First International Electronic Conference on Synthetic Organic Chemistry (ECSOC-1), www.mdpi.org/ecsoc/, September 1-30, 1997

[E0001]

Organic and Drug Molecules Spin Traps and Free Radicals Multi-frequency EPR Spectra Simulation by Fast Fourier Transform (FFT)

Hanqing Wu

Department of Chemistry, University of Wisconsin-Milwaukee, Milwaukee, WI 53201, USA. E-mail: hanqing@csd.uwm.edu

With biographical summary

Received: 13 July 1997 / Uploaded: 14 July 1997

Abstract

Fast fourier transform (FFT) has been used for simulation of **EPR** spectra. The author applied it to simulate spin traps and free radicals multi-frequency **EPR** spectra. The simulated **EPR** spectra results are discussed and compared with each other. Two methods are introduced to simulate EPR spectra at other frequencies besides **X**-band (~9.0 G Hz). The simple modified program provided here can simulate almost all the common spin traps and free radicals of organic and drug molecules.

Key words: Spin traps, free radical, EPR, simulation, multi-frequency, Fast Fourier Transform (FFT).

Introduction

The invention of the computer algorithm known as the **Fast Fourier Transform** (FFT) in the mid-1960s opened up the possibility of a wider usage of the **Fourier Transform** (FT) in computational physics and many other areas of physics, mathematics, and chemistry. Fast fourier transform is a multi grid algorithm to compute the fourier transform of a function. It performs like N*log(N) (compare with N*N for the brute forward algorithm). Every simulated spin trap or free radical EPR spectrum data is represented as a complex number with a "real" part (called *re*) and an "imaginary" part (called *im*). For the simulated organic free radical EPR spectrum data, the "imaginary" component of the data is zero, and the "real" value represents the strength of the spin trap or the free radical EPR signal. The entire waveform is an array of such complex numbers. The size of this array MUST be a power of two for the FFT algorithm to work. The author refers the interested reader to the literature [1,2].

Electron spin resonance spectroscopy (ESR) represents one of the most versatile and useful techniques for the study of spin traps and free radicals. The ESR spectroscopies also provide structural information on the configuration and conformation of transition free radicals in solution [3]. Detailed EPR theory, spin trap and free radical spin Hamiltonian equation have been presented and discussed previously in the reference [1]; the author will not repeat this introduction and discussion here.

Belford and Clarkson [4] have introduced the Multi-frequency EPR and mentioned that the low-frequency (<9 GHz) EPR experiments may lead to increased spectral resolution or enhance features due to "forbidden" transitions. High-frequency (>35 GHz) experiments also may in enhanced resolution or allow for more accurate determinations of zero-filed splittings in high-spin systems. Different frequency EPR spectrometers have been used to measure EPR spectra of some non-heme and copper proteins [5,6,7,8,9]. Recent papers reported that high-frequency EPR spectroscopies have been used for detecting or characterizing spin traps or radicals [10,11,12]. One question may be asked: what do the EPR spectra of spin traps and free radicals at different frequencies look like? The simulation of spin traps and free radicals at different frequencies is also very interesting. Several papers have reported that high spin species (S = 1, 3/2, 2 etc.) with low D values (D < 0.3 cm^{-1}, which corresponding to the frequency of X-band) also appear multiple EPR signals near g ~ 2 [13,14,15,16,17]. EPR experiments are usually carried out at X-band (~9.5 GHz) because of the good concentration sensitivity and ready availablity of this method [10]. To identify the measured EPR signals around g ~ 2, the multi-frequency EPR spectra measurements are necessary if the free radical and high spin species with low D value or anisotropic spin 1/2 systems [4,6,18] co-exist in the systems. To raise the resolution of overlaping EPR species with slightly different g values, high-frequency EPR measurements are also necessary [10,11,12].

In this poster, the author will provide two methods to simulate spin traps and free radicals EPR spectra at different frequencies (~1.5 G Hz for S-band, ~3.0 G Hz for L-band, ~9.0 G Hz for X-band, ~25 G Hz for K-band, ~35 G Hz for Q-band, ~95 G Hz for W-band, ~250 GHz for G-band, and 373 G Hz for "Z" band metioned in the references [19,20,21]). The basic idea can also be known from the author's recent published paper [19,20,21]. The simulated EPR spectra results are compared and discussed here.

Calculation

The program is modified from the reference [2]. The inputs include frequency, g value, scan range, splitting parameters, widths, and size of array (M=11 for example).

In the cited reference [3], different kinds of alkyl radical are given and their coupling constants are also provided. These radicals include methyl, ethyl, isopropyl, t-butyl, cycloakyl, bicycloalky ,a-haloalkyl, a-oxygen substituted alkyl, alkenyl, and allylic radicals. For spin traps, there are lots of data published in some papers [22,23] and can be searched from the internet. For example, one can search spin trap of $\cdot OC(CH_3)_3$ at the page of http://alfred.niehs.nih.gov/LMB/stdb/. The searching result with 100 examples has been found by current date, which has been saved to local directory with the file of occh33.htm. The simulated EPR spectra for DMPO $*\cdot OC(CH_3)_3$ in QA BHD + catalase can be seen in the following.

Results and discussion

Two methods can be used to simulate EPR spectra at different frequencies: one is a direct method, which is straight forward; the other is indirect method, in which one needs to adjust the values of some parameters. As mentioned in the reference [20], any frequency EPR spectrum can be simulated at X-band, which is convient and familiar to most people, and the X-axis scale need to be reduced by a factor, which is the ratio of frequency at X-band (9.3 G Hz) over frequency at desired band. The scan rang and the splitting parameters need to be multiplied by a certain factor {frequency at X-band (9.3 G Hz) over frequency at desired band}. Figure 1 shows that the simulated EPR spectra at X-band with different widths have different resultion, the smaller width, the higher resolution (see the top two graphs in Figure 1). The simulated EPR spectrum at S-band can be obtained from the simulated EPR spectrum at X-band, but one needs to expand the splitting parameters by a factor of 6.2 (9.3/1.5) from $\mathbf{a}_N$ = 14.5 G to 89.9 G, $\mathbf{a}_H$ = 15.70 G to 97.34 G, and expands the scan range by the same factor. After getting the spectrum (see left-bottom in Figure 1), the X-scale needs to be reduced by the same factor of 6.2, the EPR spectrum is obtained, which is totally identical to the spectrum simulated directly (see left-top figure in Figure 2). If the scan range and widths remain same for the simulation of EPR spectra at different frequencies, then the same spectra with different shift in X-scale are obtained (see Figure 2), which may not consistent with a real EPR spectrum. The lineshape of spin labeles is neither the Lorentzian nor the Gaussian, but a mixture of them.The mixture of the Gaussian and Lorentzian lineshapes is caused by both inhomogeneous and homogeneously broadening [24]. The author uses the same parameters which used above, but varies the g value. The shapes of the simulated EPR spectra are identical, but with different X-scale shift (data or figures are

not shown again). The reason is that g value(**g**), frequency (**f**), and signal position (**Hr**) have the relationships of **g·f = 714.4 ·Hr**, where, the units for frequency and signal position are G Hz and G respectively.

