

SUPPLEMENTARY DATA

The assignment and validation of metal oxidation states in the Cambridge Structural Database

GREGORY P. SHIELDS^{a, b} PAUL R. RAITHBY^b FRANK H. ALLEN^a
and W. D. SAMUEL MOTHERWELL^{*a}

^a Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, England

^b Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW England

Email: motherwell@ccdc.cam.ac.uk

A methodology has been developed for the semi-automatic assignment and checking of formal oxidation states for metal atoms in the majority of metallo-organic complexes stored in the Cambridge Structural Database (CSD). The method uses both chemical connectivity and bond length data, *via* ligand donor group templates and bond valence sums respectively. In order to use bond length data, the CSD program QUEST has been modified to allow the coordination sphere of metal atoms to be recalculated using user-defined criteria at search time. The new methodology has been used successfully to validate the +1, +2 and +3 oxidation states in 743 four-coordinate copper complexes in the CSD for which atomic coordinates are available in *ca.* 95% of structures using one or other method, and both succeed for > 86% of structures.

Ligand Templates

The following pages 2-20 comprise the ligand donor template definitions in the query language of the modified CSD Quest3D program used in the study and constitute the instruction set used in the validation procedure.

PRINT 10
 T1 *CONN
 NFRAG -99
 AT1 Cu 0
 NOSCREENS
 ELDEF MM= TR LN AN 1A 2A
 3A
 GE SN PB SB BI PO -B
 ELDEF E= HD C SI N P AS 6A
 7A -PO
 ELDEF FN= HD C SI N 7A
 ELDEF FO= C SI
 ELDEF FY= C SI 6A -PO
 ELDEF FT= HD C SI 7A
 ELDEF FX= HD C SI 6A 7A -
 PO
 ELDEF HS= HD 7A
 ELDEF CN= C N P As
 ELDEF FZ= HD C SI N 6A 7A
 -PO
 ELDEF XZ= 6A -O
 GEOM
 MEXP
 MCHK 0.05
 MECLAC CU C 0.40
 MECLAC CU O 0.80
 MECLAC CU 5A 0.50
 MECLAC CU XZ 0.60
 MECLAC CU 7A 0.60
 COMM etal-carboxylate etc.
 DEFINE TCN1 1
 DEFINE SCN1 1
 DEFINE OXN1 1
 DEFINE BVS1 1
 END
 T245 *CONN
 NFRAG -99
 COMM Halide
 LIG X1 E1 D1
 AT1 MM 1
 AT2 7A 1 T1
 BO 1 2 1
 END
 T2 *CONN
 NFRAG -99
 COMM Ethers, alcohols,
 water
 LIG E2 X0 D1
 AT1 MM 1
 AT2 6A 3 T3
 AT3 FT 1
 AT4 FT 1
 BO 1 2 99
 BO 2 3 1
 BO 2 4 1
 END
 T3 *CONN
 NFRAG -99
 COMM Amine, phosphine,
