$$

$$k_{C\theta} = \frac{2(k_{\theta 2} - k_{\theta 3})}{1 - (\sin 2\theta_0 + \cos 2\theta_0)}. \tag{7}$$

$$k_C = 4 k_F C_2, \tag{8}$$

$$k_\theta = k_{C\theta} \sin^2 \theta_0 \tag{9}$$

$$C_0 = C_2 \left(2\cos^2 \theta_0 + 1 \right) \tag{10a}$$

$$C_1 = -4 C_2 \cos \theta_0 \tag{10b}$$

$$C_2 = \frac{1}{4\sin^2 \theta_0}. \tag{10c}$$

Again we note that the function $k_{C\theta} = k_{C\theta}(k_{\theta 2}, k_{\theta 4})$ is selected over $k_{C\theta} = k_{C\theta}(k_{\theta 2}, k_{\theta 4})$ though both equations were given earlier [26]. This choice is made in order to enable parametric conversion of Eq.(A5) with $m = 3$, as adopted in EAS [1], EFF [16] and MMFF [17], to Eq.(A6). Based on [22,26] whereby

$$k_\theta = -k_F \left(C_1 \cos \theta_0 + 4 C_2 \cos 2\theta_0 \right), \tag{11}$$

$$\begin{Bmatrix} k_{\theta 2} \\ k_{\theta 3} \\ k_{\theta 4} \\ k_{\theta 5} \\ k_{\theta 6} \end{Bmatrix} = k_F \begin{Bmatrix} -\left(C_1 \cos \theta_0 + 2^2 C_2 \cos 2\theta_0 \right) \\ \dfrac{1}{3}\left(C_1 \sin \theta_0 + 2^3 C_2 \sin 2\theta_0 \right) \\ \dfrac{1}{12}\left(C_1 \cos \theta_0 + 2^4 C_2 \cos 2\theta_0 \right) \\ -\dfrac{1}{60}\left(C_1 \sin \theta_0 + 2^5 C_2 \sin 2\theta_0 \right) \\ -\dfrac{1}{360}\left(C_1 \cos \theta_0 + 2^6 C_2 \cos 2\theta_0 \right) \end{Bmatrix}. \tag{12}$$

and Eq.(10), we herein obtain

$$k_\Gamma = k_\theta = k_{\theta 2} = k_{C\theta} \sin^2 \theta_0 \tag{13}$$

$$k_{\theta3} = -\frac{1}{2}k_F\frac{C_1}{\sqrt{C_2}} \tag{14}$$

$$k_{\theta4} = -\frac{4}{3}k_F C_2\left[1 - \frac{7}{64}\left(\frac{C_1}{C_2}\right)^2\right] \tag{15}$$

$$k_{\theta5} = \frac{1}{8}k_F\frac{C_1}{\sqrt{C_2}} \tag{16}$$

$$k_{\theta6} = \frac{8}{45}k_F C_2\left[1 - \frac{31}{156}\left(\frac{C_1}{C_2}\right)^2\right]. \tag{17}$$

	F	G	H	I	J	K
1		Parametric Conversion for 3-Body Potential Functions				
2						
3	Parameter [Unit]	Input	Output			
4			Harmonic Angle	Polynomial Angle	Harmonic Cosine	Fourier Series
5		Harmonic Angle				
6	k_θ [kJ/mol/rad2]		·			
7	θ_0 [rad]		·			
8						
9		Polynomial Angle				
10	$k_{\theta2}$ [kJ/mol/rad2]			·		
11	$k_{\theta3}$ [kJ/mol/rad3]			·		
12	$k_{\theta4}$ [kJ/mol/rad4]			·		
13	$k_{\theta5}$ [kJ/mol/rad5]			·		
14	$k_{\theta6}$ [kJ/mol/rad6]			·		
15	θ_0 [rad]			·		
16						
17		Harmonic Cosine				
18	$k_{C\theta}$ [kJ/mol]				·	
19	θ_0 [rad]				·	
20						
21		Fourier Series				
22	k_F [kJ/mol]					·
23	C_0					·
24	C_1					·
25	C_2					·