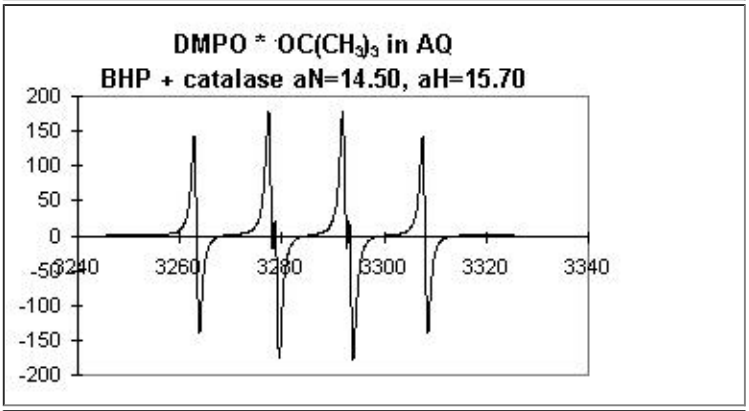
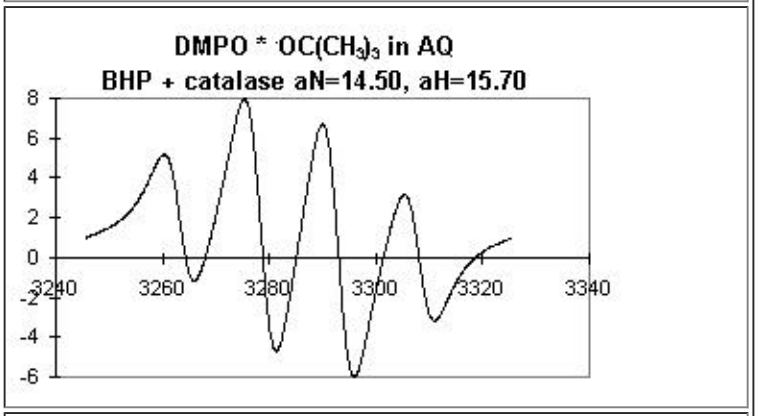
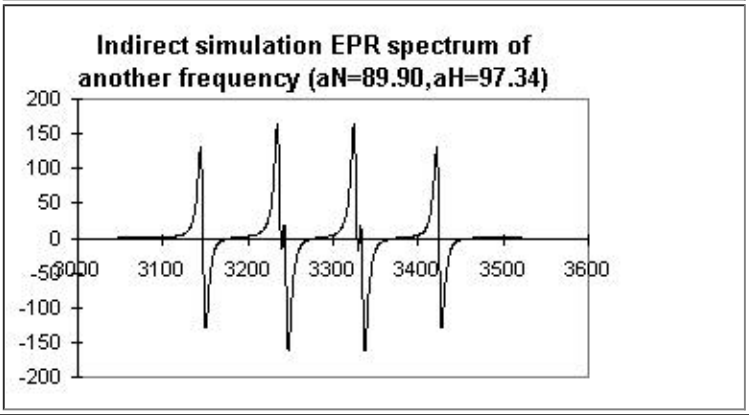
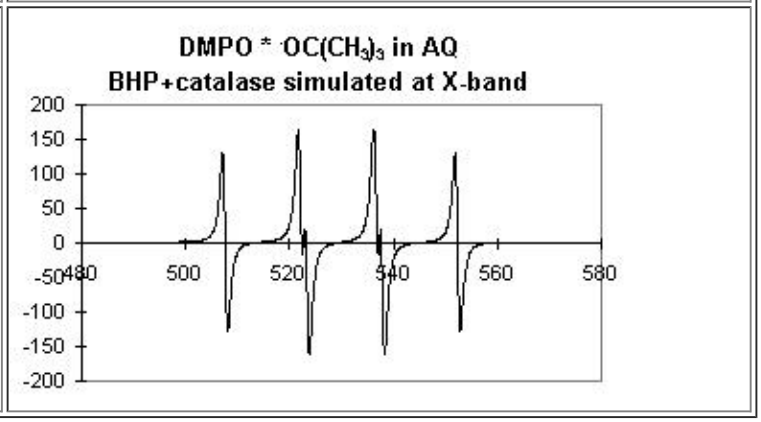
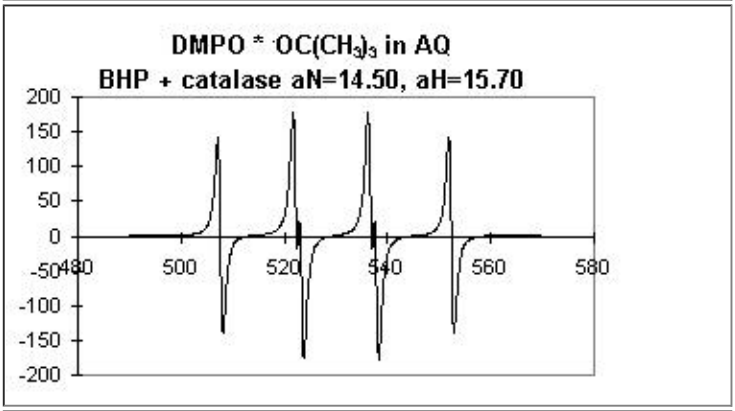
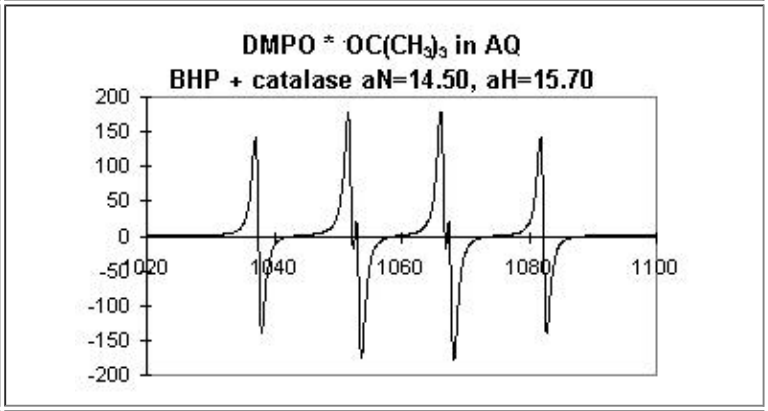
EPR simulation at **X**-Band with frequency of 9.3 G Hz; **W** = 1 G and scan range = 80 G.	EPR simulation at **X**-Band with frequency of 9.3 G Hz; **W** = 6.2 G and scan range = 80 G
	