 arsine, stibine etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 1 T4
 AT3 FT 1 99 0
 AT4 FT 1 99 0
 AT5 FT 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 2 4 1
 BO 2 5 1
 NOLN 1 3 4 5
 END
 T4 *CONN
 NFRAG -99
 COMM Phosphite, etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 4 T4
 AT3 6A 1 T2
 AT4 6A 1 T2
 AT5 6A 1 T2
 AT6 FT 1 99 0
 AT7 FT 1 99 0
 AT8 FT 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 2 4 1
 BO 2 5 1
 BO 3 6 1
 BO 4 7 1
 BO 5 8 1
 END
 T5 *CONN
 NFRAG -99
 COMM Carbonyl
 LIG E2 X0 D1
 AT1 MM 1
 AT2 C 2 T2
 AT3 6A 1 T1
 BO 1 2 99
 BO 2 3 3
 NOLN 1 3
 END
 T6 *CONN
 NFRAG -99
 COMM etal-carboxylate etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 6A 1 T1
 AT4 C 2 T3
 AT5 E 1 99 0
 BO 1 2 99
 BO 2 4 1
 BO 3 4 2
 BO 4 5 1
 NOLN 1 5
 END
 T7 *CONN
 NFRAG -99
 COMM mul-Pyridine, etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 3 T3
 AT3 C 2 T3
 AT4 CN 2
 AT5 CN 2
 AT6 CN 2
 AT7 C 2 T3
 BO 1 2 99
 BO 2 3 5
 BO 3 4 5
 BO 4 5 5
 BO 5 6 5
 BO 6 7 5
 BO 2 7 5
 END
 T8 *CONN
 NFRAG -99
 COMM etal-OC(R)=CR2 etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 FO 2 T3
 AT4 FO 1 T3 99 0
 AT5 FZ 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 3 4 2
 BO 3 5 1
 END
 T9 *CONN
 NFRAG -99
 COMM etal-O=SR2 etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 FY 1 T3
 AT4 FT 1 99 0
 AT5 FT 1 99 0
 BO 1 2 99
 BO 2 3 99
 BO 3 4 1
 BO 3 5 1
 NOLN 1 4 5
 END
 T10 *CONN
 NFRAG -99
 COMM mu2-carboxylate
 LIG X0.5,0.5 E1.5,1.5 D2
 AT1 MM 1
 AT2 MM 1
 AT3 6A 2 T2
 AT4 6A 2 T2
 AT5 C 3 T3
 AT6 FT 1 99 0
 BO 1 3 99
 BO 3 5 99
 BO 5 4 99
 BO 4 2 99
 BO 5 6 1,7
 END
 T11 *CONN
 NFRAG -99
 COMM etal-N(R)=CR2
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 2 T3
 AT3 FT 1
 AT4 C 1 T3
 AT5 FN 1 99 0
 AT6 FN 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 2 4 2
 BO 4 5 1
 BO 4 6 1
 NOLN 1 3 5 6
 END
 T12 *CONN
 NFRAG -99
 COMM etal-N(N=C)=CR2 etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 3 T3
 AT3 C 1 T3
 AT4 5A 1 T2
 AT5 C 1 T3 99 0
 AT6 FN 1 99 0
 AT7 FN 1 99 0
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 BO 4 5 2
 BO 3 6 1
 BO 3 7 1
 END
 T13 *CONN
 COMM Sulphide, selenide
 etc.
 NFRAG -99
 LIG E2 X2 D1
 AT1 MM 1
 AT2 6A 1 T1
 BO 1 2 2
 END
 T14 *CONN
 NFRAG -99
 COMM Alkoxy, etc.

LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 FO 1 T4
 AT4 FX 1 99 0
 AT5 FX 1 99 0
 AT6 FX 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 3 4 1
 BO 3 5 1
 BO 3 6 1
 END
 T15 *CONN
 NFRAG -99
 COMM hydroxide
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 HS 1 T1
 BO 1 2 1
 BO 2 3 1
 END
 T16 *CONN
 NFRAG -99
 COMM eta1-RC/S=O etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 FY 2 T3
 AT3 6A 1 T1
 AT4 E 1
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 NOLN 1 4
 END
 T17 *CONN
 COMM eta1 M...C(R)2=C
 NFRAG -99
 LIG E1 X0 D1
 AT1 MM 1
 AT2 C 2 T4
 AT3 FN 1
 AT4 FX 1 99 0
 AT5 FX 1 99 0
 BO 1 2 9
 BO 2 3 2
 BO 2 4 1
 BO 2 5 1
 END
 T18 *CONN
 COMM eta1-Cyclopentadienyl
 NFRAG -99
 LIG E5 X1 D5
 AT1 MM 1
 AT2 C 3 T4
 AT3 C 3 T4
 AT4 C 3 T4
 AT5 C 3 T4
 AT6 C 3 T4
 AT7 E 1 99 0
 AT8 E 1 99 0
 AT9 E 1 99 0
 AT10 E 1 99 0
 AT11 E 1 99 0
 BO 1 2 9
 BO 1 3 9
 BO 1 4 9
 BO 1 5 9
 BO 1 6 9
 BO 2 3 5
 BO 3 4 5
 BO 4 5 5
 BO 5 6 5
 BO 6 2 5
 BO 2 7 99
 BO 3 8 99
 BO 4 9 99
 BO 5 10 99
 BO 6 11 99
 END
 T19 *CONN
 NFRAG -99
 COMM eta2-carboxylate
 LIG E3 X1 D2
 AT1 MM 2
 AT2 6A 2 T2
 AT3 6A 2 T2
 AT4 C 3 T3
 AT5 FT 1 99 0
 BO 1 2 99
 BO 2 4 99
 BO 3 4 99
 BO 3 1 1
 BO 4 5 1
 END
 T20 *CONN
 NFRAG -99
 COMM -N(OR)=CR2
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 3 T3
 AT3 C 1 T3
 AT4 6A 1 T2
 AT5 E 1 99 0
 AT6 E 1 99 0
 AT7 E 1 99 0
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 BO 4 5 1
 BO 3 6 1
 BO 3 7 1
 END
 T21 *CONN
 NFRAG -99
 COMM mu2-chalcogen
 LIG E1,1 X1,1 D1
 AT1 MM 1
 AT2 MM 1
 AT3 6A 2 T2
 BO 1 3 99
 BO 3 2 99
 END
 T22 *CONN
 NFRAG -99
 COMM -N(O)=CR2
 LIG E1 X1 D1
 AT1 MM 1
 AT2 5A 3 T3
 AT3 C 1 T3
 AT4 6A 1 T1
 AT5 E 1 99 0
 AT6 E 1 99 0
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 BO 3 5 1
 BO 3 6 1
 END
 T23 *CONN
 COMM sigma-Aryl
 NFRAG -99
 LIG E1 X1 D1
 AT1 MM 1
 AT2 C 3 T3
 AT3 C 2
 AT4 C 2
 AT5 C 2
 AT6 C 2
 AT7 C 2
 BO 1 2 1,6

