

```
TITL gib11i in P2(1)/c
CELL 0.71073 25.0865 11.1315 23.4900 90.000 107.671 90.000
ZERR 4.00 0.0000 0.0002 0.0002 0.000 0.001 0.000
LATT 1
SYMM -X, 0.5+Y, 0.5-Z
SFAC C H N O F P
UNIT 204 312 8 72 48 8
TEMP -60

L.S. 10

BOND

FMAP 2

omit 1 0 0
omit 1 1 1
omit -2 1 3
omit 1 1 0

omit 2 0 0
omit 0 45

PLAN 20

dfix 1.587 0.001 p1 f1 p1 f2 p1 f3 p1 f4 p1 f5 p1 f6
dfix 1.587 0.001 p1 f1' p1 f2' p1 f3' p1 f4' p1 f5' p1 f6'
omit 1 2 1
size 0.5 0.3 0.3
dfix 0.880 0.000 o17 h17d o17 h17c
WGHT 0.159600 2.341400
FVAR 0.20947 0.47624
P1 6 0.39788 0.84307 0.37903 11.00000 0.05906 0.08646 =
0.07805 0.01027 0.00924 0.01190
```

P2 6 1.03433 0.10576 0.69369 11.00000 0.04054 0.03778 =
0.04093 0.00243 0.00704 0.00016

PART 1

F1 5 0.37444 0.85038 0.43453 10.50000 0.16029

F2 5 0.39962 0.71400 0.40824 10.50000 0.13372

F3 5 0.34417 0.78356 0.33364 10.50000 0.10785

F4 5 0.42481 0.82754 0.32644 10.50000 0.14828

F5 5 0.36947 0.97166 0.36592 10.50000 0.15874

F6 5 0.45165 0.91797 0.41416 10.50000 0.12501

PART 2

F1' 5 0.39875 0.88642 0.44368 10.50000 0.14316

F2' 5 0.42648 0.71669 0.39972 10.50000 0.11619

F3' 5 0.33222 0.82999 0.36555 10.50000 0.13864

F4' 5 0.38886 0.78694 0.31469 10.50000 0.13958

F5' 5 0.38776 0.96690 0.34387 10.50000 0.07919

F6' 5 0.46395 0.85551 0.39760 10.50000 0.11458

PART 0

F7 5 1.05724 0.01180 0.65578 11.00000 0.08080 0.05617 =
0.08640 -0.00848 0.04413 0.00781

F8 5 1.06614 0.21301 0.67129 11.00000 0.08686 0.04762 =
0.09799 0.00633 0.03993 -0.01587

F9 5 1.08705 0.08457 0.75062 11.00000 0.05306 0.07514 =
0.07626 0.00381 -0.01917 0.00146

F10 5 1.01075 0.20148 0.73045 11.00000 0.08072 0.07053 =
0.05302 -0.01446 0.01801 0.01733

F11 5 1.00267 -0.00080 0.71546 11.00000 0.06608 0.05918 =
0.06434 0.01378 0.02052 -0.01570

F12 5 0.98035 0.12745 0.63739 11.00000 0.06643 0.06472 =

		0.04177	0.00115	-0.00831	0.00927		
O1	4	0.80263	0.85533	0.41695	11.00000	0.04097	0.04960 =
		0.03338	0.00171	0.00816	-0.00461		
O2	4	0.90026	0.83375	0.51566	11.00000	0.04411	0.03665 =
		0.03549	-0.00367	0.00470	-0.00195		
O3	4	0.96222	0.66149	0.59680	11.00000	0.04144	0.04940 =
		0.03619	0.00690	0.00942	0.00071		
O4	4	0.95396	0.42639	0.54586	11.00000	0.04578	0.04589 =
		0.04404	0.00758	0.00082	0.00856		
O5	4	0.88680	0.26446	0.46015	11.00000	0.05234	0.05583 =
		0.04870	-0.00030	0.02261	-0.00327		
O6	4	0.73377	0.80994	0.20011	11.00000	0.04077	0.07072 =
		0.03126	0.00021	0.01351	-0.00199		
O7	4	0.77509	0.72727	0.11077	11.00000	0.06801	0.05657 =
		0.03482	0.00129	0.01165	0.01030		
O8	4	0.78654	0.49773	0.06574	11.00000	0.05653	0.05767 =
		0.04386	0.00112	0.00993	0.00000		
O9	4	0.82968	0.29497	0.14302	11.00000	0.06237	0.04669 =
		0.04059	-0.00046	0.02354	0.00895		
O10	4	0.82707	0.17793	0.24599	11.00000	0.05944	0.05130 =
		0.04681	-0.00096	0.02805	-0.00564		
O11	4	0.62051	0.70180	0.31705	11.00000	0.04373	0.04987 =
		0.04639	-0.00154	0.01382	-0.00464		
O12	4	0.53853	0.54449	0.33777	11.00000	0.04152	0.04754 =
		0.07424	-0.00303	0.02170	-0.00405		
O13	4	0.50146	0.30163	0.34438	11.00000	0.04283	0.04167 =
		0.06726	0.00083	0.01121	-0.00106		
O14	4	0.58044	0.12733	0.33765	11.00000	0.04937	0.03552 =
		0.12100	0.00903	0.04228	0.00498		

