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HEADER    METAL COMPLEX                   01-AUG-02   1PHI
TITLE     A STRUCTURE OF DELTA-cis-ALPHA-[Ru(picchxnMe2)(phi)]2+
TITLE    2 NMR, MINIMIZED STRUCTURE
COMPND    MOL_A: 1;
SOURCE    MOL_A: 1;
SOURCE   2 SYNTHETIC: YES
KEYWDS    DELTA-cis-ALPHA-[Ru(picchxnMe2)(phi)]2+ SOLUTION STRUCTURE, NMR
EXPDTA    NMR, MINIMIZED STRUCTURE
AUTHOR    P.KARUSO
REVDAT   1   01-AUG-02   1PHI    0
JRNL        AUTH   E. M. PROUDFOOT, J. P. MACKAY, P. KARUSO
JRNL        TITL   Solution structure of LAMBDA-cis-ALPHA-[Ru(S, S-picchxnMe2)
JRNL        TITL 2 (dpqC)]2+ and DELTA-cis-ALPHA-[Ru(R, R-picchxnMe2)(phi)]2+
JRNL        TITL 3 by NMR spectroscopy and molecular modelling
JRNL        TITL 4
JRNL        TITL 5
JRNL        REF    DALTON     2002  0000-0000
JRNL        REFN
REMARK   1
REMARK   2
REMARK   2 RESOLUTION. NOT APPLICABLE.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : DISCOVER3
REMARK   3   AUTHORS     : MSI
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: REFINEMENT DETAILS CAN BE FOUND
REMARK   3  IN THE JRNL CITATION ABOVE.
REMARK   4
REMARK   4 1PHI COMPLIES WITH FORMAT V. 2.2, 16-DEC-1996
REMARK 210
REMARK 210 EXPERIMENTAL DETAILS
REMARK 210  EXPERIMENT TYPE                : NMR
REMARK 210  TEMPERATURE           (KELVIN) : 288
REMARK 210  PH                             : 7.0 UNCORRECTED
REMARK 210
REMARK 210  NMR EXPERIMENTS CONDUCTED      : ROESY, 2QF-COSY, AND
REMARK 210   TOCSY
REMARK 210  SPECTROMETER FIELD STRENGTH    : 600 MHZ
REMARK 210  SPECTROMETER MODEL             : DMX600
REMARK 210  SPECTROMETER MANUFACTURER      : BRUKER
REMARK 210
REMARK 210  STRUCTURE DETERMINATION.
REMARK 210   SOFTWARE USED                 : DISCOVER3, INSIGHTII
REMARK 210   METHOD USED                   : ROE-RESTRAINED MOLECULAR
REMARK 210   DYNAMICS/MECHANICS
REMARK 210
REMARK 210 CONFORMERS, NUMBER CALCULATED   : 20
REMARK 210 CONFORMERS, NUMBER SUBMITTED    : 1
REMARK 210 CONFORMERS, SELECTION CRITERIA  : THIS STRUCTURE PROVIDED
REMARK 210   THE BEST-FIT FOR THE NOE DATA BASED ON THE TWELVE
REMARK 210   OBSERVED NOES AND WAS FOUND 19 TIMES OUT OF 20 STRUCTURES
REMARK 210
REMARK 210 REMARK:
REMARK 210 IONIC_STRENGTH: 10mM NaCl, 10mM PHOSPHATE
REMARK 210 PRESSURE: NULL
REMARK 210 SOLVENT SYSTEM: H2O
REMARK 210
REMARK 210 SEE JRNL CITATION ABOVE FOR ADDITIONAL NMR EXPERIMENTAL
REMARK 210 DETAILS.
REMARK 215
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REMARK 215 NMR STUDY
REMARK 215 THE COORDINATES IN THIS ENTRY WERE GENERATED FROM SOLUTION
REMARK 215 NMR DATA.  PROTEIN DATA BANK CONVENTIONS REQUIRE THAT
REMARK 215 CRYST1 AND SCALE RECORDS BE INCLUDED, BUT THE VALUES ON
REMARK 215 THESE RECORDS ARE MEANINGLESS.