EPR simulation at **X**-Band with frequency of 9.3 G Hz; **W** = 6.2 G and scan range = 496 G	EPR spectrum at **S**-Band (1.5 G Hz) which is obtained from the left spectrum by reducing the X-scale of 6.2
	

Figure 1. EPR simulation of DMPO ·$OC(CH_3)_3$ in AQ, BHP + catalase with $\mathbf{a}_N$ = 14.50 G, $\mathbf{a}_H$ = 15.70 G, with two different widths and two different frequencies.

EPR simulate at S-Band with frequency of 1.5 G Hz	EPR simulation at B-Band with frequency of 3.0 G Hz
	
EPR simulation at K-Band with frequency of 25 G Hz	EPR simulation at Q-band with frequency of 35 G Hz

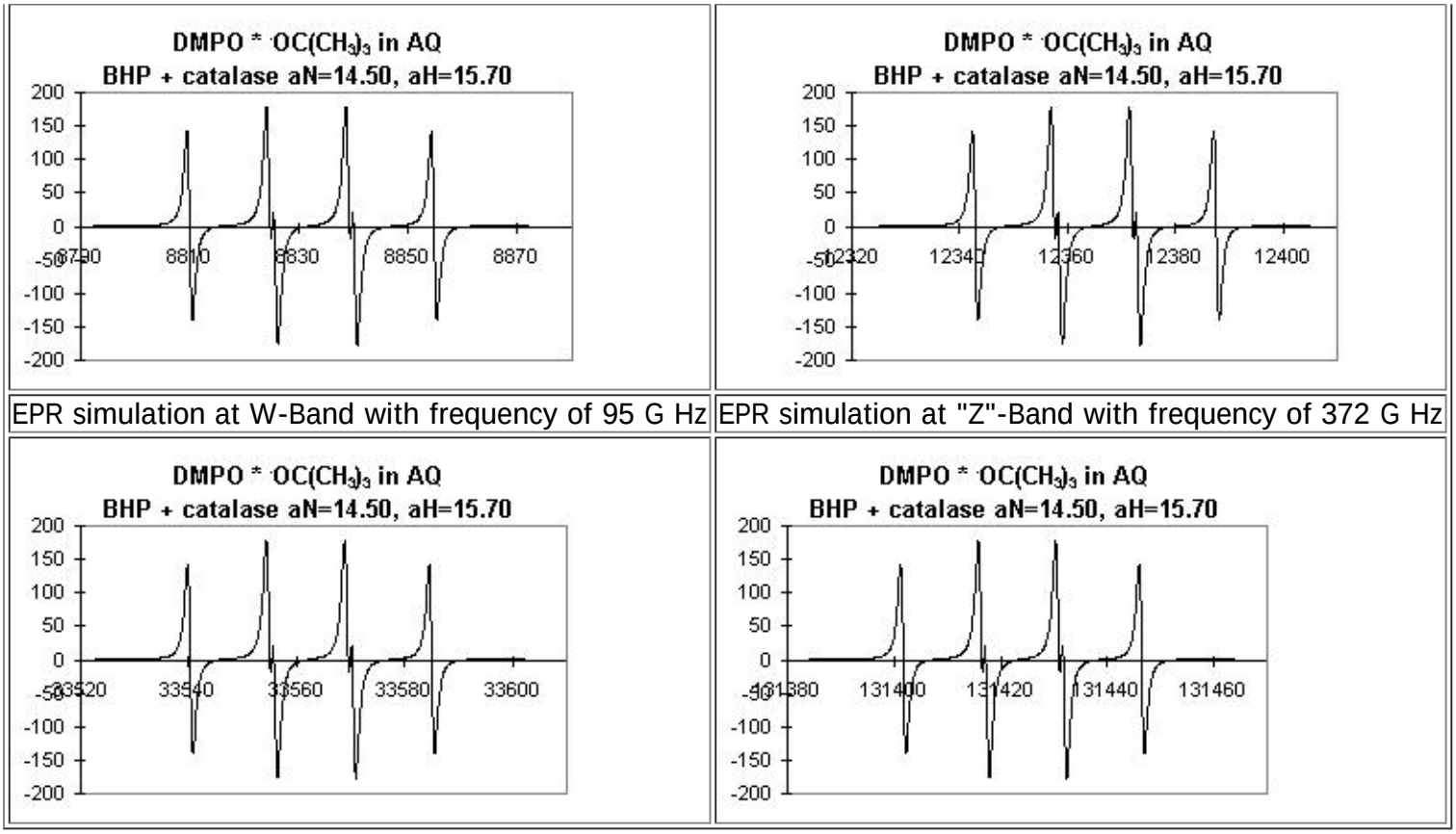


Figure 2. EPR simulation of DMPO ·$OC(CH_3)_3$ in AQ, BHP + catalase with $\mathbf{a}_N$ = 14.50 G, $\mathbf{a}_H$ = 15.70 G, at different frequencies

---

More spin traps simulated EPR spectra can be seen in Figure 3 according to the parameters given in the reference [23]. The simulated EPR spectrum of DMPO spin adduct of C(phenyl) free radical and that of DMPO spin adduct of N(alkyl) free radical are very similar, the simulated EPR spectra of DMPO spin adducts of O_2R and S cysteinyl free radicals are also similar with each other. Recent paper also reports that: at X-band, the ESR parameters of DMPO-glutathionyl radical adduct (DMPO/·SG) and DMPO-hydroxyl radical adduct (DMPO/·OH) are nearly similar in aqueous solutions, most spectral lines of DMPO/·SG virtually over-lap with those of the DMPO/·OH adduct [12]; The phenyl-PBN and the trichloromethyl-PBN spin adducts have the similar situation [10]. These papers have examined how high-field (HF) EPR at high frequencies (either Q-band or W-band) with enhanced g value resolution and sensitity to rotational motion can provide additional information on these spin adducts [10,11,12].