O15	4	0.70496	0.13670	0.36592	11.00000	0.04757	0.05002 =
		0.06232	-0.00327	0.01920			
O16	4	0.63478	0.63486	0.50746	11.00000	0.13585	
O17	4	0.86610	0.58676	0.48026	11.00000	0.05761	0.04714 =
		0.05892	-0.00224	-0.01575		0.00245	
H17C	2	0.86983	0.66323	0.49019	11.00000	-1.50000	
H17D	2	0.88707	0.53441	0.50530	11.00000	-1.50000	
O18	4	0.72380	1.12427	0.11036	11.00000	0.17579	0.11951 =
		0.24624	0.00843	0.06516		-0.00660	
N1	3	0.83345	0.54444	0.24472	11.00000	0.03827	0.03622 =
		0.04328	-0.00053	0.00901		0.00035	
N2	3	0.65735	0.39044	0.41726	11.00000	0.04289	0.03791 =
		0.06413	0.00311	0.01243		-0.00243	
C1	1	0.76361	0.82364	0.36359	11.00000	0.04082	0.02460 =
		0.03809	0.00189	0.00975		0.00147	
C2	1	0.77297	0.83659	0.30783	11.00000	0.03391	0.03264 =
		0.03760	-0.00063	0.01333		0.00453	
AFIX	43						
H2A	2	0.80690	0.86751	0.30486	11.00000	-1.20000	
AFIX	0						
C3	1	0.73012	0.80190	0.25701	11.00000	0.02990	0.03260 =
		0.04186	0.00863	0.00760		0.00794	
C4	1	0.68070	0.75390	0.26160	11.00000	0.04528	0.03482 =
		0.03378	0.00186	0.00610		0.00365	
AFIX	43						
H4A	2	0.65291	0.72780	0.22712	11.00000	-1.20000	
AFIX	0						
C5	1	0.67216	0.74430	0.31701	11.00000	0.04035	0.02693 =

		0.04588	0.00368	0.01581	0.00399		
C6	1	0.71453	0.77705	0.36874	11.00000	0.04468	0.03019 =
		0.03756	0.00493	0.01090	0.00400		
AFIX	43						
H6A	2	0.70952	0.76732	0.40654	11.00000	-1.20000	
AFIX	0						
C7	1	0.85583	0.89811	0.41550	11.00000	0.04081	0.03615 =
		0.04412	0.00307	0.00928	-0.00302		
AFIX	23						
H7A	2	0.85087	0.96637	0.38803	11.00000	-1.20000	
H7B	2	0.87570	0.83441	0.40144	11.00000	-1.20000	
AFIX	0						
C8	1	0.88870	0.93580	0.47685	11.00000	0.04996	0.03653 =
		0.04178	-0.00158	0.01415	-0.00178		
AFIX	23						
H8A	2	0.92390	0.97281	0.47601	11.00000	-1.20000	
H8B	2	0.86752	0.99549	0.49180	11.00000	-1.20000	
AFIX	0						
C9	1	0.93199	0.86446	0.57579	11.00000	0.03783	0.04322 =
		0.04019	-0.01039	0.00362	0.00157		
AFIX	23						
H9A	2	0.91459	0.93288	0.58953	11.00000	-1.20000	
H9B	2	0.97009	0.88740	0.57722	11.00000	-1.20000	
AFIX	0						
C10	1	0.93379	0.75953	0.61513	11.00000	0.05113	0.06171 =
		0.02913	-0.00555	0.01239	0.00879		
AFIX	23						
H10A	2	0.95347	0.78113	0.65665	11.00000	-1.20000	
H10B	2	0.89562	0.73522	0.61276	11.00000	-1.20000	