BO 2 3 5
 BO 3 4 5
 BO 4 5 5
 BO 5 6 5
 BO 6 7 5
 BO 2 7 5
 END
 T24 *CONN
 NFRAG -99
 COMM mu2-halide
 LIG E1.5,1.5 X0.5,0.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 7A 2 T2
 BO 1 3 99
 BO 3 2 99
 END
 T25 *CONN
 COMM mul-aryloxy
 NFRAG -99
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 C 3 T3
 AT4 C 1
 AT5 C 1
 BO 1 2 99
 BO 2 3 1
 BO 3 4 5
 BO 3 5 5
 END
 T199 *CONN
 COMM mul-pyridyloxy
 NFRAG -99
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 C 3 T3
 AT4 N 2
 AT5 C 2 T3
 BO 1 2 99
 BO 2 3 1
 BO 3 4 5
 BO 3 5 5
 END
 T26 *CONN
 NFRAG -99
 COMM mul-nitrosyl
 LIG E100 X100 D1
 AT1 MM 1
 AT2 5A 2 T2
 AT3 6A 1 T1
 BO 1 2 99
 BO 2 3 99
 END
 T27 *CONN
 NFRAG -99
 COMM Alkyl, silyl etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 FO 4 T4
 AT3 FX 1
 AT4 FX 1
 AT5 FX 1
 BO 1 2 99
 BO 2 3 1
 BO 2 4 1
 BO 2 5 1
 END
 T198 *CONN
 NFRAG -99
 COMM C(R)2NR2 etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 FO 4 T4
 AT3 5A 1 T3

```

AT4 FX 1          BO 2 3 3          AT7 FX 1 99 0
AT5 FX 1          BO 3 4 1          BO 1 3 99
AT6 FT 1          END               BO 3 2 1
AT7 FT 1          T30 *CONN        BO 3 4 1
BO 1 2 99         NFRAG -99       BO 4 5 1
BO 2 3 1          COMM eta1-S=C(NR2)(R) etc.
BO 2 4 1          LIG E2 X0 D1    BO 4 6 1
BO 2 5 1          AT1 MM 1        BO 4 7 1
BO 3 6 1          AT2 6A 2 T2    END
BO 3 7 1          AT3 FY 3 T3    T34 *CONN
END               AT4 5A 1 T3    NFRAG -99
T28 *CONN         AT5 FT 1        COMM mu2-hydroxide etc.
NFRAG -99         AT6 FN 1        LIG E1.5,1.5 X0.5,0.5 D1
COMM P(R)(OR)2 etc. AT7 FN 1        AT1 MM 1
LIG E2 X0 D1      BO 1 2 99       AT2 MM 1
AT1 MM 1          BO 2 3 2,7     AT3 6A 3 T3
AT2 5A 4 T4       BO 3 4 1,7     AT4 HD 1 T1
AT3 6A 1 T2       BO 3 5 1        BO 1 3 1
AT4 6A 1 T2       BO 4 6 1        BO 3 2 1
AT5 FT 1 99 0     BO 4 7 1        BO 3 4 1
AT6 FT 1 99 0     NOLN 1 5       END
AT7 FT 1 99 0     END               T35 *CONN
BO 1 2 99         T31 *CONN        NFRAG -99
BO 2 3 1          NFRAG -99       COMM O-mu2-OC(R)=C etc.
BO 2 4 1          COMM eta1-N(NR2)=CR2 etc.
BO 2 5 1          LIG E2 X0 D1    LIG E1.5,1.5 X0.5,0.5 D1
BO 3 6 1          AT1 MM 1        AT1 MM 1