The linewidth at different frequencies has different values, which has been detailed disscussed in the literature [10,25], the author does not introduce here. From equation 1 in the reference [10], the author can get the equation as the following:

$$^{\Delta}H \sim 357.2 * {}^{\Delta}g * f \qquad {}^{\Delta\Delta}H \sim 357.2 * {}^{\Delta}g * {}^{\Delta}f$$

where $^{\Delta}H$ is the difference in th field position of the two spin adducts at certain frequency EPR measurement; and $^{\Delta\Delta}H$ is the difference of $^{\Delta}H$; $^{\Delta}g$ is the difference of the g values of two spin adducts (free radicals); f is the frequency; $^{\Delta}f$ is the difference of the frequencies.

The author takes the example from the reference [10] and considers the isotropic EPR simulation by current

program, the isotropic magnetic parameters of phenyl-PBM and trichloromethyl-PBM spin adducts are given as the following:

phenyl-PBM	trichoromethyl-PBM
g_{iso} = 2.00614 a_N = 14.263 a_H = 2.148	g_{iso} = 2.00626 a_N = 13.878 a_H = 1.540

Assuming two spin adducts are measured at two frequencies: 9.5 GHz for X-band and 95 GHz for W-band, then f1 = 9.5 GHz, f2 = 95 GHz; $^{\Delta}$f = f2 - f1 = 95 - 9.5 = 85.5 GHz; $^{\Delta}$g = 2.00626 - 2.00614 = 0.00012; $^{\Delta}$H1 = 357.2* $^{\Delta}$g*f1 = 357.2*0.00012*9.5 = 0.41 (G); $^{\Delta}$H2 = 357.2* $^{\Delta}$g*f2 = 357.2*0.00012*95 = 4.1 (G); $^{\Delta\Delta}$H = $^{\Delta}$H2 - $^{\Delta}$H1 = 4.1 -0.41 = 3.7 (G). For easy comparison, the author simulate their EPR spectra with width of 1 G at X-band with frequency of 9.5 GHz and at W-band with frequency of 95 GHz, the simulated EPR spectra with scan range of 50 G can be seen in Figure 4, which tells us how better resolution (seperation) at W-band than at X-band if two spin adducts mix together, the same situation for other spin adducts and other free radicals with slightly differenct g values.

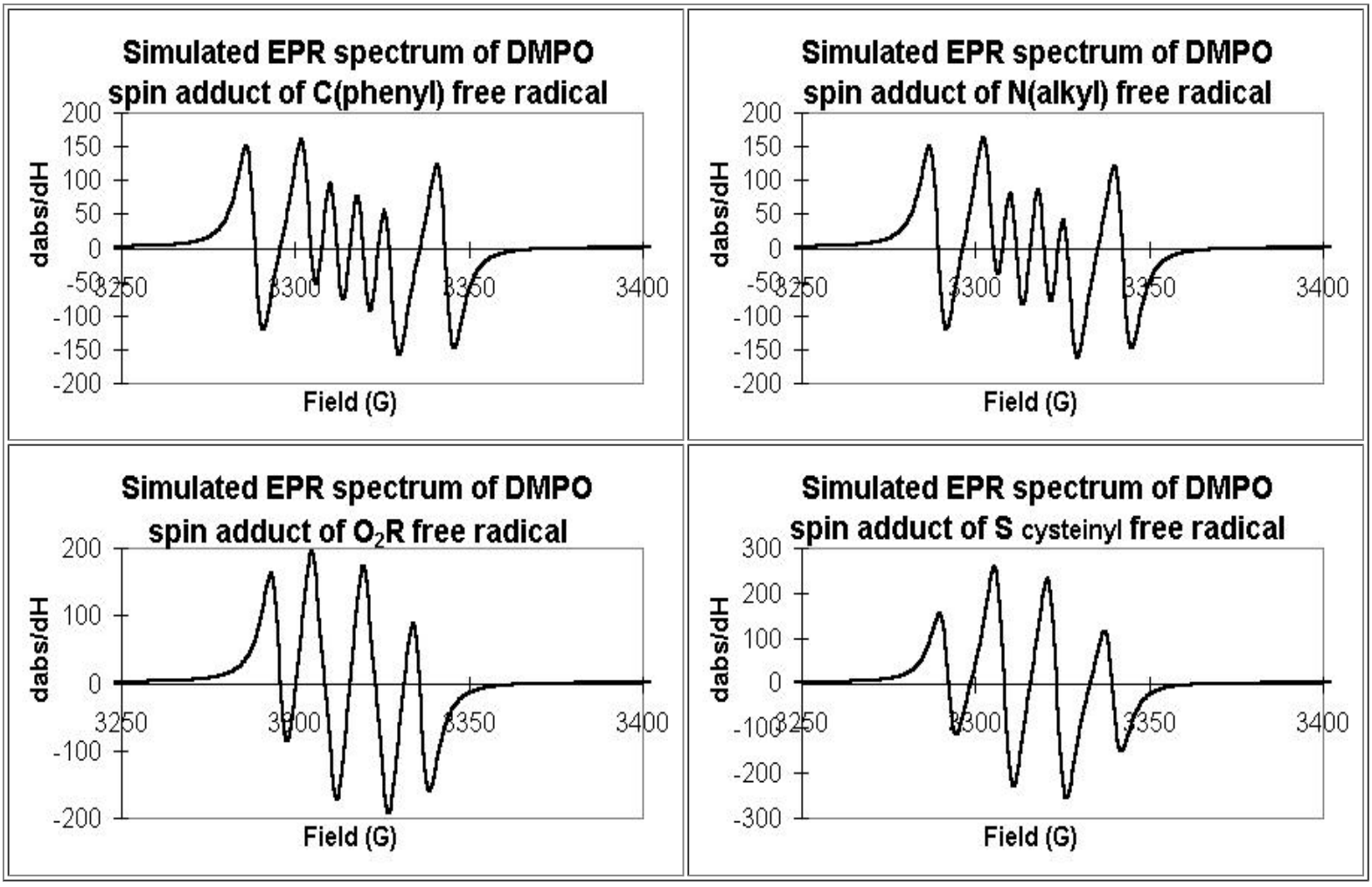


Figure 3. Simulated EPR spectra of DMPO spin adducts of C (phenyl), N (alkyl), O_2R, S cysteinyl free radicals. g = 2.0026, frequency = 9.3 GHz, scan range 400 G, M = 11