AFIX 0
C11 1 0.95911 0.55354 0.62906 11.00000 0.06104 0.05471 =
0.03979 0.01266 0.01374 -0.00214

AFIX 23
H11A 2 0.91989 0.53439 0.62446 11.00000 -1.20000
H11B 2 0.97851 0.56531 0.67167 11.00000 -1.20000

AFIX 0
C12 1 0.98543 0.45260 0.60581 11.00000 0.05432 0.04634 =
0.05267 0.01707 0.00287 -0.00145

AFIX 23
H12A 2 1.02375 0.47441 0.60758 11.00000 -1.20000
H12B 2 0.98712 0.38125 0.63073 11.00000 -1.20000

AFIX 0
C13 1 0.97588 0.32555 0.52327 11.00000 0.04501 0.05041 =
0.06235 0.00989 0.01181 0.00711

AFIX 23
H13A 2 0.97513 0.25469 0.54776 11.00000 -1.20000
H13B 2 1.01483 0.34107 0.52513 11.00000 -1.20000

AFIX 0
C14 1 0.94130 0.30216 0.45923 11.00000 0.04749 0.05031 =
0.05555 0.00748 0.02335 0.00394

AFIX 23
H14A 2 0.93841 0.37541 0.43533 11.00000 -1.20000
H14B 2 0.95874 0.23932 0.44168 11.00000 -1.20000

AFIX 0
C15 1 0.78373 0.86020 0.19180 11.00000 0.04746 0.04986 =
0.04355 -0.00143 0.01813 0.00074

AFIX 23

H15A	2	0.81677	0.81506	0.21487	11.00000	-1.20000	
H15B	2	0.78817	0.94428	0.20476	11.00000	-1.20000	
AFIX	0						
C16	1	0.77647	0.85094	0.12544	11.00000	0.05072	0.06018 =
		0.05190	0.00787	0.02106	0.00160		
AFIX	23						
H16A	2	0.74158	0.89001	0.10242	11.00000	-1.20000	
H16B	2	0.80768	0.89058	0.11607	11.00000	-1.20000	
AFIX	0						
C17	1	0.76457	0.70547	0.04837	11.00000	0.05625	0.07344 =
		0.03233	0.00980	0.01211	0.00764		
AFIX	23						
H17A	2	0.79899	0.71657	0.03749	11.00000	-1.20000	
H17B	2	0.73639	0.76192	0.02499	11.00000	-1.20000	
AFIX	0						
C18	1	0.74390	0.57870	0.03546	11.00000	0.05517	0.07731 =
		0.03966	0.00057	0.00473	0.00254		
AFIX	23						
H18A	2	0.71079	0.56669	0.04866	11.00000	-1.20000	
H18B	2	0.73326	0.56368	-0.00765	11.00000	-1.20000	
AFIX	0						
C19	1	0.76743	0.37713	0.05467	11.00000	0.07279	0.07628 =
		0.04869	-0.02398	0.01519	0.00088		
AFIX	23						
H19A	2	0.75125	0.36381	0.01161	11.00000	-1.20000	
H19B	2	0.73851	0.36116	0.07388	11.00000	-1.20000	
AFIX	0						
C20	1	0.81705	0.29358	0.07986	11.00000	0.09116	0.06393 =
		0.04482	-0.01503	0.02574	-0.00075		

