jp993505o

Data taken from the ValRay Binary Data File:

File label - Glycine at 23 K

Cell constants (A,B,C,cosines of angles)
and e.s.d.s

5.0866	11.7731	5.4595	.0000	-.3744	.0000
.0020	.0030	.0020	.0000	.0005	.0000

Cell Volume (A**3) 303.1572

Metric tensor

25.8735	.0000	-10.3984
.0000	138.6059	.0000
-10.3984	.0000	29.8061

Reciprocal Metric tensor

.0450	.0000	.0157
.0000	.0072	.0000
.0157	.0000	.0390

Orthogonalization matrix and its inverse

O			OI		
4.71655	.00000	.00000	.21202	.00000	.00000
.00000	11.77310	.00000	.00000	.08494	.00000
-1.90465	.00001	5.45950	.07397	.00000	.18317

Matrices defining multipole coordinate system
VE transforms orthogonal coordinates (OV) into fractional ones (FV),
i.e. FV = VE * OV
(VE is stored by columns)

.19659	.00000	.07939
.00000	.08494	.00000
.00000	.00000	.19754

VR transforms fractional coordinates (FV) into orthogonal ones (OV),
i.e. OV = VR * FV
VR is the inverse of VE and is stored by rows,
i.e. it is the inverse transpose of VE.

5.0866	.65027E-05	-2.0443
-.12765E-12	11.773	.41446E-05

SUPPLEMENTARY MATERIAL

-.21803E-06 .33088E-13 5.0623

Population coefficients read from BDF are multiplied by 1.01920 (ReScal)

Information on Extinction (REX array)

G11	G22	G33	G12	G13	G23
1.00941	.08277	.42862	-.16124	-.10609	-.07935

Crystal coordinates of atoms with e.s.d.s

Atom	X	Y	Z
C1	.06933	.12516	.06579
	.00002	.00001	.00002
C2	.05797	.14585	-.21406
	.00002	.00001	.00002
N1	.29496	.08838	-.25956
	.00002	.00001	.00002
O1	.30208	.09379	.23642
	.00002	.00001	.00002
O2	-.15523	.14238	.10655
	.00002	.00001	.00002
HH1	.27761	.10030	-.45288
	.00107	.00039	.00123
HH2	.48838	.11700	-.13376
	.00123	.00042	.00106
HH3	.28948	.00291	-.22658
	.00083	.00047	.00079
HH4	.07488	.23597	-.24163
	.00085	.00044	.00082
HH5	-.14166	.11490	-.35901
	.00106	.00042	.00096

Thermal parameters (Beta or B) with e.s.d.s

Atom						
C1	.003487	.000643	.002939	.000025	.001513	.000007
	.000020	.000004	.000018	.000006	.000015	.000006
C2	.004353	.000846	.003233	.000318	.001669	.000250
	.000021	.000004	.000019	.000006	.000016	.000006
N1	.004604	.000932	.003293	.000347	.001926	.000074
	.000020	.000004	.000018	.000006	.000015	.000006
O1	.004238	.001129	.003053	.000471	.001187	.000296
	.000023	.000004	.000021	.000007	.000018	.000007
O2	.003957	.001201	.004481	.000141	.002454	-.000128
	.000023	.000004	.000022	.000007	.000018	.000008

HH1	.020701	.003344	.008796	.000914	.006506	.000530
	.000000	.000000	.000000	.000000	.000000	.000000
HH2	.008971	.002773	.011762	-.000569	.003555	-.000537
	.000000	.000000	.000000	.000000	.000000	.000000
HH3	.015998	.001739	.013741	.000480	.006589	.000079
	.000000	.000000	.000000	.000000	.000000	.000000
HH4	.024694	.001784	.017346	.000842	.010871	.001169
	.000000	.000000	.000000	.000000	.000000	.000000
HH5	.007986	.004036	.011461	-.000551	.001976	-.001312
	.000000	.000000	.000000	.000000	.000000	.000000

Thermal parameters (Uij*100) with e.s.d.s

Atom						
C1	.39303	.45185	.38152	.00717	.18298	.00225
	.00221	.00246	.00239	.00165	.00179	.00177
C2	.49063	.59393	.41970	.08952	.20187	.07554
	.00236	.00269	.00252	.00178	.00193	.00195
N1	.51890	.65410	.42748	.09757	.23291	.02246
	.00227	.00252	.00238	.00170	.00183	.00181
O1	.47761	.79275	.39633	.13257	.14353	.08933
	.00262	.00294	.00267	.00206	.00214	.00217
O2	.44599	.84365	.58179	.03963	.29686	-.03852
	.00259	.00304	.00286	.00205	.00221	.00233
HH1	2.33300	2.34800	1.14200	.25700	.78700	.16000
	.00000	.00000	.00000	.00000	.00000	.00000
HH2	1.01100	1.94700	1.52700	-.16000	.43000	-.16200
	.00000	.00000	.00000	.00000	.00000	.00000
HH3	1.80300	1.22100	1.78400	.13500	.79700	.02400
	.00000	.00000	.00000	.00000	.00000	.00000
HH4	2.78300	1.25300	2.25200	.23700	1.31500	.35300
	.00000	.00000	.00000	.00000	.00000	.00000
HH5	.90000	2.83400	1.48800	-.15500	.23900	-.39600
	.00000	.00000	.00000	.00000	.00000	.00000