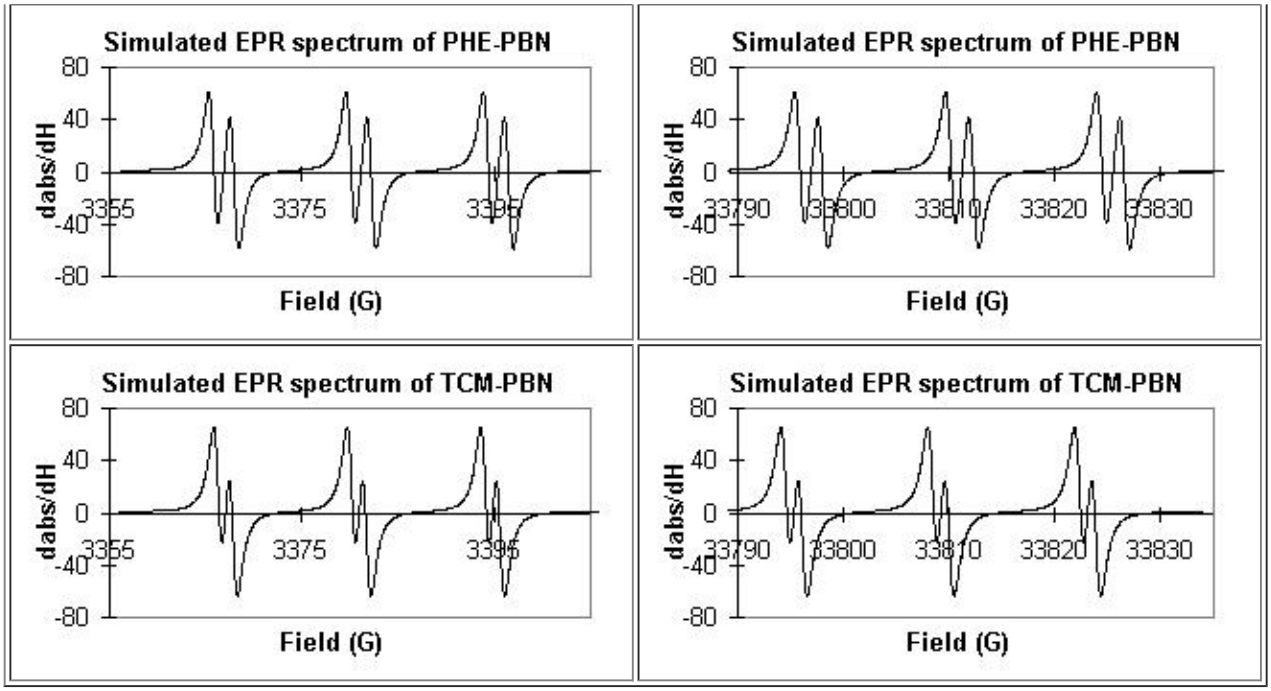


Figure 4. Simulated EPR spectra of Phenyl-PBN (PHE-PBN) and Trichloromethyl-PBN (TCM-PBN) at X-band (9.5 GHz) (Left) and at W-band (95 GHz) (Right).

Figure 5 shows two kinds of free radicals: one is $\cdot OC(CH_3)_3$ with $\mathbf{a}_H$=10 G, $\mathbf{a}_C$=30 G; the other is $\cdot CH_3$ with $\mathbf{a}_H$=20 G (data from reference [3]). Their multi-frequency EPR spectra can also be obtained by two methods mentioned above (data are not shown here). Many free radical simulated EPR spectra can be obtained according to the splitting parameters given in the references [3]. By the program, almost all the free radical EPR spectra can be simulated.

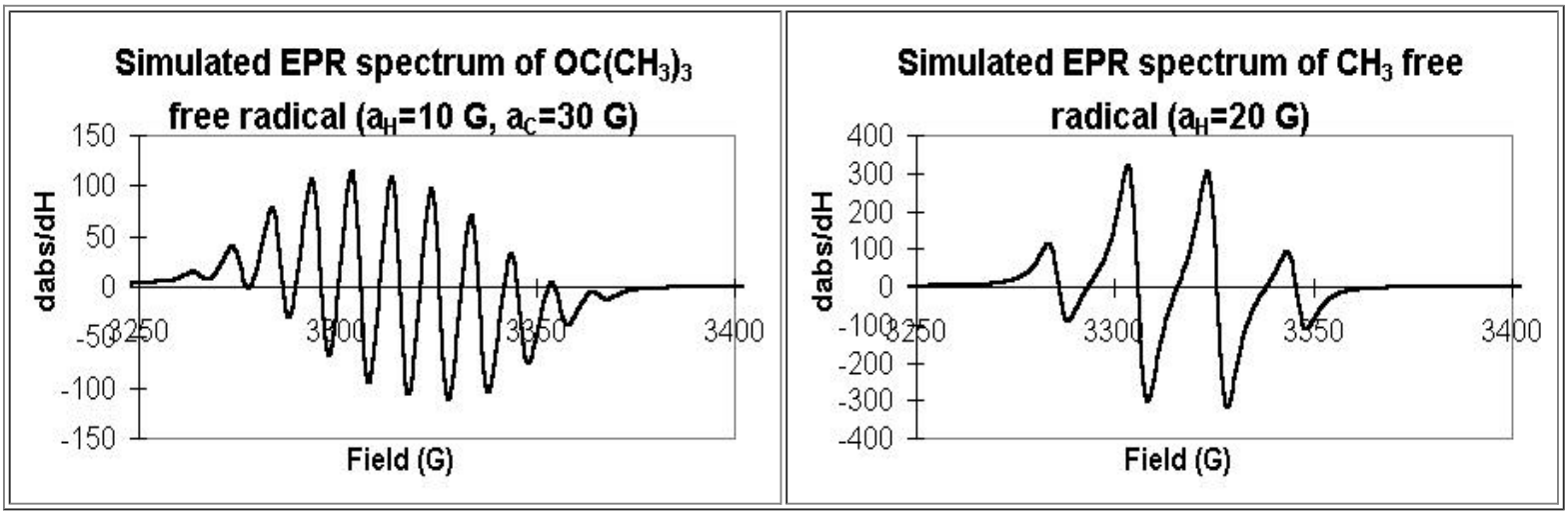


Figure 5. Simulated EPR spectra of $\cdot OC(CH_3)_3$ and $\cdot CH_3$ free radicals. g = 2.0026, frequency = 9.3 GHz, scan range 400 G, M = 11