AFIX 23

H20A 2 0.80762 0.21190 0.06453 11.00000 -1.20000

H20B 2 0.84933 0.32135 0.06824 11.00000 -1.20000

AFIX 0

C21 1 0.87121 0.21008 0.17234 11.00000 0.05708 0.04723 =
0.05380 -0.00838 0.03390 0.00166

AFIX 23

H21A 2 0.90660 0.22870 0.16469 11.00000 -1.20000

H21B 2 0.85957 0.12911 0.15726 11.00000 -1.20000

AFIX 0

C22 1 0.87875 0.21589 0.23837 11.00000 0.04820 0.04042 =
0.05509 0.00886 0.01976 0.00732

AFIX 23

H22A 2 0.90923 0.16278 0.26030 11.00000 -1.20000

H22B 2 0.88762 0.29808 0.25317 11.00000 -1.20000

AFIX 0

C23 1 0.60858 0.69591 0.37270 11.00000 0.04836 0.03532 =
0.06070 -0.00285 0.01408 -0.00538

AFIX 23

H23A 2 0.61624 0.77356 0.39323 11.00000 -1.20000

H23B 2 0.63199 0.63472 0.39852 11.00000 -1.20000

AFIX 0

C24 1 0.54823 0.66436 0.35937 11.00000 0.05665 0.04263 =
0.06414 0.00171 0.02690 -0.00069

AFIX 23

H24A 2 0.53708 0.67256 0.39571 11.00000 -1.20000

H24B 2 0.52548 0.71982 0.32932 11.00000 -1.20000

AFIX 0

C25 1 0.48122 0.51166 0.32579 11.00000 0.04377 0.05141 =
0.07984 0.00736 0.01767 -0.00571

AFIX 23

H25A 2 0.45739 0.56899 0.29770 11.00000 -1.20000

H25B 2 0.47101 0.51371 0.36287 11.00000 -1.20000

AFIX 0

C26 1 0.47218 0.38712 0.29951 11.00000 0.04417 0.05639 =
0.08921 0.00486 0.00929 -0.00608

AFIX 23

H26A 2 0.43212 0.36841 0.28606 11.00000 -1.20000

H26B 2 0.48624 0.38259 0.26493 11.00000 -1.20000

AFIX 0

C27 1 0.48664 0.17891 0.32565 11.00000 0.04745 0.04929 =
0.08740 -0.00633 0.01886 -0.01237

AFIX 23

H27A 2 0.47930 0.17224 0.28235 11.00000 -1.20000

H27B 2 0.45250 0.15615 0.33502 11.00000 -1.20000

AFIX 0

C28 1 0.53311 0.09652 0.35687 11.00000 0.05359 0.04363 =
0.08712 0.00127 0.03158 -0.00646

AFIX 23

H28A 2 0.54227 0.10610 0.40026 11.00000 -1.20000

H28B 2 0.52222 0.01282 0.34667 11.00000 -1.20000

AFIX 0

C29 1 0.61834 0.03258 0.34223 11.00000 0.04100 0.03836 =
0.07123 0.00291 0.01382 0.00004

AFIX 23

H29A 2 0.59920 -0.03626 0.31879 11.00000 -1.20000

H29B 2 0.63349 0.00738 0.38402 11.00000 -1.20000

AFIX 0
C30 1 0.66501 0.07386 0.31927 11.00000 0.05611 0.03545 =
0.06082 0.00447 0.02034 0.00868

AFIX 23
H30A 2 0.68271 0.00454 0.30664 11.00000 -1.20000
H30B 2 0.65027 0.12684 0.28473 11.00000 -1.20000

AFIX 0
C31 1 0.84886 0.23160 0.40622 11.00000 0.04429 0.03292 =
0.04899 0.00222 0.02293 0.00556
C32 1 0.86183 0.22553 0.35278 11.00000 0.04575 0.03230 =
0.05046 0.00586 0.02659 0.00342

AFIX 43
H32A 2 0.89768 0.24537 0.35089 11.00000 -1.20000

AFIX 0
C33 1 0.81920 0.18856 0.30174 11.00000 0.05841 0.02747 =
0.05247 0.00779 0.02652 0.00753
C34 1 0.76625 0.15779 0.30394 11.00000 0.04847 0.02948 =
0.05536 0.00402 0.02019 0.00749

AFIX 43
H34A 2 0.73831 0.13345 0.26920 11.00000 -1.20000

AFIX 0
C35 1 0.75536 0.16353 0.35796 11.00000 0.04276 0.03059 =
0.06270 0.00797 0.02544 0.00345
C36 1 0.79700 0.20141 0.40951 11.00000 0.05664 0.04207 =
0.04736 0.00265 0.02337 0.00675

