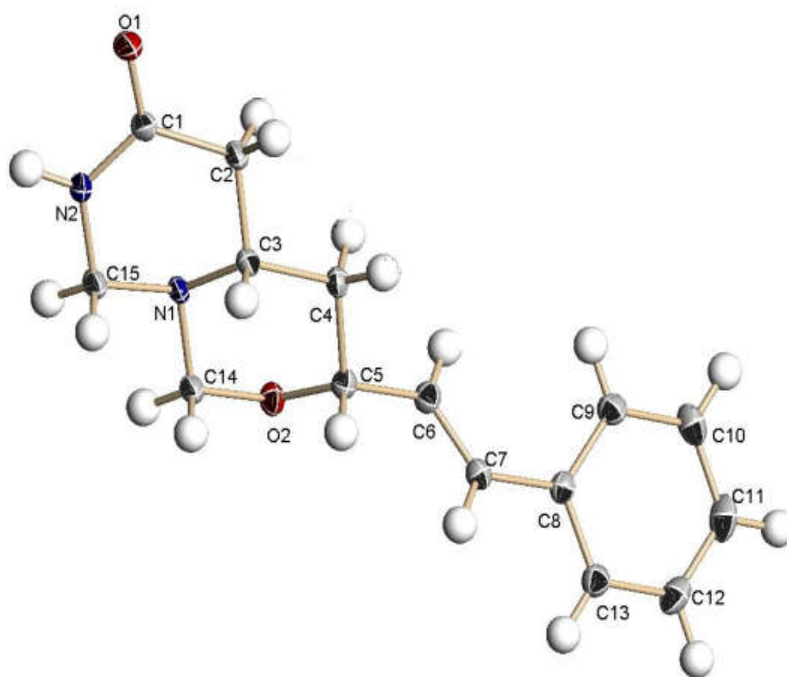




TITL Nadiiah4240\_0m in P2(1)2(1)2(1)  
 CELL 0.71073 6.1025 6.3610 36.1031 90.000 90.000 90.000  
 ZERR 4.00 0.0006 0.0006 0.0033 0.000 0.000 0.000  
 LATT -1  
 SYMM 0.5-X, -Y, 0.5+Z  
 SYMM -X, 0.5+Y, 0.5-Z  
 SYMM 0.5+X, 0.5-Y, -Z  
 SFAC C H N O  
 UNIT 60 72 8 8  
 OMIT 0 0 2  
 L.S. 4  
 ACTA  
 BOND \$H  
 FMAP 2  
 PLAN 5  
 HTAB  
 TEMP -173.00  
 WGHT 0.041600 0.300300  
 FVAR 0.21304  
 O1 4 1.235535 0.329901 0.763544 11.00000 0.02620 0.01948  
 =  
 0.02699 -0.00055 0.01030 -0.00092  
 C1 1 1.100460 0.271924 0.787530 11.00000 0.01961 0.01588  
 =  
 0.01947 -0.00331 0.00099 -0.00112  
 C2 1 0.935639 0.424309 0.802819 11.00000 0.02204 0.01344  
 =  
 0.02042 0.00090 0.00522 0.00151  
 AFIX 23  
 H2A 2 0.871708 0.505254 0.782040 11.00000 -1.20000  
 H2B 2 1.012298 0.525031 0.819224 11.00000 -1.20000  
 AFIX 0  
 C3 1 0.750730 0.321509 0.824492 11.00000 0.01865 0.01315  
 =  
 0.01636 0.00027 0.00014 0.00095  
 AFIX 13  
 H3A 2 0.649598 0.247913 0.806974 11.00000 -1.20000  
 AFIX 0