Drug free radical, like the semiquinone of the anthracycline drug daunomycin, obtained in deuterated solvent, can also be simulated by the program, with $\mathbf{a}_H$=2.15 G, $\mathbf{a}_H$=1.92 G, $\mathbf{a}_H$=1.56 G, $\mathbf{a}_H$=1.49 G, $\mathbf{a}_H$=0.98 G, $\mathbf{a}_H$=0.9 G. The simulated spectrum (see Figure 6) with width of 0.3 G is very similar as the observed and simulated spectra (see Figure 3 in the reference [25]).

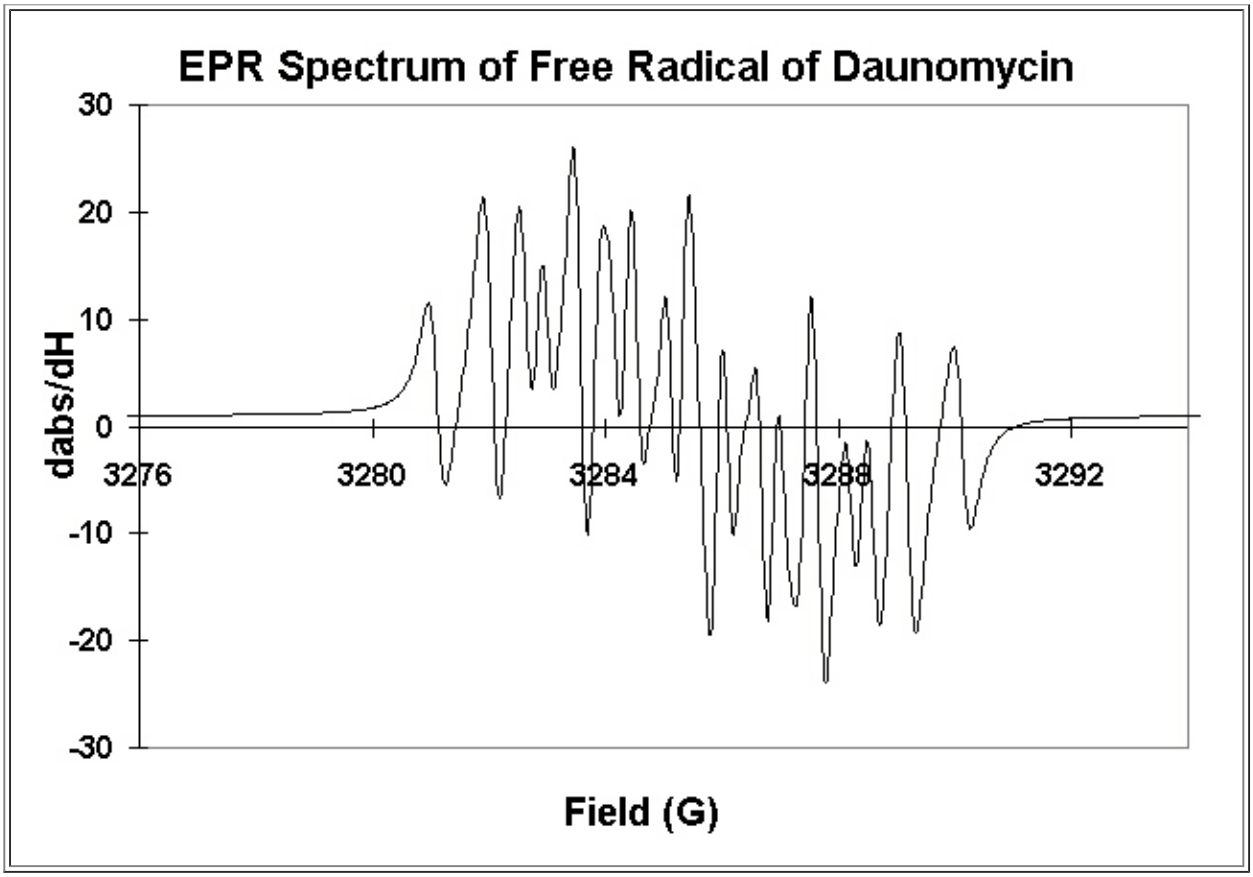


Figure 6. Simulated EPR spectrum of free radical of daunomycin with $\mathbf{a}_H$=2.15 G, $\mathbf{a}_H$=1.92 G, $\mathbf{a}_H$=1 .56 G, $\mathbf{a}_H$=1.49 G, $\mathbf{a}_H$=0.98 G, $\mathbf{a}_H$=0.9 G.

Conclusion

Almost all the spin traps and free radicals EPR spectra at any frequency can be simulated by the simple and modified program. The simulated EPR spectra at different frequencies are identifical to the simulated EPR spectrum at X-band by shifting the midpoint of the simulated spectrum from 714.4*(frequency at X-band)/(g value) to 714.4*(frequency at any frequency)/(g value). The resolution of over-lap EPR signals can be enhanced at high-frequencies if they have slightly different g values based on EPR simulation and simple calculation.

Two methods can be used to simulate any frequency EPR spectrum: one is direct method, which simulates EPR spectrum at the desired frequency with certain width; the other is indirect method, which can be used to simulate EPR spectrum at convient band (like X-band at 9.3 G Hz), then the spectrum need to be shifted as mentioned above; or one simulates the EPR spectrum at X-band by changing the coupling counstants {multify by a factor of 9.3/(desired frequency)} , then rescales the x-axis scale by multiplying the factor {(desired frequency)/9.3}.

Acknowledgments

This article is dedicated to my father **Shuren Wu** who has given years and years of encouragement.