BO 4 7 1          AT2 5A 3 T3    AT2 MM 1
END               AT3 C 1 T3    AT3 6A 3 T3
T240 *CONN         AT4 5A 1 T3    AT4 C 1
NFRAG -99         AT5 FN 1 99 0   AT5 6A 1 T1
COMM P(NR2)(OR)2 etc. AT6 FN 1 99 0   AT6 FT 1
LIG E2 X0 D1      AT7 FN 1 99 0   BO 1 3 99
AT1 MM 1          AT8 FN 1 99 0   BO 3 2 99
AT2 5A 4 T4       BO 1 2 99       BO 3 4 1
AT3 6A 1 T2       BO 2 3 2        BO 4 5 2
AT4 6A 1 T2       BO 2 4 1        BO 4 6 1
AT5 5A 3 T3 0     BO 4 5 1       END
AT6 FT 1 99 0     BO 4 6 1       T36 *CONN
AT7 FT 1 99 0     BO 3 7 1       NFRAG -99
AT8 FT 1 99 0     BO 3 8 1       COMM O,O-mu2-carboxylate
AT9 FT 1 99 0     END               etc.
BO 1 2 99         T32 *CONN        LIG E1.5,1.5 X0.5,0.5 D1
BO 2 3 1          NFRAG -99       AT1 MM 1
BO 2 4 1          COMM eta3-allyl  AT2 MM 1
BO 2 5 99         LIG E3 X1 D3    AT3 6A 3 T3
BO 3 6 1          AT1 MM 3        AT4 C 1
BO 4 7 1          AT2 C 2 T4    AT5 C 1 T3
BO 5 8 1          AT3 C 3 T4    AT6 FT 1
BO 5 9 1          AT4 C 2 T4    BO 1 3 99
END               AT5 FX 1        BO 3 2 99
T237 *CONN         AT6 FX 1        BO 3 4 1
NFRAG -99         AT7 FX 1        BO 4 5 2
COMM P(R)2(OR) etc. AT8 FX 1        BO 4 6 1
LIG E2 X0 D1      AT9 FX 1       END
AT1 MM 1          BO 1 2 9         T37 *CONN
AT2 5A 4 T4       BO 2 3 99       COMM mu2-aryloxy
AT3 6A 1 T2       BO 3 4 99       NFRAG -99
AT4 FT 1 99 0     BO 4 1 9        LIG E1.5,1.5 X0.5,0.5 D1
AT5 FT 1 99 0     BO 3 1 9        AT1 MM 1
AT6 FT 1 99 0     BO 2 5 1        AT2 MM 1
BO 1 2 99         BO 2 6 1        AT3 6A 2 T3
BO 2 3 1          BO 3 7 1        AT4 C 3 T3
BO 2 4 1          BO 4 8 1        AT5 CN 1
BO 2 5 1          BO 4 9 1        AT6 CN 1
BO 3 6 1          END               BO 1 3 99
END               T33 *CONN        BO 3 2 99
T29 *CONN         NFRAG -99       BO 3 4 1
COMM -CNR etc.    COMM mu2-alkoxy etc. BO 4 5 5
NFRAG -99         LIG E1.5,1.5 X0.5,0.5 D1 BO 4 6 5
LIG E2 X0 D1      AT1 MM 1       END
AT1 MM 1          AT2 MM 1       T38 *CONN
AT2 5A 2 T2       AT3 6A 3 T3    NFRAG -99
AT3 C 2 T2       AT4 FO 1       COMM terminal hydride
AT4 FN 1          AT5 FX 1 99 0   LIG E1 X1 D1
BO 1 2 99         AT6 FX 1 99 0   AT1 MM 1