|      |    |           |          |          |          |          |         |
|------|----|-----------|----------|----------|----------|----------|---------|
| C4   | 1  | 0.622704  | 0.483901 | 0.846699 | 11.00000 | 0.01948  | 0.01493 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.01935   | -0.00006 | 0.00073  | 0.00321  |          |         |
| AFIX | 23 |           |          |          |          |          |         |
| H4A  | 2  | 0.538096  | 0.573772 | 0.829475 | 11.00000 | -1.20000 |         |
| H4B  | 2  | 0.726837  | 0.575095 | 0.860262 | 11.00000 | -1.20000 |         |
| AFIX | 0  |           |          |          |          |          |         |
| C5   | 1  | 0.466193  | 0.382159 | 0.874248 | 11.00000 | 0.01799  | 0.01808 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.01834   | -0.00152 | 0.00026  | 0.00168  |          |         |
| AFIX | 13 |           |          |          |          |          |         |
| H5A  | 2  | 0.348500  | 0.304769 | 0.860628 | 11.00000 | -1.20000 |         |
| AFIX | 0  |           |          |          |          |          |         |
| C6   | 1  | 0.365696  | 0.543113 | 0.899150 | 11.00000 | 0.01990  | 0.01991 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.01927   | -0.00272 | -0.00004 | 0.00115  |          |         |
| AFIX | 43 |           |          |          |          |          |         |
| H6A  | 2  | 0.458497  | 0.648083 | 0.909362 | 11.00000 | -1.20000 |         |
| AFIX | 0  |           |          |          |          |          |         |
| C7   | 1  | 0.154488  | 0.548100 | 0.907842 | 11.00000 | 0.02106  | 0.01646 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.01906   | -0.00108 | -0.00045 | 0.00022  |          |         |
| AFIX | 43 |           |          |          |          |          |         |
| H7A  | 2  | 0.063826  | 0.439529 | 0.898270 | 11.00000 | -1.20000 |         |
| AFIX | 0  |           |          |          |          |          |         |
| C8   | 1  | 0.049933  | 0.709377 | 0.931229 | 11.00000 | 0.01812  | 0.02006 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.01632   | -0.00055 | -0.00081 | 0.00368  |          |         |
| C9   | 1  | 0.140017  | 0.910288 | 0.935840 | 11.00000 | 0.02291  | 0.02219 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.02089   | -0.00016 | 0.00142  | -0.00039 |          |         |
| AFIX | 43 |           |          |          |          |          |         |
| H9A  | 2  | 0.274827  | 0.944728 | 0.924164 | 11.00000 | -1.20000 |         |
| AFIX | 0  |           |          |          |          |          |         |
| C10  | 1  | 0.033406  | 1.059154 | 0.957363 | 11.00000 | 0.03846  | 0.01856 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.02486   | -0.00464 | -0.00314 | 0.00277  |          |         |
| AFIX | 43 |           |          |          |          |          |         |
| H10A | 2  | 0.095596  | 1.194956 | 0.960429 | 11.00000 | -1.20000 |         |
| AFIX | 0  |           |          |          |          |          |         |
| C11  | 1  | -0.163839 | 1.010252 | 0.974428 | 11.00000 | 0.03836  | 0.03103 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.02169   | -0.00529 | 0.00227  | 0.01404  |          |         |
| AFIX | 43 |           |          |          |          |          |         |
| H11A | 2  | -0.236908 | 1.112668 | 0.989065 | 11.00000 | -1.20000 |         |
| AFIX | 0  |           |          |          |          |          |         |
| C12  | 1  | -0.253570 | 0.813163 | 0.970129 | 11.00000 | 0.02308  | 0.03598 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.02151   | 0.00212  | 0.00432  | 0.00741  |          |         |
| AFIX | 43 |           |          |          |          |          |         |
| H12A | 2  | -0.388188 | 0.779654 | 0.981952 | 11.00000 | -1.20000 |         |
| AFIX | 0  |           |          |          |          |          |         |
| C13  | 1  | -0.148651 | 0.663690 | 0.948676 | 11.00000 | 0.02096  | 0.02210 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.02189   | 0.00125  | 0.00030  | 0.00228  |          |         |
| AFIX | 43 |           |          |          |          |          |         |
| H13A | 2  | -0.212423 | 0.528443 | 0.945782 | 11.00000 | -1.20000 |         |
| AFIX | 0  |           |          |          |          |          |         |
| O2   | 4  | 0.589808  | 0.236990 | 0.896892 | 11.00000 | 0.02437  | 0.01780 |
| =    |    |           |          |          |          |          |         |
|      |    | 0.01784   | -0.00006 | 0.00288  | 0.00422  |          |         |