References

[1]. Dunham, W. R.; Fee, J. A. Application of Fast Fourier Transforms to EPR Spectra of Free Radicals in Solution, *Journal of Magnetic Resonance* 1980, **40**, 351-359 *1, 2*

[2]. Brumby, Steven An account of two computer programs for the simulation of magnetic resonance spectra by

the fast fourier transform method, *Computers & Chemistry* 1984, **8**(1), 75-80 *1*, *2*

[3]. Kochi, Jay K. Configurations and conformations of transient alkyl radicals in solution by electron spin resonance spectroscopy, p189-318, Advances in Free-radical Chemistry, Vol. V, Edited by G. H. Williams, 1975, Academic Press, New York London San Francisco *1*, *2*, *3*, *4*

[4]. Belford, R. L.; Clarkson, R. B. Multiple frequency electron paramagnetic resonance. 77, 504-511, Magnetic resonance of carbonanceous solids, edited by Robert E. Botto and Yuzo Sanada,ACS, 1993 *1*, *2*

[5]. Yang, An-Suei; Gaffney, B. J. Determination of Relative Spin Concentration in Some High-Spin Ferric Proteins Using E/D-Distribution in Electron Paramagnetic Resonance Simulations, *Biophys. J.* 1987, **51**, 55-67 *1*

[6]. Yuan, Hua; Collins, M. L. P.; Antholine, W. E. Low-Frequency EPR of the Copper in Particulate Methane Monooxygenase from Methylomicrobium albus BG8, *J. Am. Chem. Soc.* 1997, **119** (21), 5073 -5074 *1*, *2*

[7]. Antholine, W. E.; Hanna, P. M.; McMillin, D. R. Low frequency EPR of Pseudomonas aeruginosa azurin: analysis of ligand superhyperfine structure from a type 1 copper site. *Biophys. J.* 1993, **64**, 267-272 *1*

[8]. Antholine, W. E.; Kastrau, D. H. W.; Steffen, G. C. M.; Buse G.; Zumft, W. G.; Kroneck, P. M. H. Electron paramagnetic resonance investigations of the multi-copper proteins nitrous oxide reductase and cytochrome c oxidase. *Eur. J. Biochem.* 1992, **209**, 875-881 *1*

[9]. Kroneck, P. M. H.; Antholine, W. E.; Kastrau, D. H. W.; Buse, G.; Steffen, G. C. M.; Zumft, W. G. Multifrequency electron spin resonance evidence for a bimetallic center at the CuA site of cytochrome c oxidase. *FEBS Lett.* 1990, **268**, 274-276 *1*

[10]. Smirnova, T. I.; Smirnov, A. I.; Clarkson, R. B.; Belford, R. L.; Kotake, Y.; Janzen, E. G. High-frequency (95 GHz) EPR spectroscopy to characterize spin adducts, *J. Phys. Chem.* B 1997, **101**, 3877-3885 *1*, *2*, *3*, *4*, *5*, *6*, *7*, *8*

[11]. Smirnova, T. I.; Smirnov, A. I.; Clarkson, R. B.; Belford, R. L. W-band (95 GHz) EPR spectroscopy of nitroxide radicals with complex proton hyperfine structure: fast motion, *J. Phys. Chem.* 1995, **99**, 9008-9016 *1*, *2*, *3*

[12]. Kalyanaraman, B.; Karoui, H.; Singh, R. J.; Felix, C. C. Detection of thiyl radical adducts formed during hydroxyl radical-and peroxynitrite-mediated oxidation of thiols - a high resolution ESR spin-trapping study at Q-band (35 GHz), *Analytical Biochemistry* 1996, **241**, 75-81 *1*, *2*, *3*

[13]. Adam, Waldemar et al. EPR characterization of the quintet state for a hydrocarbon tetraradical with two localized 1,3-cyclopentanediyl biradicals linked by *meta*-phenylene as a ferromagnetic coupler, *J. Am. Chem. Soc.* 1996, **118**, 3874-3975 *1*

14]. Jacobs, S. Joshua et al. Evaluation of potential ferromagnetic coupling units: the bis(TMM) approach to high-spin organic molecules, *J. Am. Chem. Soc.* 1993, **115**, 1744-1753 *1*

[15]. Nakamura, Toshihiro et al. Novel organic ions of high-spin states. 5. generation of a high-spin ground-state anion from an intramolecularly spin-frustrated system, *J. Am. Chem. Soc.* 1996, **118**, 8684-8687 *1*

[16]. Wienk, Martijn M.; Janssen, Rene A. J. Triplet-state phosphinyl diradicals, *Chem. Commun.* 1996, 1919-1920 *1*

[17]. Wright, Bradford B.; Platz, Mattew S. Electron spin resonance spectroscopy of the triplet state of *m*-Xylylene, *J. Am. Chem. Soc.* 1993, **105**, 628-630 *1*

[18]. Wu, Hanqing, EPR Spectra Simulation of Anisotropic Spin 1/2 System, WATOC96, E-Posters at http://www.ch.ic.ac.uk/watoc/ *1*

[19]. Wu, Hanqing, Why spin = 1, 2 species have no electron paramagnetic resonance signal under normal conditions: Possible detection by electron paramagnetic resonance at frequency close to D value? *Journal of Molecular Graphics* 1996, **14** (6), 328-330 *1*, *2*

[20]. Wu, Hanqing, Low Frequency as well as High Frequency EPR Spectra of Spin S = 1, 3/2 System can be predicted by EPR Spectra Simulation at X-band Using Adjusted D value, ECCC3, November, 1996 at http://hackberry.chem.niu.edu/ECCC3/ *1*, *2*

[21]. Wu, Hanqing, Prediction of high-frequency electron paramagnetic resonance spectra of Spin S = 3/2, 5/2 Systems, *Journal of Molecular Graphics* 1996, **14** (6), 338-340 *1*, *2*

[22]. Janzen , Edward G.; Zhang, Yong-Kang EPR spin trapping alkoxyl radicals with 2-substituted 5,5-dimethylpryrroline-*N*-oxide (2-XM_2PO's), *Journal of Magnetic Resonance*, Series B 1993, **101**, 91-93 *1*

[23] Li, Anson S. W.; Chignell, Colin F. The NoH value in EPR spin trapping: a new parameter for the identification of 5,5-dimethyl-1-pyrroline-*N*-oxide spin adducts, *Journal of Biochemical and Biophysical Methods* 1991, **22**, 83-87 *1*, *2*

