

```

TITL  DSNII296

CELL  1.54184 10.7679 15.6775 32.4528  90.000  93.196  90.000

ZERR  4

LATT  1

SYMM  -X,0.5+Y,0.5-Z

SFAC  P    F    O    N    C    H

UNIT  4  24  52   8 180 256

L.S.  4

P1    1    0.66313    0.31695    0.52723 11.00000 0.12680 0.06923 =
      0.07866  -0.01132    0.01290    0.00846

P2    1    0.19391    0.14305    0.24361 11.00000 0.10692 0.09851 =
      0.10023  -0.01666   -0.00711    0.02390

F1    2    0.59332    0.36015    0.49081 11.00000 0.16248 0.27471 =
      0.17340    0.12651   -0.00052    0.03978

F2    2    0.73506    0.26657    0.56329 11.00000 0.17990 0.22707 =
      0.16714    0.08335   -0.01771    0.01505

F3    2    0.74018    0.39397    0.53964 11.00000 0.34048 0.12963 =
      0.27547  -0.03921   -0.01626   -0.06415

F4    2    0.58373    0.23926    0.51994 11.00000 0.41536 0.14903 =
      0.29987    0.06269   -0.17014   -0.13971

F5    2    0.76732    0.29536    0.49876 11.00000 0.19450 0.31243 =
      0.14645  -0.00170    0.04348    0.08334

F6    2    0.56458    0.34193    0.55560 11.00000 0.26841 0.32643 =
      0.19365  -0.00641    0.12518    0.10502

F7    2    0.13552    0.10775    0.20184 11.00000 0.19898 0.18703 =
      0.14554  -0.02407   -0.03392   -0.06619

F8    2    0.25589    0.17973    0.28275 11.00000 0.41200 0.21917 =
      0.15480  -0.10016   -0.16542    0.17764

F9    2    0.23783    0.05327    0.25587 11.00000 0.27593 0.11350 =

```

| | | | | | | | | |
|-----|---|---------|----------|----------|----------|----------|---------|---|
| | | 0.18654 | -0.00921 | -0.03699 | 0.08764 | | | |
| F10 | 2 | 0.15086 | 0.23881 | 0.23404 | 11.00000 | 0.13727 | 0.10354 | = |
| | | 0.23371 | 0.02580 | -0.01877 | | 0.01713 | | |
| F11 | 2 | 0.31463 | 0.15852 | 0.22221 | 11.00000 | 0.12269 | 0.22330 | = |
| | | 0.33301 | -0.13907 | 0.05956 | | -0.03321 | | |
| F12 | 2 | 0.06995 | 0.12801 | 0.26151 | 11.00000 | 0.26489 | 0.15014 | = |
| | | 0.28592 | 0.05413 | 0.16476 | | 0.03672 | | |
| O1 | 3 | 0.68476 | 0.24728 | 0.36228 | 11.00000 | 0.09674 | 0.06128 | = |
| | | 0.06319 | 0.01268 | 0.00971 | | 0.00155 | | |
| O2 | 3 | 0.59291 | 0.42644 | 0.36081 | 11.00000 | 0.06950 | 0.07433 | = |
| | | 0.13113 | 0.04129 | 0.00568 | | 0.00066 | | |
| O3 | 3 | 0.38123 | 0.51688 | 0.33176 | 11.00000 | 0.06575 | 0.05867 | = |
| | | 0.12729 | -0.00332 | 0.01198 | | 0.00864 | | |
| O4 | 3 | 0.14919 | 0.44737 | 0.33723 | 11.00000 | 0.08070 | 0.06213 | = |
| | | 0.14106 | 0.01509 | -0.00324 | | 0.00587 | | |
| O5 | 3 | 0.03156 | 0.32042 | 0.38204 | 11.00000 | 0.08834 | 0.06257 | = |
| | | 0.16060 | -0.02295 | 0.00242 | | 0.00405 | | |
| O6 | 3 | 0.03672 | 0.01220 | 0.39170 | 11.00000 | 0.09002 | 0.09540 | = |
| | | 0.16938 | -0.04889 | 0.00285 | | -0.00213 | | |
| O7 | 3 | 0.10866 | -0.13450 | 0.34570 | 11.00000 | 0.08592 | 0.05840 | = |
| | | 0.12068 | -0.02421 | 0.00197 | | 0.00559 | | |
| O8 | 3 | 0.26646 | -0.20838 | 0.28348 | 11.00000 | 0.08269 | 0.09628 | = |
| | | 0.09057 | -0.02340 | 0.01133 | | -0.00171 | | |
| O9 | 3 | 0.48586 | -0.12225 | 0.26337 | 11.00000 | 0.09705 | 0.07749 | = |
| | | 0.07205 | -0.02683 | 0.01279 | | -0.00143 | | |
| O10 | 3 | 0.66176 | -0.04602 | 0.32448 | 11.00000 | 0.10442 | 0.07128 | = |
| | | 0.05179 | 0.00140 | 0.00950 | | -0.00168 | | |
| O11 | 3 | 0.68277 | -0.05985 | 0.47654 | 11.00000 | 0.13085 | 0.07857 | = |