Figure 3. Spreadsheet layout for 3-body potential function converter

Though Eq.(12) is theoretically valid [22], the choice of Eqs.(13) to (17) is more practical since the equilibrium bond angle does not appear in the Fourier series potential, as evident from Eq.(A7). Needless to say, given the Fourier series

parameters (k_F, C_0, C_1, C_2), the converter calculates the polynomial angle series parameters (k_{θ_n} & θ_0; $n = 2,3,4,5,6$) based on Eqs.(13) to (17). To execute Eqs.(5) to (17), we program the 3-body potential function converter (Fig.3) as follows:

```
H10 = G6
H11 = 0
H12 = 0
H13 = 0
H14 = 0
H15 = G7
H18 = G6/(sin(G7))^2
H19 = G7
H22 = G6
H23 = H25*(2*cos(G7)*cos(G7)+ 1)
H24 = -4*H25*cos(G7)
H25 = 1/4/(sin(G7))^2
I6 = G10
I7 = G15
I18 = 2*(G10-G11)/(1-(sin(2*G15)+cos(2*G15)))
I19 = G15
I22 = G10
I23 = I25*(2*cos(G15)*cos(G15)+ 1)
I24 = -4*I25*cos(G15)
I25 = 1/4/(sin(G15))^2
J6 = G18*(sin(G10))^2
J7 = G19
J10 = G18*(sin(G19))^2
J11 = G18*sin(G19)*cos(G19)
J12 = G18/4*cos(G19))^2-G18/3*(sin(G19))^2
J13 = -G18/4*sin(G19)*cos(G19)
J14 = 2*G18/45*(sin(G19))^2-G18/24*(cos(G19))^2
J15 = G19
J22 = G18*(sin(G19))^2
J23 = J25*(2*cos(G19)*cos(G19)+ 1)
J24 = -4*J25*cos(G19)
J25 = 1/4/(sin(G19))^2
K6 = G22
K7 = acos(-G24/G25/4)
K10 = G22
K11 = -0.5*G22*G24/sqrt(G25)
K12 = -(4/3)*G22*G25*(1-(7/64)*(G24/G25)^2)
K13 = 0.125*G22*G24/sqrt(G25)
```

```
K14 = (8/45)*G22*G25*(1-(31/256)*(G24/G25)^2)
K15 = acos(-G24/G25/4)
K18 = 4*G22*G25
K19 = acos(-G24/G25/4)
```

Here the input elements are: (i) G6 and G7, (ii) G10 to G15, (iii) G18 and G19, or (iv) G22 to G25. With reference to Eqs.(A8) and (A9), parametric conversions for 4-body potential functions have been given as [23,26]

$$
\begin{Bmatrix} k_{T0} \\ k_{Ti} \\ k_{T2} \\ k_{T3} \\ k_{T4} \\ k_{T5} \end{Bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 2 & 1 & 0 & 1 \\ 1 & 0 & -3 & 0 & 5 \\ 0 & -2 & 0 & 8 & 0 \\ 0 & 0 & 4 & 0 & -20 \\ 0 & 0 & 0 & -8 & 0 \\ 0 & 0 & 0 & 0 & 16 \end{bmatrix} \begin{Bmatrix} k_{\phi 1} \\ k_{\phi 2} \\ k_{\phi 3} \\ k_{\phi 4} \\ k_{\phi 5} \end{Bmatrix}
\tag{18}
$$

and

$$
\begin{Bmatrix} k_{\phi 1} \\ k_{\phi 2} \\ k_{\phi 3} \\ k_{\phi 4} \\ k_{\phi 5} \end{Bmatrix} = \frac{1}{8} \begin{bmatrix} 16 & 0 & 12 & 0 & 10 \\ 0 & -8 & 0 & -8 & 0 \\ 0 & 0 & 4 & 0 & 5 \\ 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} k_{T1} \\ k_{T2} \\ k_{T3} \\ k_{T4} \\ k_{T5} \end{Bmatrix}.
\tag{19}
$$