[24]. Peric, Miroslav; Halpern, Howard J. Fitting of the derivative voigt EPR line under conditions of modulation broading, *Journal of Magnetic Resonance*, Series A 1994, **109**, 198-202 *1*

[25]. Motten, Ann G.; Duling, David R.; Schreiber, Jorg Proton Coupling Constant Extraction. A Fast Method for Analyzing ESR Spectra by Computer, *Journal of Magnetic Resonance* 1987, **71**, 34-44 *1*, *2*

Source code of the program.

```
COMPLEX*8 A(2048)
REAL*8 H(2048)
1 FORMAT (I1,F8.0)
2 FORMAT (3F8.0)
3 FORMAT (' SCAN RANGE =',F8.2)
4 FORMAT (20X,'PRONTONS',20X,'HFS')
5 FORMAT (18X, 34('-'))
6 FORMAT (22X, I2,20X,F8.4)
7 FORMAT (18X, '13C NUCLEI', 19X, 'HFS')
8 FORMAT (' 14N HFS =',F8.4)
9 FORMAT (' LINEWIDTHS =',F8.4,',',F8.4,' AND',F8.4)
OPEN(UNIT=5,NAME='FFT.DAT',STATUS='OLD')
OPEN(UNIT=6,NAME='FFT.COPY',STATUS='NEW')
READ (5,*) M
READ (5,*) F
READ (5,*) G
READ (5,*) SPAN
WRITE (6** ,3) SPAN
PI = 3.1415927
60 WRITE(6,5)
READ(5,*) HFS
WRITE(6,8) HFS
C
C
C
C
READ(5,*) W1,W2,W3
WRITE(6,9) W1,W2,W3
CLOSE(UNIT=6)
CLOSE(UNIT=5)
W1=W1*ROOT3*B
W2=W3*ROOT3*B
W3=W3*ROOT3*B
X1=-2.*HFS*B+PI
X2=PI
X3=2.*HFS*B+PI
DO 130 I =2,NP2
Y1=W1*(I-1)
```

```
ROOT3 = 1.7320508
NP=2M
NP2=NP/2+1
B=PI/SPAN
C
C
DO 10 I=1,NP2
10 A(I)=CMPLX(1.0,0.0)
C
WRITE(6,5)
WRITE(6,4)
WRITE(6,5)
20 READ(5,*) NH,HFS
IF(NH .EQ. 0.0) GO TO 40
WRITE(6,6) NH,HFS
X=B*HFS
DO 30 I=2,NP2
Y=X*(I-1) Z=COS(Y)
30 A(I)=A(I)*(Z**NH)
GO TO 20
40 WRITE(6,5)
C
C
WRITE(6,7)
WRITE(6,5)
45 READ(5,*) NC,HFS
IF (NC .EQ. 0.0) GO TO
60 WRITE(6,6) NC,HFS
X=B*HFS
DO 50 I=2,NP2
IF(Y1 .GT. 20.) GO TO 70
Y1=EXP(-Y1) GO TO 80 70
Y1=0.0 80
Y2=W2*(I-1)
IF(Y2 .GT. 20.) GO TO 90
Y2=EXP(-Y2) GO TO 100
90 Y2=0.0
100 Y3=W3*(I-1)
IF(Y3 .GT. 20.) GO TO 110
Y3=EXP(-Y3) GO TO 120
110 Y3=0.0
120 Z1=X1*(I-1)
Z2=X2*(I-1)
Z3=X3*(I-1)
RR=Y1*COS(Z1)+Y2*COS(Z2)+Y3*COS(Z3)
RI=-Y1*SIN(Z1)-Y2*SIN(Z2)-Y3*SIN(Z3)
130 A(I)=A(I)*CMPLX(RR,RI)*CMPLX(0.,FLOAT(I-1))
C
C
A(NP2)=CMPLX(REAL(A(NP2)),0.0)
NP3=NP2+1
DO 140 I=NP3,NP
140 A(I)=CONJG(A(NP+2-I))
CALL FOUR1(A,NP,1)
OPEN(UNIT=9,NAME='FFT.OUT',STATUS='NEW')
DO II=1,NP
STEP=SPAN/(NP-1)
BR=F*714/G
H(II) = BR-SPAN/2.0+(II-1)*STEP
WRITE(9,*) H(II),REAL(A(II))
```

```
Y=X*(I-1)                    ENDDO
Z=0.9889+0.0111*COS(Y)       CLOSE(UNIT=9)
50 A(I)=A(I)*(Z**NC)         STOP
GO TO 45                     END
```

The program can be downloaded here (Fortran code), input file, output file, and copy file.

Hanqing Wu

Hanqing Wu was born in November 1962 in Jiaxing, Zhejiang Province, China. He served as one of the editors for the student journal of *March on Science* (*Xiang Ke Xue Jin Jun*) USTC Press in 1982-83, and graduated with a B.S. from Department of Applied Chemistry, University of Science and Technology of China (USTC) in 1984, major in polymer chemistry. He had worked as instructor and research associate in the same department since then (1984-1990) and also studied for a M.S. in computer chemistry under Professor Yuankai Wen in USTC (1987-1989). He obtained his M.A. degree in 1994 from Department of Biophyscis, Johns Hopkins University (JHU), and had finished sixteen graduate level courses in the fields of biophyscs, biology, chemistry, and physics. In Jan. 1994, he came to Department of Chemistry, University of Wisconsin-Milwaukee (UWM) as a Ph.D student, and became a Ph.D candidate after 1995. He will hopefully graduate in June 1998 and try to find a job in either academia or industry (*please contact with him if you have opening position*). He has broad interests in several research fields, and he is the main author of 60 publications and presentations. He has two beautiful daughters (one daughter, **Yiling**, born in March, 1991, and the other, **Tesia**, born in Aug. 1997). His present address is: 2865 N. Bartlett Ave. #4, Milwaukee, WI 53211, USA, Tel. and FAX: (414) 332-8563, E-mail: hanqing@csd.uwm.edu, wuhanqing@geocities.com.

Comments

During 1-30 September 1997, all comments on this poster should be sent by e-mail to ecsoc@listserv.arizona.edu with **E0001** as the message subject of your e-mail. After the conference, please send all the comments and reprints requests to the author(s).