| | | | | | | | | |
|------|---|---------|----------|----------|----------|----------|---------|---|
| | | 0.05690 | 0.01730 | 0.01616 | 0.00320 | | | |
| O12A | 3 | 0.07398 | 0.12155 | 0.53594 | 10.50000 | 0.10348 | 0.09675 | = |
| | | 0.13690 | 0.00706 | 0.01651 | | 0.02164 | | |
| O12B | 3 | 0.14628 | 0.18296 | 0.53292 | 10.50000 | 0.13600 | 0.10735 | = |
| | | 0.12472 | -0.00442 | 0.02309 | | 0.02552 | | |
| N1 | 4 | 0.34524 | 0.33754 | 0.42421 | 11.00000 | 0.06155 | 0.05941 | = |
| | | 0.08801 | 0.00100 | 0.00908 | | 0.00707 | | |
| N2 | 4 | 0.40403 | -0.09504 | 0.37577 | 11.00000 | 0.08128 | 0.06162 | = |
| | | 0.05386 | 0.00100 | 0.01629 | | -0.00677 | | |
| C1 | 5 | 0.34286 | 0.27813 | 0.45414 | 11.00000 | 0.10229 | 0.06169 | = |
| | | 0.06594 | 0.01256 | 0.00788 | | 0.00947 | | |
| C2 | 5 | 0.34910 | 0.19562 | 0.44452 | 11.00000 | 0.10222 | 0.06148 | = |
| | | 0.05543 | 0.02224 | 0.01611 | | 0.02029 | | |
| C3 | 5 | 0.35813 | 0.16756 | 0.40474 | 11.00000 | 0.04724 | 0.05471 | = |
| | | 0.06129 | 0.00244 | 0.00675 | | 0.00007 | | |
| C4 | 5 | 0.36315 | 0.23016 | 0.37473 | 11.00000 | 0.08281 | 0.06524 | = |
| | | 0.06035 | 0.00513 | 0.01092 | | 0.00479 | | |
| C5 | 5 | 0.35726 | 0.31471 | 0.38406 | 11.00000 | 0.07462 | 0.06228 | = |
| | | 0.07933 | 0.01272 | 0.00895 | | -0.00426 | | |
| C6 | 5 | 0.33838 | 0.43182 | 0.43476 | 11.00000 | 0.14713 | 0.04133 | = |
| | | 0.13283 | -0.00489 | 0.02259 | | 0.01026 | | |
| C7 | 5 | 0.37844 | -0.03858 | 0.34601 | 11.00000 | 0.08239 | 0.08216 | = |
| | | 0.05820 | -0.00560 | -0.00323 | | -0.00370 | | |
| C8 | 5 | 0.36083 | 0.04685 | 0.35422 | 11.00000 | 0.08581 | 0.06367 | = |
| | | 0.05857 | 0.00440 | -0.00029 | | 0.00778 | | |
| C9 | 5 | 0.36873 | 0.07644 | 0.39460 | 11.00000 | 0.05121 | 0.06061 | = |
| | | 0.05226 | 0.00036 | 0.00924 | | 0.00684 | | |
| C10 | 5 | 0.38784 | 0.01431 | 0.42529 | 11.00000 | 0.09143 | 0.06229 | = |
| | | 0.05379 | 0.00139 | 0.01719 | | -0.00746 | | |