|      |    |          |           |          |          |          |         |
|------|----|----------|-----------|----------|----------|----------|---------|
| C14  | 1  | 0.684730 | 0.079633  | 0.874658 | 11.00000 | 0.02117  | 0.01377 |
| =    |    |          |           |          |          |          |         |
|      |    | 0.02107  | -0.00026  | 0.00354  | 0.00059  |          |         |
| AFIX | 23 |          |           |          |          |          |         |
| H14A | 2  | 0.568906 | 0.010001  | 0.859888 | 11.00000 | -1.20000 |         |
| H14B | 2  | 0.753440 | -0.027898 | 0.890723 | 11.00000 | -1.20000 |         |
| AFIX | 0  |          |           |          |          |          |         |
| N1   | 3  | 0.850104 | 0.167175  | 0.849721 | 11.00000 | 0.01862  | 0.01111 |
| =    |    |          |           |          |          |          |         |
|      |    | 0.01664  | 0.00075   | 0.00285  | 0.00134  |          |         |
| C15  | 1  | 0.944657 | -0.002406 | 0.828155 | 11.00000 | 0.02412  | 0.01295 |
| =    |    |          |           |          |          |          |         |
|      |    | 0.02110  | -0.00091  | 0.00509  | 0.00123  |          |         |
| AFIX | 23 |          |           |          |          |          |         |
| H15A | 2  | 0.826518 | -0.079089 | 0.815092 | 11.00000 | -1.20000 |         |
| H15B | 2  | 1.019206 | -0.102519 | 0.844948 | 11.00000 | -1.20000 |         |
| AFIX | 0  |          |           |          |          |          |         |
| N2   | 3  | 1.101537 | 0.077833  | 0.801182 | 11.00000 | 0.02028  | 0.01393 |
| =    |    |          |           |          |          |          |         |
|      |    | 0.02385  | -0.00100  | 0.00588  | 0.00272  |          |         |
| AFIX | 43 |          |           |          |          |          |         |
| H2C  | 2  | 1.204366 | -0.008439 | 0.793374 | 11.00000 | -1.20000 |         |
| AFIX | 0  |          |           |          |          |          |         |
| O3   | 4  | 0.366799 | 0.749581  | 0.771429 | 11.00000 | 0.02656  | 0.01677 |
| =    |    |          |           |          |          |          |         |
|      |    | 0.03313  | -0.00072  | 0.01116  | 0.00091  |          |         |
| H1W  | 2  | 0.489430 | 0.761043  | 0.759453 | 11.00000 | 0.04233  |         |
| H2W  | 2  | 0.316841 | 0.636120  | 0.768673 | 11.00000 | 0.05036  |         |

HKLF 4

REM Nadiiah4240\_0m in P2(1)2(1)2(1)

REM R1 = 0.0426 for 3655 Fo > 4sig(Fo) and 0.0533 for all 4240 data

REM 189 parameters refined using 0 restraints

END

WGHT 0.0415 0.2993

REM Highest difference peak 0.252, deepest hole -0.207, 1-sigma level 0.044

|    |   |         |        |        |          |      |      |
|----|---|---------|--------|--------|----------|------|------|
| Q1 | 1 | 0.6803  | 0.3999 | 0.8350 | 11.00000 | 0.05 | 0.25 |
| Q2 | 1 | -0.0376 | 0.6940 | 0.9441 | 11.00000 | 0.05 | 0.23 |
| Q3 | 1 | 0.0649  | 0.8200 | 0.9317 | 11.00000 | 0.05 | 0.20 |
| Q4 | 1 | 0.7849  | 0.1275 | 0.8648 | 11.00000 | 0.05 | 0.20 |
| Q5 | 1 | 0.0776  | 1.0084 | 0.9395 | 11.00000 | 0.05 | 0.20 |