AFIX 43
H36A 2 0.78931 0.20604 0.44620 11.00000 -1.20000

AFIX 0

C37 1 0.87200 0.57001 0.20903 11.00000 0.04589 0.05314 =
0.05135 -0.00298 0.01278 -0.00384

AFIX 33

H37A 2 0.90688 0.60210 0.23497 11.00000 -1.50000

H37B 2 0.85490 0.62825 0.17817 11.00000 -1.50000

H37C 2 0.87937 0.49636 0.19066 11.00000 -1.50000

AFIX 0

C38 1 0.78230 0.49884 0.21784 11.00000 0.04213 0.06364 =
0.04577 -0.01442 0.00528 -0.01345

AFIX 43

H38A 2 0.77079 0.48437 0.17646 11.00000 -1.20000

AFIX 0

C39 1 0.74684 0.47339 0.25090 11.00000 0.03601 0.06016 =
0.05225 -0.01986 0.00450 -0.01424

AFIX 43

H39A 2 0.71121 0.44182 0.23141 11.00000 -1.20000

AFIX 0

C40 1 0.76207 0.49294 0.31245 11.00000 0.03178 0.02368 =
0.04877 -0.00080 0.00703 0.00555

C41 1 0.81557 0.54101 0.33839 11.00000 0.03909 0.04396 =
0.03295 0.00667 -0.00160 -0.00090

AFIX 43

H41A 2 0.82827 0.55566 0.37974 11.00000 -1.20000

AFIX 0

C42 1 0.84937 0.56673 0.30425 11.00000 0.04125 0.04254 =
0.03674 0.00348 -0.00090 -0.00758

AFIX 43

H42A 2 0.88471 0.60088 0.32250 11.00000 -1.20000

AFIX 0

C43 1 0.62271 0.34719 0.45453 11.00000 0.06351 0.07880 =
0.08738 0.00600 0.02875 -0.02277

AFIX 33

H43A 2 0.64245 0.36146 0.49637 11.00000 -1.50000

H43B 2 0.61572 0.26183 0.44798 11.00000 -1.50000

H43C 2 0.58739 0.39009 0.44354 11.00000 -1.50000

AFIX 0

C44 1 0.70897 0.43758 0.44361 11.00000 0.05369 0.04783 =
0.04851 0.00225 0.01907 0.00587

AFIX 43

H44A 2 0.72165 0.44544 0.48542 11.00000 -1.20000

AFIX 0

C45 1 0.74258 0.47347 0.41151 11.00000 0.04092 0.04127 =
0.04602 -0.00065 0.00801 0.00227

AFIX 43

H45A 2 0.77783 0.50675 0.43107 11.00000 -1.20000

AFIX 0

C46 1 0.72495 0.46119 0.34850 11.00000 0.03142 0.02783 =
0.04892 0.00268 0.00895 0.00210

C47 1 0.67096 0.41551 0.32319 11.00000 0.04261 0.04011 =
0.05089 -0.00069 0.00309 -0.00035

AFIX 43

H47A 2 0.65648 0.40870 0.28143 11.00000 -1.20000

AFIX 0

C48 1 0.63874 0.38047 0.35812 11.00000 0.04136 0.03184 =
0.07139 -0.00419 0.00997 -0.00313

AFIX 43

H48A 2 0.60286 0.34883 0.33991 11.00000 -1.20000

AFIX 0
C49 1 0.60712 0.64041 0.59026 11.00000 0.31042

AFIX 33
H49A 2 0.62045 0.55824 0.59239 11.00000 -1.50000
H49B 2 0.56987 0.64140 0.59457 11.00000 -1.50000
H49C 2 0.63221 0.68717 0.62211 11.00000 -1.50000

AFIX 0
C50 1 0.60537 0.69170 0.53320 11.00000 0.15648
C51 1 0.58580 0.81873 0.52353 11.00000 0.27437

AFIX 33
H51A 2 0.58607 0.84497 0.48424 11.00000 -1.50000
H51B 2 0.61051 0.86952 0.55375 11.00000 -1.50000
H51C 2 0.54808 0.82433 0.52629 11.00000 -1.50000

HKLF 4

END

WGHT 0.1637 2.9056
Q1 1 0.3412 0.9096 0.3855 11.00000 0.05 0.84
Q2 1 0.5390 0.5894 0.5183 11.00000 0.05 0.74
Q3 1 0.4012 0.9129 0.3192 11.00000 0.05 0.55
Q4 1 0.3511 0.7357 0.4039 11.00000 0.05 0.53
Q5 1 0.3611 0.7661 0.3125 11.00000 0.05 0.42
Q6 1 0.4511 0.7708 0.3807 11.00000 0.05 0.42
Q7 1 0.5990 0.6081 0.5896 11.00000 0.05 0.39
Q8 1 0.6191 0.7829 0.5830 11.00000 0.05 0.39
Q9 1 0.4011 0.6713 0.3814 11.00000 0.05 0.35
Q10 1 0.4312 0.9572 0.4394 11.00000 0.05 0.35
Q11 1 0.4612 0.8465 0.3568 11.00000 0.05 0.33

Q12	1	0.4112	0.9943	0.3796	11.00000	0.05	0.31
Q13	1	0.4011	0.8280	0.4535	11.00000	0.05	0.31
Q14	1	1.1010	0.0723	0.7080	11.00000	0.05	0.31
Q15	1	0.5989	0.1268	0.3882	11.00000	0.05	0.30
Q16	1	0.9291	0.7661	0.6604	11.00000	0.05	0.29
Q17	1	0.5592	0.6667	0.2872	11.00000	0.05	0.28
Q18	1	0.9788	0.0490	0.7294	11.00000	0.05	0.27
Q19	1	0.4211	0.7865	0.3115	11.00000	0.05	0.27
Q20	1	0.7791	0.7584	0.0215	11.00000	0.05	0.25