C11 5 0.40728 -0.06864 0.41503 11.00000 0.11218 0.04966 =
0.06587 0.01489 0.00484 -0.00142

C12 5 0.44015 -0.18348 0.36594 11.00000 0.13816 0.04075 =
0.10914 -0.00474 0.01373 0.00010

C13 5 0.68742 0.16426 0.37431 11.00000 0.06131 0.04939 =
0.05943 0.00481 0.00746 -0.00440

C14 5 0.69793 0.13899 0.41501 11.00000 0.06269 0.06748 =
0.05249 0.00011 0.00806 0.00115

C15 5 0.69738 0.05170 0.42355 11.00000 0.06654 0.05701 =
0.04806 0.01063 0.00811 0.00490

C16 5 0.68932 -0.00690 0.39276 11.00000 0.06444 0.05596 =
0.05519 0.00743 0.01178 -0.00438

C17 5 0.67696 0.02006 0.35291 11.00000 0.06293 0.05751 =
0.05407 -0.00401 0.00771 0.00126

C18 5 0.67500 0.10408 0.34272 11.00000 0.07965 0.06359 =
0.05607 0.00753 0.01313 -0.00126

C19 5 0.70946 0.02670 0.46841 11.00000 0.11422 0.07748 =
0.07167 0.01577 0.00380 0.00045

C20 5 0.70422 0.31092 0.39355 11.00000 0.07081 0.05261 =
0.08953 -0.00185 -0.00915 0.00299

C21 5 0.71192 0.39671 0.37417 11.00000 0.06662 0.08805 =
0.12133 -0.00276 -0.01514 -0.00578

C22 5 0.59753 0.50370 0.33663 11.00000 0.08643 0.07779 =
0.18616 0.05317 0.02268 -0.00352

C23 5 0.49461 0.55571 0.34322 11.00000 0.08494 0.06081 =
0.14365 0.01718 0.00013 -0.00082

C24 5 0.27957 0.56905 0.33683 11.00000 0.09782 0.05515 =
0.11506 0.01481 0.01971 0.01311

C25 5 0.16250 0.52679 0.32096 11.00000 0.07116 0.07790 =
0.14203 0.01107 0.01633 0.01352

C26 5 0.03598 0.40714 0.32167 11.00000 0.08238 0.07624 =
0.17327 -0.00530 -0.02109 0.00336

C27 5 0.03518 0.31953 0.33738 11.00000 0.07977 0.05662 =
0.17481 -0.01074 -0.00167 0.00078

C28 5 0.03136 0.24420 0.40354 11.00000 0.05434 0.04393 =
0.16964 -0.01857 0.00205 0.00906

C29 5 0.02921 0.24783 0.44508 11.00000 0.08306 0.08479 =
0.13505 -0.03808 -0.01365 0.01826

C30 5 0.03073 0.17592 0.46871 11.00000 0.08777 0.06853 =
0.16017 -0.01022 -0.02291 0.02445

C31 5 0.03596 0.09883 0.44881 11.00000 0.08691 0.06628 =
0.15082 -0.00567 -0.01644 0.01567

C32 5 0.03722 0.09400 0.40690 11.00000 0.05790 0.04970 =
0.17089 -0.03471 -0.00174 0.00967

C33 5 0.03542 0.16537 0.38240 11.00000 0.06471 0.05218 =
0.15551 -0.01296 0.01745 -0.00337

C34 5 0.02439 0.18353 0.51574 11.00000 0.13316 0.13131 =
0.13267 -0.02667 -0.03992 0.02779

C35 5 0.01715 0.00365 0.35055 11.00000 0.07737 0.05343 =