	L	M	N	O
1		Parametric Conversion for 4-Body Potential Functions		
2				
3	Parameter [Unit]	Input	Output	
4			Trigonometric Series	Cosine Power Series
5		Trigonometric Series		
6	$k_{\phi 1}$ [kJ/mol]		-	
7	$k_{\phi 2}$ [kJ/mol]		-	
8	$k_{\phi 3}$ [kJ/mol]		-	
9	$k_{\phi 4}$ [kJ/mol]		-	
10	$k_{\phi 5}$ [kJ/mol]		-	
11				
12		Cosine Power Series		
13	k_{T0} [kJ/mol]			-
14	k_{T1} [kJ/mol]			-
15	k_{T2} [kJ/mol]			-
16	k_{T3} [kJ/mol]			-
17	k_{T4} [kJ/mol]			-
18	k_{T5} [kJ/mol]			-

Figure 4. Spreadsheet layout for 4-body potential function converter

For execution of Eqs.(18) and (19), the 4-body potential function converter (Fig.4) is programmed as

```
N13 = 0.5*M6+ M7+ 0.5*M8+ 0.5*M10
N14 = 0.5*M6-1.5*M8+ 2.5*M10
N15 = -M7+ 4*M9
N16 = 2*M8-10*M10
N17 = -4*M9
N18 = 8*M10
O6 = 2*M14+ 1.5*M16+ 1.25*M18
O7 = -M15-M17
O8 = 0.5*M16+ (5/8)*M18
O9 = -0.25*M17
O10 = 0.125*M18
```

in which inputs can either be from (i) M6 to M10, or (ii) M13 to M18. Figure 5 shows the spreadsheet layout for the van der Waals potential function converter. Relationships among van der Waals potential functions – given by Eqs.(A10) to (A12) – has been developed [24] and summarized as [26]

$$A = 162755 D_{12-6}^{LJ} = 16206.2 D_{9-6}^{LJ} \tag{20}$$

$$B = \frac{12}{R_{12-6}^{LJ}} = \frac{9}{R_{9-6}^{LJ}} \tag{21}$$

$$C = 2 D_{12-6}^{LJ} \left(R_{12-6}^{LJ} \right)^6 = 3 D_{9-6}^{LJ} \left(R_{9-6}^{LJ} \right)^6 \tag{22}$$

for long range approximation, and

$$A = 739132 D_{12-6}^{LJ} = 18153.1 D_{9-6}^{LJ} \tag{23}$$

$$B = \frac{13.772}{R_{12-6}^{LJ}} = \frac{11.162}{R_{9-6}^{LJ}} \tag{24}$$

$$C = 1.772 D_{12-6}^{LJ} \left(R_{12-6}^{LJ} \right)^6 = 2.1623 D_{9-6}^{LJ} \left(R_{9-6}^{LJ} \right)^6 \tag{25}$$

for near equilibrium case. Inferring from Eqs.(20) and (21), the long range relationship between Lennard-Jones (12-6) and (9-6) are