DBREF  1PHI A    1    10  PDB    1PHI     1PHI             1     10
DBREF  1PHI B    1    11  PDB    1PHI     1PHI             1     11
SEQRES   1 A   10    C   G   C   G   A   T   C   G   C   G
SEQRES   1 B   11    G   C   G   C   T   A   G   C   G   C
HETNAM       MOL_A DELTA-cis-ALPHA-[Ru(picchxnMe2)(phi)]2+
FORMUL   1   MOL_A    C34 H38 N6 RU
CRYST1    1.000    1.000    1.000  90.00  90.00  90.00 P 1           1
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      1.000000  0.000000  0.000000        0.00000
SCALE2      0.000000  1.000000  0.000000        0.00000
SCALE3      0.000000  0.000000  1.000000        0.00000
REMARK   4 DAPH COMPLIES WITH FORMAT V. 2.0, 10-AUG-2002
ATOM      1  C   MOL A   1      12.419   9.347   7.600  1.00  1.00           C
ATOM      2  C1  MOL A   1      11.960  11.699   8.102  1.00  1.00           C
ATOM      3  C2  MOL A   1      11.642  14.032   9.160  1.00  1.00           C
ATOM      4  N   MOL A   1      12.308  10.367   8.690  1.00  1.00           N
ATOM      5  C3  MOL A   1      14.906  10.414   8.774  1.00  1.00           C
ATOM      6  C4  MOL A   1       6.696  10.337   8.485  1.00  1.00           C
ATOM      7  C5  MOL A   1       6.733  10.626   7.104  1.00  0.00           C
ATOM      8  C6  MOL A   1       5.564  10.800   6.366  1.00  0.00           C
ATOM      9  N1  MOL A   1       9.081  10.252   8.653  1.00  1.00           N
ATOM     10  C7  MOL A   1      11.459  12.642   9.184  1.00  1.00           C
ATOM     11  C8  MOL A   1      11.075  14.817  10.167  1.00  1.00           C
ATOM     12  C9  MOL A   1       7.879  10.160   9.224  1.00  1.00           C
ATOM     13  C10 MOL A   1      13.558  10.446   9.555  1.00  1.00           C
ATOM     14  C11 MOL A   1      10.105   7.124   8.816  1.00  1.00           C
ATOM     15  C12 MOL A   1      16.140  10.408   9.686  1.00  1.00           C
ATOM     16  C13 MOL A   1       5.442  10.221   9.139  1.00  1.00           C
ATOM     17  C14 MOL A   1       4.275  10.403   8.363  1.00  0.00           C
ATOM     18  C15 MOL A   1       4.333  10.688   6.999  1.00  0.00           C
ATOM     19  C16 MOL A   1      10.202   5.728   8.817  1.00  1.00           C
ATOM     20  N2  MOL A   1      10.747  12.087  10.189  1.00  1.00           N
ATOM     21  RU  MOL A   1      10.645   9.955  10.006  1.00  1.00          Ru
ATOM     22  C17 MOL A   1      10.323  14.198  11.170  1.00  1.00           C
ATOM     23  N3  MOL A   1      10.660   7.819   9.827  1.00  1.00           N
ATOM     24  C18 MOL A   1      10.161  12.809  11.162  1.00  1.00           C
ATOM     25  C19 MOL A   1      10.857   5.077   9.866  1.00  1.00           C
ATOM     26  C20 MOL A   1      13.496   9.329  10.646  1.00  1.00           C
ATOM     27  C21 MOL A   1       7.828   9.878  10.604  1.00  1.00           C
ATOM     28  C22 MOL A   1       5.390   9.930  10.529  1.00  1.00           C
ATOM     29  C23 MOL A   1       4.168   9.803  11.227  1.00  0.00           C
ATOM     30  C24 MOL A   1       4.122   9.518  12.591  1.00  0.00           C
ATOM     31  C25 MOL A   1      16.080   9.246  10.684  1.00  1.00           C
ATOM     32  C26 MOL A   1      11.278   7.233  10.875  1.00  1.00           C
ATOM     33  N4  MOL A   1       8.984   9.732  11.253  1.00  1.00           N
ATOM     34  C27 MOL A   1      11.393   5.836  10.909  1.00  1.00           C
ATOM     35  N5  MOL A   1      12.198   9.467  11.427  1.00  1.00           N
ATOM     36  C28 MOL A   1       6.591   9.758  11.264  1.00  1.00           C