0.28886 -0.02289 0.00818 0.00693

C36 5 -0.00344 -0.09104 0.33962 11.00000 0.06892 0.09614 =
0.26217 -0.06612 -0.00510 0.00689

C37 5 0.10168 -0.21855 0.32832 11.00000 0.09592 0.06556 =
0.18115 -0.02851 0.03130 -0.00867

C38 5 0.13855 -0.22168 0.28528 11.00000 0.09481 0.10980 =
0.11681 -0.04415 0.00913 -0.00442

C39 5 0.30202 -0.19613 0.24333 11.00000 0.10831 0.12094 =

| | | | | | | | |
|------|----|---------|----------|----------|----------|----------|-----------|
| | | 0.07953 | -0.03663 | -0.00800 | 0.01311 | | |
| C40 | 5 | 0.44137 | -0.19412 | 0.24178 | 11.00000 | 0.11852 | 0.09669 = |
| | | 0.07768 | -0.04211 | 0.01248 | | 0.00423 | |
| C41 | 5 | 0.61422 | -0.10799 | 0.25890 | 11.00000 | 0.12067 | 0.09949 = |
| | | 0.05982 | -0.01933 | 0.02366 | | -0.00512 | |
| C42 | 5 | 0.65029 | -0.02670 | 0.28135 | 11.00000 | 0.11507 | 0.08084 = |
| | | 0.06923 | -0.01048 | 0.02646 | | -0.01257 | |
| O1S | 3 | 0.18050 | 0.12571 | 0.03104 | 10.50000 | 0.09648 | |
| C1S | 5 | 0.11594 | 0.08952 | 0.05268 | 10.50000 | 0.13353 | |
| C2S | 5 | 0.05186 | 0.01485 | 0.04095 | 10.50000 | 0.19255 | |
| C3S | 5 | 0.06127 | 0.10839 | 0.08971 | 10.50000 | 0.09613 | |
| O1W | 3 | 0.17737 | 0.14227 | 0.06920 | 10.50000 | 0.27552 | |
| AFIX | 01 | | | | | | |
| H1 | 6 | 0.33674 | 0.29499 | 0.48209 | 11.00000 | 0.09948 | |
| H2 | 6 | 0.34722 | 0.15468 | 0.46607 | 11.00000 | 0.09439 | |
| H4 | 6 | 0.37093 | 0.21364 | 0.34681 | 11.00000 | 0.08998 | |
| H5 | 6 | 0.36142 | 0.35675 | 0.36310 | 11.00000 | 0.09347 | |
| H7 | 6 | 0.37203 | -0.05754 | 0.31816 | 11.00000 | 0.09688 | |
| H8 | 6 | 0.34322 | 0.08551 | 0.33212 | 11.00000 | 0.09037 | |
| H10 | 6 | 0.38724 | 0.03016 | 0.45355 | 11.00000 | 0.08929 | |
| H11 | 6 | 0.42369 | -0.10906 | 0.43646 | 11.00000 | 0.09868 | |
| H14 | 6 | 0.70534 | 0.17976 | 0.43667 | 11.00000 | 0.07893 | |
| H16 | 6 | 0.69228 | -0.06608 | 0.39897 | 11.00000 | 0.07568 | |
| H18 | 6 | 0.66537 | 0.12145 | 0.31466 | 11.00000 | 0.08592 | |
| H19A | 6 | 0.79247 | 0.03787 | 0.47839 | 11.00000 | 0.11420 | |
| H19B | 6 | 0.65387 | 0.06098 | 0.48299 | 11.00000 | 0.11420 | |
| H20A | 6 | 0.77961 | 0.29936 | 0.40915 | 11.00000 | 0.09291 | |
| H20B | 6 | 0.63690 | 0.30998 | 0.41127 | 11.00000 | 0.09291 | |