$$D_{9-6}^{LJ} = 10.043 D_{12-6}^{LJ} \tag{26}$$

$$R_{9-6}^{LJ} = \frac{3}{4} R_{12-6}^{LJ}. \tag{27}$$

	P	Q	R	S	T
1	Parametric Conversion for van der Waals Potential Functions (long range)				
2					
3	Parameter [Unit]	Input	Output		
4			Lennard-Jones (12-6)	Lennard-Jones (9-6)	Exponential-6
5		Lennard-Jones (12-6)			
6	D$_{12\text{-}6}$ [kJ/mol]		-		
7	R$_{12\text{-}6}$ [m]		-		
8					
9		Lennard-Jones (9-6)			
10	D$_{9\text{-}6}$ [kJ/mol]			-	
11	R$_{9\text{-}6}$ [m]			-	
12					
13		Exponential-6			
14	A [kJ/mol]				-
15	B [/m]				-
16	C [kJm6/mol]				-
17					
18					
19	Parametric Conversion for van der Waals Potential Functions (near equilibrium)				
20					
21	Parameter [Unit]	Input	Output		
22			Lennard-Jones (12-6)	Lennard-Jones (9-6)	Exponential-6
23		Lennard-Jones (12-6)			
24	D$_{12\text{-}6}$ [kJ/mol]		-		
25	R$_{12\text{-}6}$ [m]		-		
26					
27		Lennard-Jones (9-6)			
28	D$_{9\text{-}6}$ [kJ/mol]			-	
29	R$_{9\text{-}6}$ [m]			-	
30					
31		Exponential-6			
32	A [kJ/mol]				-
33	B [/m]				-
34	C [kJm6/mol]				-

Figure 5. Spreadsheet layout for van der Waals potential function converter

Discrepancy between both sets of Lennard-Jones parameters, as shown in Eqs.(26) and (27), is due to the requirement to ensure energistic correlation when compared over long range non-bonded distance. In the case of near-equilibrium, parametric relations between both Lennard-Jones potentials are

$$D_{9-6}^{LJ} = D_{12-6}^{LJ} \tag{28}$$

$$R_{9-6}^{LJ} = R_{12-6}^{LJ} \tag{29}$$

as obviously dictated by the minimum well-depth $U_{min} = -D$ at equilibrium distance $r = R$.

Practical implementation of Eqs.(20) to (29) for conversion of van der Waals functional parameters are as follows:

```
R10 = 10.043*Q6
R11 = 0.75*Q7
R14 = 162755*Q6
R15 = 12/Q7
R16 = 2*Q6*Q7^6
R28 = Q24
R29 = Q25
R32 = 739132*Q24
R33 = 13.772/Q25
R34 = 1.772*Q24*Q25^6
S6 = 0.099574*Q10
S7 = (4/3)*Q11
S14 = 16206.2*Q10
S15 = 9/Q11
S16 = 3*Q10*Q11^6
S24 = Q28
S25 = Q29
S32 = 18153.1*Q28
S33 = 11.162/Q29
S34 = 2.1623*Q28*Q29^6
T6 = Q14/162755
T7 = 12/Q15
T10 = Q14/16206.2
T11 = 9/Q15
T24 = Q32/739132
T25 = 13.772/Q33
T28 = Q32/18153.1
T29 = 11.162/Q33
```

As in the case of 2-, 3- and 4-body converters, the user is required to provide input for (i) Q6 and Q7, (ii) Q10 and Q11, or (iii) Q14 to Q16, in the case of long range conversion; or entering input in (i) Q24 and Q25, (ii) Q28 and Q28, or (iii) Q32 to Q34, for the case of near-equilibrium.

4. Illustration

As a sample illustration, keying in 694.12 (for $k_{C\theta}$ =694.12kJ/mol) and 1.9373 (for θ_0 =1.9373rad) into the cells G18 and G19 respectively gives inputs of harmonic cosine angle potential parameters. The results for harmonic angle potential, polynomial series angle potential and Fourier series potential functions are simultaneously generated in column J, as shown in Figure 6. Good agreement is found between the presently generated results and previously verified results [22]. Input and output are bolded in Figure 6 for clarity.