Population Coefficients

Population coefficients in this order
  Monopoles:
        Pcore PL-sh PM-sh
  Dipoles:
        dx dy dz
  Quadrupoles:
        Qx2-y2 Qxy Qxz Qyz Q3z2-1

Octopoles:

Ox3yQx O3xyQy OxyQz Oxyz O5zQ1x O5zQ1y O5zQ1z

Hexadecapoles

Hx4y4 HxyQxy HxyQxz HxyQyz HzQxyQ HzQxy HzQxz HzQyz Hz4zQ

C1

2.11728 .00000 3.98402
.00141 .00000 .02343
-.03187 -.21459 .20064
.02784 .03155 .03032
1.32592 -1.35690 .45542 -.98536 .62799
.03333 .05871 .06700 .05991 .06067
-1.29853 .08404 3.58433 -8.57137 3.26807 -.15368 -1.56808
.07710 .08691 .20050 .45810 .06899 .07065 .05394
.05641 -4.97766 1.91918 -2.76023 .29340 -.78035 -.51209 .07036 .58295
.31681 1.24948 .94689 .92156 .28075 .51373 .41462 .33467 .33775

C2

2.11728 .00000 4.08633
.00141 .00000 .02359
-.27634 .36426 -.07511
.03577 .03388 .04045
-.48566 1.02358 .73608 -.18355 .16659
.03661 .07121 .07263 .07150 .06039
-.54247 -2.91527 -.96313 -2.45520 -2.13704 -1.01834 1.30490
.11158 .09826 .27696 .49099 .08154 .07268 .06533
-.32421 -6.67981 .39891 6.90384 2.30348 2.42415 -.78852 -1.18238 1.80478
.36070 1.53005 1.18788 1.07772 .29195 .58372 .41233 .40631 .33667

N1

2.11728 .00000 5.15059
.00141 .00000 .01981
.15397 -.05071 -.06882
.02735 .02922 .02938
-.20234 .37330 .16700 -.03572 .28004
.02854 .05086 .06019 .04962 .04825
.22471 1.83500 .03531 1.13370 1.28853 .51657 -.99623
.06683 .06244 .16692 .32215 .04935 .05084 .04059
.10656 -2.49144 2.38392 3.80145 .88161 1.31905 -.95205 .07088 .83203
.21341 .81259 .68502 .54623 .18062 .30441 .23336 .22558 .19206

O1

2.11728 .00000 6.29515
.00141 .00000 .01264
.11994 -.04865 .09588
.00608 .00654 .00635
.03535 -.00822 -.11033 -.02247 .04734
.00530 .00936 .01060 .00954 .00902
.00572 .00786 -.05820 .14573 -.02729 .00643 .02242

```
          .00517   .00531   .01285   .02637   .00387   .00416   .00324
         -.02177   .00718   .10405  -.01626  -.00071  -.03837   .00408   .02016  -.01181
          .01165   .04208   .03413   .02982   .00896   .01660   .01224   .01158   .01007
O2
         2.11728   .00000  6.34349
          .00141   .00000   .01236
         -.16106   .03979   .03312
          .00615   .00657   .00651
          .00257  -.01192   .06228  -.07097   .14953
          .00530   .00972   .01069   .00991   .00922
          .01689  -.01765  -.04037   .08492  -.03664   .00711   .00900
          .00530   .00521   .01306   .02665   .00398   .00403   .00327
          .01581   .06176   .04315   .02727  -.02004  -.00077   .03098  -.00615   .02446
          .01192   .04300   .03405   .03155   .00926   .01658   .01234   .01162   .01016
HH1
          .00000   .00000   .66956
          .00000   .00000   .01056
         -.04235  -.05683   .44601
          .02770   .02735   .02719
          .03454  -.01041  -.34730  -.14029  1.17591
          .06054   .11792   .11876   .13488   .11645
HH2
          .00000   .00000   .65734
          .00000   .00000   .01047
         -.34508  -.16731  -.32259
          .02635   .02818   .02958
          .10355   .63952  1.04377   .07461   .06902
          .06400   .12635   .12769   .13261   .11268
HH3
          .00000   .00000   .68798
          .00000   .00000   .01003
          .12335   .49004  -.10280
          .02510   .02319   .02555
         -.26282   .39468  -.00681  -.60141  -.15984
          .05825   .11287   .11210   .13103   .09819
HH4
          .00000   .00000   .77806
          .00000   .00000   .01085
         -.09894  -.39519   .02249
          .02778   .02216   .02961
         -.28515   .25309  -.05366   .12638  -.19910
          .05961   .12573   .11846   .13885   .11455
HH5
          .00000   .00000   .76108
          .00000   .00000   .01123
```

```
          .31971    .14995    .31642
          .02507    .02922    .02785
          .22862   -.25995    .33503    .63240   -.30471
          .06486    .12335    .13886    .13778    .11529
The number of atoms in the asymmetric unit (NA) is .....   10
The number of atoms in a molecule (NAMol) is .....   10
The number of atoms in the unit cell (NACell) is .....   40
The number of atoms which describe the crystal (NACrys) is ...  160
Calculation is done over a molecule
Actually, only the atoms in the asymmetric unit will be included in calculation
```