```

```

END
T229 *CONN
COMM eta1 M...C(R)=-C
NFRAG -99
LIG E1 X0 D1
AT1 MM 1
AT2 C 2 T3
AT3 FN 1
AT4 FX 1 99 0
BO 1 2 9
BO 2 3 3
BO 2 4 1
END
T39 *CONN
NFRAG -99
COMM eta2 .../-C(R)=X
LIG E1,1 X0,0 D1
AT1 MM 1
AT2 MM 1
AT3 C 3 T4
AT4 E 1
AT5 E 1 99 0
BO 1 3 9
BO 3 2 1
BO 3 4 2
BO 3 5 1
END
T197 *CONN
NFRAG -99
COMM eta2 .../-N(R)=X
LIG E1,2 X0,0 D1
AT1 MM 1
AT2 MM 1
AT3 N 3 T4
AT4 E 1
AT5 E 1 99 0
BO 1 3 9
BO 3 2 1
BO 3 4 2
BO 3 5 1
END
T40 *CONN
NFRAG -99
COMM mu1-eta1-imidazole
LIG E1 X1 D1
AT1 MM 1
AT2 5A 3 T3
AT3 C 2 T3
AT4 N 2 T3
AT5 C 2 T3
AT6 C 2 T3
AT7 FT 1 99 0
AT8 FT 1 99 0
AT9 FN 1 99 0
AT10 FN 1 99 0
BO 1 2 99
BO 2 3 1,5,7
BO 3 4 99
BO 4 5 99
BO 5 6 99
BO 6 2 99
BO 3 7 1
BO 4 8 1
BO 5 9 99
BO 6 10 99
END
T41 *CONN
NFRAG -99
COMM isothiocyanate
LIG E100 X1 D1
AT1 MM 1
AT2 5A 2 T2
AT3 C 2 T2
AT4 6A 1 T1
BO 1 2 99
BO 2 3 99
BO 3 4 99
BO 4 5 99
BO 5 6 99
BO 6 2 99
BO 3 7 1
BO 4 8 1
BO 5 9 99
BO 6 10 99
END
T42 *CONN
NFRAG -99
COMM deloc-diketonate
LIG E3 X1 D2
AT1 MM 1
AT2 6A 2 T2
AT3 6A 2 T2
AT4 C 2 T3
AT5 C 2 T3 99 0
AT6 C 2 T3
AT7 E 1 99 0
AT8 E 1 99 0
AT9 E 1 99 0
BO 1 2 99 C
BO 2 4 7 C
BO 4 5 7 C
BO 5 6 7 C
BO 6 3 7 C
BO 3 1 99 C
BO 4 7 1
BO 5 8 1
BO 6 9 1
END
T43 *CONN
NFRAG -99
COMM eta3-RB(N~N)3
LIG E5 X1 D3
AT1 MM 3
AT2 N 3 T3
AT3 N 3 T3
AT4 N 3 T3
AT5 N 3 T3
AT6 N 3 T3
AT7 N 3 T3
AT8 B 3 T4
AT9 FT 1
BO 1 2 99
BO 2 5 1,5
BO 5 8 1
BO 8 6 1
BO 6 3 1,5
BO 3 1 99
BO 1 4 99
BO 4 7 1,5
BO 7 8 1
BO 8 9 1
END
T44 *CONN
NFRAG -99
COMM mu3-OR etc.
LIG E1.67,1.67,1.67
X0.34,0.34,0.34 D1
AT1 MM 1
AT2 MM 1
AT3 MM 1
AT4 6A 3 T4
AT5 FT 1
BO 1 4 99
BO 4 2 99
BO 4 3 99
BO 4 5 1
END
T45 *CONN
NFRAG -99
COMM eta1-S=C(NR2)2 etc.
LIG E2 X0 D1
AT1 MM 1
AT2 6A 2 T2
AT3 FY 3 T3
AT4 5A 1 T3
AT5 5A 1 T3
AT6 E 1
AT7 E 1
AT8 E 1
AT9 E 1
BO 1 2 99
BO 2 3 2
BO 3 4 1
BO 3 5 1
BO 4 6 1
BO 4 7 1
BO 5 8 1
BO 5 9 1
END
T46 *CONN
NFRAG -99
COMM eta2-carbamate etc.
LIG E3 X1 D2
AT1 MM 2
AT2 6A 2 T2
AT3 6A 2 T2
AT4 C 3 T3
AT5 5A 1 T3 99 0
AT6 E 1 99 0
AT7 E 1 99 0
BO 1 2 99
BO 2 4 99
BO 3 4 99
BO 3 1 1
BO 4 5 99
BO 5 6 1
BO 5 7 1
END
T47 *CONN
NFRAG -99
COMM eta2 .../..C(R)=-X
LIG E1,1 X0,0 D1
AT1 MM 2
AT2 MM 2
AT3 C 3 T4
AT4 E 1
AT5 FX 1 99 0
BO 1 3 9
BO 3 2 9
BO 3 4 3
BO 3 5 1
END
T48 *CONN
NFRAG -99
COMM mu2-CO etc.
LIG E1,1 X0,0 D1
AT1 MM 1
AT2 MM 1
AT3 C 3 T3
AT4 6A 1 T1
BO 1 3 99
BO 3 2 99
BO 3 4 2
END
T49 *CONN
NFRAG -99
COMM eta6-aryl
LIG E6 X0 D1
AT1 MM 1
AT2 C 3
AT3 C 2
AT4 C 2
AT5 C 2
AT6 C 2
AT7 C 2
BO 1 2 9
BO 2 3 5
BO 3 4 5
BO 4 5 5
BO 5 6 5
BO 6 7 5
BO 7 2 5
NOLN 1 3 7
END
T50 *CONN

