Supporting Information

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/*rat_tc_chch_amp.c */
/*compile with 'cc -o xx xx.c -lm -lc_s' */
/* University of Frankfurt/M. 1998 */

#include <stdio.h>
#include <math.h>
#define gamma1H  26.7519e7    /*       gyromag. ratio 1H  [sec* A* kg-1] */
#define gamma15N  2.75e7      /*       gyromag. ratio 15N [sec* A* kg-1] */
#define gamma13C  6.726e7     /*       gyromag. ratio 13C [sec* A* kg-1] */
#define Hq        1.0546e-34  /*       Planck's h/2pi  [J*sec]    */
#define m0        1e-7
                            /* permeability of vacuum [m*kg*sec-2*A-2] */
#define dNH       1.02e-10    /* distance N H */
#define dCH       1.09e-10    /* distance C H */
#define dCC       1.54e-10    /* distance C C */



/* bond angle taken from cns2.0 force field for C3'-endo:*/

/*H1,C1,C2 112.45  */
#define ah1_c1_c2 112.45

/*H2,C2,C1 111.44  */
#define ah2_c2_c1 111.44

/*H2,C2,C3 110.30  */
#define ah2_c2_c3 110.30

/*H3,C3,C2 112.65  */
#define ah3_c3_c2 112.65

/*H3,C3,C4 111.86  */
#define ah3_c3_c4 111.86

/*H4,C4,C3 106.60   */
#define ah4_c4_c3 106.60


FILE   *ascout;
char   s1[80];
int    i,j;
double  numax1,temp,a1,a2,a3,factor,
        phi_h1h2,phi_h2h3,phi_h3h4,phi,tc,iminus144,iplus0,iplus144,
        rate12,theta12,theta112,temp12,
        rate23,theta23,theta123,temp23,
        rate34,theta34,theta134,temp34,
       noe12,noe23,noe34,dist12,dist23,dist34,
       Rnull,omegaH,cross12,cross23,cross34,r112,r123,r134,
       Jkl,disttemp,numax;
double densityf();



main ()
{
  printf("out file"); scanf("%s",s1);
  printf("tc: (ns)\n "); scanf("%lf",&tc);
  printf("Pseudo rotation amplitude: (degree)\n "); scanf("%lf",&numax);
  (void)printf("Enter Omega 1H      [MHz]    : ");
  (void)scanf("%lf",&omegaH);
  omegaH *= M_PI*1.0e6;

  ascout=fopen(s1,"w");
  tc *= 1.0e-9;


  a1 = gamma1H*gamma13C/dCH/dCH/dCH;

  a2 = gamma1H*gamma13C/dCH/dCH/dCH;

  a3 = m0*m0*Hq*Hq;

  Jkl = 0.1*pow(gamma1H,4.0)*Hq*Hq*1.0e-14;
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  factor=a1*a2*a3/5;

fprintf(ascout,"#P rateh1h2   rateh2h3   rateh3h4 rateh3h4/rateh1h2 crossh1h2 crossh1h2*10 crossh2h3
crossh3h4 P2h1h2 P2h2h3 P2h3h4 phi_h1h2 phi_h2h3 phi_h3h4\n");

/* Distance for two synclinal protons  */
Rnull=dCC+2*dCH*sin(19*M_PI/180);


/* Pseudorotation Amplitude */
  numax1=numax*M_PI/180.0;

/* Pseudorotation Phase */
 for(i=0;i<360;i++){
  iminus144=(double)(i-144);
  iplus0=(double)(i);
  iplus144=(double)(i+144);
/* formula to convert P into phi_h1h2,phi_h2h3,phi_h3h4 */

  phi_h1h2=(123.3*M_PI/180.0)
  + 1.102*numax1*cos(iminus144*M_PI/180.0);

  phi_h2h3=(0.2*M_PI/180.0)
  + 1.090*numax1*cos(iplus0*M_PI/180.0);

  phi_h3h4=(-124.9*M_PI/180.0)
  + 1.095*numax1*cos(iplus144*M_PI/180.0);

/* distance for protons with an angle of phi_h1h2,phi_h2h3,phi_h3h4 */

   dist12=2*dCH*cos(phi_h1h2);
   dist12=sqrt(dist12*dist12+Rnull*Rnull);
   dist12 = Jkl*(pow(dist12,-6));


   dist23=2*dCH*cos(phi_h2h3);
   dist23=sqrt(dist23*dist23+Rnull*Rnull);
   dist23 = Jkl*(pow(dist23,-6));

   dist34=2*dCH*cos(phi_h3h4);
   dist34=sqrt(dist34*dist34+Rnull*Rnull);
   dist34 = Jkl*(pow(dist34,-6));

/* noe for protons with an angle of phi_h1h2,phi_h2h3,phi_h3h4 */


   cross12 = 1.0/4.0*dist12*(12.0*densityf(omegaH+omegaH,tc)
                        - 2.0*densityf(0.0,tc));


   cross23 = 1.0/4.0*dist23*(12.0*densityf(omegaH+omegaH,tc)
                        - 2.0*densityf(0.0,tc));

   cross34 = 1.0/4.0*dist34*(12.0*densityf(omegaH+omegaH,tc)
                        - 2.0*densityf(0.0,tc));

/* projection angle between HnCnCn+1Hn+1 and dipole,dipole cross correlated relaxation rate*/

  theta12=(-1)*cos(ah1_c1_c2*M_PI/180.0)*cos(ah2_c2_c1*M_PI/180.0)
        + sin(ah1_c1_c2*M_PI/180.0)*sin(ah2_c2_c1*M_PI/180.0)*cos(phi_h1h2);
  theta112=acos(theta12);
  temp12=cos(theta112)*cos(theta112);
  rate12=tc*factor*((3*temp12)-1);


  theta23=(-1)*cos(ah2_c2_c3*M_PI/180.0)*cos(ah3_c3_c2*M_PI/180.0)
        + sin(ah2_c2_c3*M_PI/180.0)*sin(ah3_c3_c2*M_PI/180.0)*cos(phi_h2h3);
  theta123=acos(theta23);
  temp23=cos(theta123)*cos(theta123);
  rate23=tc*factor*((3*temp23)-1);

  theta34=(-1)*cos(ah3_c3_c4*M_PI/180.0)*cos(ah4_c4_c3*M_PI/180.0)
        + sin(ah3_c3_c4*M_PI/180.0)*sin(ah4_c4_c3*M_PI/180.0)*cos(phi_h3h4);
  theta134=acos(theta34);
  temp34=cos(theta134)*cos(theta134);
  rate34=tc*factor*((3*temp34)-1);

/* would you kindly print what you want */
```

```
  fprintf(ascout,"%d %.3e %.3e %.3e \n",
  i,rate12,rate34,rate12/rate34);


    }
}

double densityf(omega,tc)
 double tc, omega;
{
double r;

r = tc / ( 1.0 + omega*omega*tc*tc) ;
return(2.0 * r);
}
```