ATOM     37  C29 MOL A   1       6.524   9.469  12.645  1.00  0.00           C
ATOM     38  C30 MOL A   1       5.303   9.350  13.304  1.00  0.00           C
ATOM     39  C31 MOL A   1      14.790   9.299  11.513  1.00  1.00           C
ATOM     40  C32 MOL A   1      11.750   8.154  11.989  1.00  1.00           C
ATOM     41  C33 MOL A   1      12.284  10.482  12.524  1.00  1.00           C
ATOM     42  H1  MOL A   1      13.170   9.635   6.837  1.00  1.00           H
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ATOM     43  H2  MOL A   1      11.455   9.224   7.069  1.00  1.00           H
ATOM     44  H3  MOL A   1      11.150  11.595   7.355  1.00  1.00           H
ATOM     45  H4  MOL A   1      14.995  11.280   8.091  1.00  1.00           H
ATOM     46  H5  MOL A   1      12.804  12.140   7.534  1.00  1.00           H
ATOM     47  H6  MOL A   1      12.701   8.352   7.994  1.00  1.00           H
ATOM     48  H7  MOL A   1      12.205  14.506   8.369  1.00  0.00           H
ATOM     49  H8  MOL A   1      14.966   9.504   8.147  1.00  1.00           H
ATOM     50  H9  MOL A   1       7.663  10.724   6.571  1.00  0.00           H
ATOM     51  H10 MOL A   1       5.607  11.022   5.309  1.00  0.00           H
ATOM     52  H11 MOL A   1       9.287  10.479   7.695  1.00  0.00           H
ATOM     53 2H1  MOL A   1      17.059  10.323   9.073  1.00  1.00           H
ATOM     54  H13 MOL A   1      11.205  15.891  10.165  1.00  0.00           H
ATOM     55  H14 MOL A   1       9.588   7.613   8.002  1.00  0.00           H
ATOM     56  H15 MOL A   1       3.291  10.330   8.793  1.00  0.00           H
ATOM     57  H16 MOL A   1       3.420  10.821   6.436  1.00  0.00           H
ATOM     58  H17 MOL A   1      13.566  11.404  10.114  1.00  1.00           H
ATOM     59 8H1  MOL A   1      16.205  11.368  10.235  1.00  1.00           H
ATOM     60  H19 MOL A   1       9.769   5.153   8.011  1.00  0.00           H
ATOM     61  H20 MOL A   1       9.866  14.795  11.946  1.00  0.00           H
ATOM     62  H21 MOL A   1       9.569  12.345  11.940  1.00  0.00           H
ATOM     63  H22 MOL A   1      10.937   3.998   9.875  1.00  0.00           H
ATOM     64 3H2  MOL A   1      16.136   8.283  10.138  1.00  1.00           H
ATOM     65  H24 MOL A   1      13.496   8.370  10.086  1.00  1.00           H
ATOM     66  H25 MOL A   1       3.217   9.921  10.734  1.00  0.00           H
ATOM     67  H26 MOL A   1       3.169   9.427  13.094  1.00  0.00           H
ATOM     68 7H2  MOL A   1      16.960   9.289  11.356  1.00  1.00           H
ATOM     69  H28 MOL A   1       9.115   9.498  12.223  1.00  0.00           H
ATOM     70  H29 MOL A   1      11.881   5.338  11.734  1.00  0.00           H
ATOM     71  H30 MOL A   1       7.413   9.329  13.237  1.00  0.00           H
ATOM     72  H31 MOL A   1       5.266   9.128  14.361  1.00  0.00           H
ATOM     73 2H3  MOL A   1      14.852  10.206  12.144  1.00  1.00           H
ATOM     74 3H3  MOL A   1      12.969  10.161  13.334  1.00  1.00           H
ATOM     75 4H3  MOL A   1      12.534   7.675  12.610  1.00  1.00           H
ATOM     76 5H3  MOL A   1      14.794   8.431  12.199  1.00  1.00           H
ATOM     77 6H3  MOL A   1      10.898   8.296  12.681  1.00  1.00           H
ATOM     78 7H3  MOL A   1      12.637  11.463  12.150  1.00  1.00           H
ATOM     79 8H3  MOL A   1      11.294  10.651  12.990  1.00  1.00           H
END
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