Coordinates of atoms in the asymmetric unit

I	Label	Orthogonal Coordinates X	Y	Z	Fractional Coordinates X	Y	Z
1	C1	.2182	1.4736	.3330	.0693	.1252	.0658
2	C2	.7325	1.7171	-1.0836	.0580	.1459	-.2141
3	N1	2.0309	1.0405	-1.3140	.2950	.0884	-.2596
4	O1	1.0532	1.1042	1.1968	.3021	.0938	.2364
5	O2	-1.0074	1.6762	.5394	-.1552	.1424	.1066
6	H1	2.3379	1.1808	-2.2926	.2776	.1003	-.4529
7	H2	2.7576	1.3775	-.6771	.4884	.1170	-.1338
8	H3	1.9357	.0343	-1.1470	.2895	.0029	-.2266
9	H4	.8748	2.7781	-1.2232	.0749	.2360	-.2416
10	H5	.0133	1.3527	-1.8174	-.1417	.1149	-.3590

ValRay BDF orientation and charges

Center Number	Center Label	Atomic Number	Coordinates (fractional) X	Y	Z	Coordinates (Angstroms) X	Y	Z	Atomic Charge (esds)
1	C1	6	.069334	.125163	.065788	.218188	1.473562	.333042	-.101 (.023)
2	C2	6	.057969	.145851	-.214056	.732458	1.717118	-1.083618	-.204 (.024)
3	N1	7	.294958	.088380	-.259560	2.030944	1.040509	-1.313974	-.268 (.020)
4	O1	8	.302077	.093790	.236421	1.053234	1.104202	1.196841	-.412 (.013)
5	O2	8	-.155229	.142376	.106552	-1.007409	1.676208	.539401	-.461 (.012)
6	H1	1	.277610	.100300	-.452880	2.337904	1.180840	-2.292623	.330 (.011)
7	H2	1	.488380	.117000	-.133760	2.757637	1.377452	-.677136	.343 (.010)
8	H3	1	.289480	.002910	-.226580	1.935661	.034259	-1.147020	.312 (.010)
9	H4	1	.074880	.235970	-.241630	.874845	2.778097	-1.223208	.222 (.011)
10	H5	1	-.141660	.114900	-.359010	.013349	1.352728	-1.817423	.239 (.011)

Center of Mass	.119992	.117853	-.018031	.647211	1.387499	-.091281
Molecular Charge						.000 (.049)
Total number of electrons						40.000 (.049)
Principal Moments of Inertia (amu-Angstrom**2)				48.853911	128.110750	169.095357
Rotational constants (GHZ)				36.941591	14.087352	10.672920

Molecular Electrostatic Moments and Estimated Standard Deviations

Origin: Center of Mass
Orientation: BDF

Moments		Values			E.s.d.'s		
Charge		.000			.049		
Dipole	(X, Y, Z)	9.188	-1.103	-11.711	.265	.172	.289
	Magnitude	14.926			.279		
Quadrupole	(XX, XY, XZ)	-1.848	-.557	-7.704	.650	.334	.558
	(YY, YZ)		.036	3.705		.504	.370
	(ZZ)			1.812			.670
Octapole	(XXX, YYY, ZZZ)	19.597	15.584	14.600	1.898	1.280	1.966
	(XYY, XXY, XXZ)	-15.200	-10.565	-24.757	1.094	1.026	1.825
	(XZZ, YZZ, YYZ)	-2.877	2.536	12.368	1.842	1.128	1.182
	(XYZ)			17.747			1.045

Molecular Electrostatic Moments and Estimated Standard Deviations

Origin: Center of Mass
Orientation: Eigen-axes of the inertial tensor

Moments		Values			E.s.d.'s		
Charge		.000			.049		

Dipole	(X,	Y,	Z)	-14.679	2.692	.243	.275	.271	.185
	Magnitude			14.926			.275		
Quadrupole	(XX,	XY,	XZ)	7.991	-2.206	-2.778	.605	.588	.389
	(	YY,	YZ)		-8.009	-.402		.577	.402
	(		ZZ)			.018			.478
Octapole	(XXX,	YYY,	ZZZ)	-34.881	25.479	-8.368	1.831	1.696	1.233
	(XYY,	XXY,	XXZ)	11.135	-23.363	6.378	1.735	1.780	1.170
	(XZZ,	YZZ,	YYZ)	24.960	-2.306	-5.932	1.131	1.151	1.177
	(		XYZ)			-2.636			1.172