	F	G	H	I	J	K
1		Parametric Conversion for 3-Body Potential Functions				
2						
3	Parameter [Unit]	Input	Output			
4			Harmonic Angle	Polynomial Angle	Harmonic Cosine	Fourier Series
5		Harmonic Angle				
6	kθ [kJ/mol/rad2]		-	0.000E+00	6.050E+02	0.000E+00
7	θ0 [rad]		-	0.000E+00	1.937E+00	#DIV/0!
8						
9		Polynomial Angle				
10	kθ2 [kJ/mol/rad2]		0.000E+00	-	6.050E+02	0.000E+00
11	kθ3 [kJ/mol/rad3]		0.000E+00	-	-2.322E+02	#DIV/0!
12	kθ4 [kJ/mol/rad4]		0.000E+00	-	-1.794E+02	#DIV/0!
13	kθ5 [kJ/mol/rad5]		0.000E+00	-	5.806E+01	#DIV/0!
14	kθ6 [kJ/mol/rad6]		0.000E+00	-	2.317E+01	#DIV/0!
15	θ0 [rad]		0.000E+00	-	1.937E+00	#DIV/0!
16						
17		Harmonic Cosine				
18	kCθ [kJ/mol]	694.12	#DIV/0!	#DIV/0!	-	0.000E+00
19	θ0 [rad]	1.9373	0.000E+00	0.000E+00	-	#DIV/0!
20						
21		Fourier Series				
22	kF [kJ/mol]		0.000E+00	0.000E+00	6.050E+02	-
23	C0		#DIV/0!	#DIV/0!	3.605E-01	-
24	C1		#DIV/0!	#DIV/0!	4.112E-01	-
25	C2		#DIV/0!	#DIV/0!	2.868E-01	-

Figure 6. Sample illustration whereby input in cells G18 and G19 generates output in column J.

5. Conclusion

A molecular potential function converter has been developed using Microsoft Excel® spreadsheet on the basis of recently formulated mathematical relationships [21-24]. The present prototype converter has been illustrated to be technically workable, thereby paving way for further refinements in terms of user-friendliness and pleasant appearance.

References

[1]   E.M. Engler, J.D. Andose, P.v.R. Schleyer, J. Am. Chem. Soc. **95** (1973) 8005

[2]   S. Lifson, A.T. Hagler and P. Dauber, J. Am. Chem. Soc. **101** (1979) 5111

[3]   R. Brooks, R.E. Bruccoleri, B.D. Olafson, D.J. States, S. Swaminathan and M. Karplus, J. Comput. Chem. **4** (1983) 187

[4]   W.F. van Gunsterenm and H.J.C. Berendsen, Groningen Molecular Simulation (GROMOS) Library Manual (1987)

[5]   M. Clark, R.D. Cramer III and N. van Opdenbosch, J. Comput. Chem. **10** (1989) 982

[6]   S.L. Mayo, B.D. Olafson and W.A. Goddard III, J. Phys. Chem. **94** (1990) 162

[7]   S.D. Morley, R.J. Abraham, I.S. Haworth, D.E. Jackson, M.R. Saunders and J.G. Vinter, J. Comput.-Aided Mol. Des. **5** (1991) 475.

[8]   V.S. Allured, C.M. Kelly and C.R. Landis, J. Am. Chem. Soc. **113** (1991) 1

[9]   A.K. Rappe, C.J. Casewit, K.S. Colwell, W.A. Goddard and W.M. Skiff, J. Am. Chem. Soc. **114** (1992) 10024

[10] W.D. Cornell, P. Cieplak, C.I. Bayly, I.R. Gould, K.M. Merz Jr, D.M. Ferguson, D.C. Spellmeyer, T. Fox, J.W. Caldwell and P.A. Kollman, J. Am. Chem. Soc. **117** (1995) 5179

[11] P. Comba and T.W. Humbley, Molecular Modeling of Inorganic Compounds, VCH (1995)

[12] W. Damm, A. Frontera, J. Tirado-Rives and W.L. Jorgensen, J. Comput. Chem. **18** (1997) 1955