| | | | | | | |
|------|---|----------|----------|---------|----------|---------|
| H21A | 6 | 0.74823 | 0.43557 | 0.39381 | 11.00000 | 0.12056 |
| H21B | 6 | 0.76234 | 0.39317 | 0.35111 | 11.00000 | 0.12056 |
| H22A | 6 | 0.59735 | 0.48923 | 0.30818 | 11.00000 | 0.15104 |
| H22B | 6 | 0.67160 | 0.53395 | 0.34440 | 11.00000 | 0.15104 |
| H23A | 6 | 0.49528 | 0.56955 | 0.37175 | 11.00000 | 0.12566 |
| H23B | 6 | 0.50171 | 0.60647 | 0.32755 | 11.00000 | 0.12566 |
| H24A | 6 | 0.29007 | 0.62070 | 0.32212 | 11.00000 | 0.11545 |
| H24B | 6 | 0.27400 | 0.58123 | 0.36536 | 11.00000 | 0.11545 |
| H25A | 6 | 0.09385 | 0.56087 | 0.32794 | 11.00000 | 0.12560 |
| H25B | 6 | 0.16352 | 0.52209 | 0.29177 | 11.00000 | 0.12560 |
| H26A | 6 | 0.03267 | 0.40660 | 0.29233 | 11.00000 | 0.14512 |
| H26B | 6 | -0.03367 | 0.43740 | 0.33089 | 11.00000 | 0.14512 |
| H27A | 6 | -0.03599 | 0.29052 | 0.32584 | 11.00000 | 0.13521 |
| H27B | 6 | 0.10823 | 0.29092 | 0.32978 | 11.00000 | 0.13521 |
| H29 | 6 | 0.02657 | 0.30191 | 0.45819 | 11.00000 | 0.13217 |
| H31 | 6 | 0.03877 | 0.04779 | 0.46461 | 11.00000 | 0.13280 |
| H33 | 6 | 0.03679 | 0.16210 | 0.35317 | 11.00000 | 0.11744 |
| H35A | 6 | 0.08750 | 0.02432 | 0.33722 | 11.00000 | 0.18181 |
| H35B | 6 | -0.05431 | 0.03549 | 0.34153 | 11.00000 | 0.18181 |
| H36A | 6 | -0.06307 | -0.11472 | 0.35686 | 11.00000 | 0.18572 |
| H36B | 6 | -0.03268 | -0.09596 | 0.31154 | 11.00000 | 0.18572 |
| H37A | 6 | 0.01845 | -0.23831 | 0.32908 | 11.00000 | 0.14727 |
| H37B | 6 | 0.15517 | -0.25499 | 0.34456 | 11.00000 | 0.14727 |
| H38A | 6 | 0.11781 | -0.27599 | 0.27389 | 11.00000 | 0.13912 |
| H38B | 6 | 0.09519 | -0.17861 | 0.26974 | 11.00000 | 0.13912 |
| H39A | 6 | 0.26892 | -0.14355 | 0.23319 | 11.00000 | 0.13446 |
| H39B | 6 | 0.27006 | -0.24146 | 0.22645 | 11.00000 | 0.13446 |
| H40A | 6 | 0.47605 | -0.24418 | 0.25423 | 11.00000 | 0.12659 |
| H40B | 6 | 0.46364 | -0.19100 | 0.21388 | 11.00000 | 0.12659 |

| | | | | | | |
|------|---|---------|----------|---------|----------|---------|
| H41A | 6 | 0.62976 | -0.10261 | 0.23047 | 11.00000 | 0.12045 |
| H41B | 6 | 0.66105 | -0.15432 | 0.27049 | 11.00000 | 0.12045 |
| H42A | 6 | 0.72735 | -0.00635 | 0.27237 | 11.00000 | 0.11388 |
| H42B | 6 | 0.58794 | 0.01539 | 0.27618 | 11.00000 | 0.11388 |
| HKLF | 4 | | | | | |