[13] N.L. Allinger, J. Am. Chem. Soc. **99** (1977) 8127

[14] N.L. Allinger, Y.H. Yuh and J.H. Lii, J. Am. Chem. Soc. **111** (1989) 8551

[15] M.J. Hwang, T.P. Stockfisch and A.T. Hagler, J. Am. Chem. Soc. **116** (1994) 2515

[16] J.L.M. Dillen, J. Comput. Chem. **16** (1995) 595

[17] T.A. Halgren, J. Comput. Chem. **17** (1996) 490

[18] N.L. Allinger, K. Chen, J.H. Lii, J. Comput. Chem. **17** (1996) 642

[19] S. Barlow, A.H. Rohl, S. Shi, C.M. Freeman and D. O'Hare, J. Am. Chem. Soc. **118** (1996) 7578

[20] G. Nemethy, K.D. Gibsen, K.A. Palmer, C.N. Yoon, G. Paterlini, A. Zagari, S. Rumsey and H.A. Scheraga, J. Phys. Chem. **96** (1992) 6472

[21] T.C. Lim, J. Math. Chem. **33** (2003) 29

[22] T.C. Lim, J. Math. Chem. **32** (2002) 249

[23] T.C. Lim, J. Math. Chem. **31** (2002) 421

[24] T.C. Lim, J. Math. Chem. **33** (2003) 279

[25] T.C. Lim, J. Math. Chem. **34** (2003) 221

[26] T.C. Lim, MATCH Commun. Math. Comput. Chem. **49** (2003) 155

Appendix

The appendix lists molecular potential functions that are considered for parametric conversion. The 2-body potential functions being related are the harmonic potential

$$U_H = \frac{1}{2} k_H (r - r_0)^2 = \frac{1}{2} k_H (\delta r)^2 ,$$

(A1)

the polynomial series potential

$$U_S = \frac{1}{2} \sum_{n=2}^{m} k_{Sn} (\delta r)^n \quad ; \quad (m = 3,4,5,6)$$

(A2)

and the Morse potential

$$U_M = D_M \left[1 - \exp(- \alpha \, \delta r) \right]^2 .$$

(A3)

The 3-body potential functions being related are the harmonic angle potential

$$U_\theta = \frac{1}{2}k_\theta(\theta - \theta_0)^2 = \frac{1}{2}k_\theta(\delta\theta)^2,$$

(A4)

the polynomial angle series potential

$$U_{S\theta} = \frac{1}{2}\sum_{n=2}^{m}k_{\theta n}(\delta\theta)^n \quad ; \quad (m = 3,4,5,6),$$

(A5)

the harmonic cosine angle potential

$$U_{C\theta} = \frac{1}{2}k_{C\theta}(\cos\theta - \cos\theta_0)^2$$

(A6)

and the Fourier series potential

$$U_F = k_F \sum_{n=0}^{2}C_n \cos(n\theta).$$

(A7)

The 4-body potential functions being related are the trigonometric series potential

$$U_\phi = \frac{1}{2}\sum_{n=1}^{5}k_{\phi n}\left[1 - (-1)^n \cos(n\phi)\right]$$

(A8)

and the cosine power series potential

$$U_T = \sum_{n=0}^{5}k_{Tn} \cos^n \phi.$$

(A9)

The van der Waals potential functions being related are the Lennard-Jones (12-6) potential

$$U_{12-6}^{LJ} = D_{12-6}^{LJ}\left[\left(\frac{R_{12-6}^{LJ}}{r}\right)^{12} - 2\left(\frac{R_{12-6}^{LJ}}{r}\right)^6\right],$$

(A10)

the Lennard-Jones (9-6) potential

$$U_{9-6}^{LJ} = D_{9-6}^{LJ}\left[2\left(\frac{R_{9-6}^{LJ}}{r}\right)^9 - 3\left(\frac{R_{9-6}^{LJ}}{r}\right)^6\right]$$

(A11)

and the Exponential-6 potential

(A12)

$$U_{X6} = A\exp(-Br) - \frac{C}{r^6}.$$