```

NFRAG -99
 COMM terminal cyanide,etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 C 2 T2
 AT3 5A 1 T1
 BO 1 2 99
 BO 2 3 3
 NOLN 1 3
 END
 T51 *CONN
 NFRAG -99
 COMM thiocyanate etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 C 2 T2
 AT4 5A 1 T1
 BO 1 2 99
 BO 2 3 1
 BO 3 4 3
 END
 T52 *CONN
 NFRAG -99
 COMM mu2-ethers, alcohols,
 water etc.
 LIG E2,2 X0,0 D1
 AT1 MM 1
 AT2 MM 1
 AT3 6A 2 T4
 AT4 FT 1
 AT5 FT 1
 BO 1 3 99
 BO 2 3 99
 BO 3 4 1
 BO 3 5 1
 END
 T53 *CONN
 NFRAG -99
 COMM eta1-RC=NR2 etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 C 2 T3
 AT3 5A 1 T3
 AT4 FX 1
 AT5 FX 1
 AT6 FX 1
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 BO 3 5 1
 BO 3 6 1
 NOLN 1 3
 END
 T54 *CONN
 COMM isocyanate
 NFRAG -99
 LIG E2 X0 D1
 AT1 MM 1
 AT2 C 2 T2
 AT3 5A 2 T2
 AT4 E 1
 BO 1 2 99
 BO 2 3 3
 BO 3 4 1
 END
 T55 *CONN
 NFRAG -99
 COMM mu2-PR2 etc
 LIG E1.5,1.5 X0.5,0.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 5A 4 T4
 AT4 FT
 AT5 FT
 BO 1 3 99
 BO 3 2 99
 BO 3 5 1
 END
 T56 *CONN
 NFRAG -99
 COMM mu2-hydride
 LIG E0.5,0.5 X0.5,0.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 HD 2 T2
 BO 1 3 1
 BO 3 2 1
 END
 T57 *CONN
 NFRAG -99
 COMM eta1-NR
 LIG E101 X2 D1
 AT1 MM 1
 AT2 5A 1 T2
 AT3 FT 1
 BO 1 2 99
 BO 2 3 1
 END
 T58 *CONN
 NFRAG -99
 COMM N(C(R)=C)2 etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 5A 1 T3
 AT3 C 2 T3
 AT4 C 2 T3
 AT5 C 1 T3 99 0
 AT6 C 1 T3 99 0
 AT7 FN 1 99 0
 AT8 FN 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 2 4 1
 BO 3 5 99
 BO 4 6 99
 BO 3 7 1,5
 BO 4 8 1,5
 END
 T59 *CONN
 NFRAG -99
 COMM eta2-O~C~NR etc
 LIG E1.5,1.5 X0.5,0.5 D2
 AT1 MM 1
 AT2 MM 1
 AT3 6A 2 T2
 AT4 N 2 T3
 AT5 C 2 T3
 AT6 E 1 99 0
 AT7 E 1 99 0
 BO 1 3 99
 BO 3 5 99
 BO 5 4 99
 BO 4 2 99
 BO 5 7 1
 BO 4 6 1
 END
 T60 *CONN
 NFRAG -99
 COMM N(CR3)2 etc.
 LIG E100 X1 D1
 AT1 MM 1
 AT2 5A 3 T3
 AT3 FO 1 T4
 AT4 FO 1 T4
 AT5 FN 1 99 0
 AT6 FN 1 99 0
 AT7 FN 1 99 0
 AT8 FN 1 99 0
 AT9 FN 1 99 0
 AT10 FN 1 99 0
 BO 1 2 99
 BO 2 3 7
 BO 3 4 7
 BO 4 5 7
 BO 5 6 7
 BO 3 1 9
 BO 4 1 9
 BO 5 1 9
 BO 6 1 9
 BO 2 7 1
 BO 2 8 1
 BO 6 9 1
 BO 6 10 1
 NOLN 2 6
 END
 T61 *CONN
 NFRAG -99
 COMM mu3-phosphinidine
 etc.
 LIG E1.34,1.34,1.34
 X0.67,0.67,0.67 D1
 AT1 MM 2
 AT2 MM 2
 AT3 MM 2
 AT4 5A 3 T4
 AT5 FT 1
 BO 1 4 9
 BO 4 2 9
 BO 3 4 9
 BO 4 5 1
 END
 T62 *CONN
 NFRAG -99
 COMM eta1-hydrazine etc.
 LIG E2 X0 D1
 AT1 MM 2
 AT2 5A 2 T4
 AT3 5A 1 T3
 AT4 FT 1 99 0
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 AT7 FT 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 2 4 1
 BO 2 5 1
 BO 3 6 1
 BO 3 7 1
 END
 T63 *CONN
 NFRAG -99
 COMM eta5-pentadienyl
 LIG E5 X1 D5
 AT1 MM 5
 AT2 C 2 T4
 AT3 C 3 T4
 AT4 C 3 T4
 AT5 C 3 T4
 AT6 C 2 T4
 AT7 FX 1
 AT8 FX 1
 AT9 FX 1
 AT10 FX 1
 BO 1 2 9
 BO 2 3 7
 BO 3 4 7
 BO 4 5 7
 BO 5 6 7
 BO 3 1 9
 BO 4 1 9
 BO 5 1 9
 BO 6 1 9
 BO 2 7 1
 BO 2 8 1
 BO 6 9 1
 BO 6 10 1
 NOLN 2 6
 END
 T64 *CONN
 NFRAG -99
 COMM eta1-N(R)=NR

```

LIG X0 E2 D1          BO 3 5 1          BO 3 2 99
AT1 MM 1              BO 4 6 1          BO 3 4 1
AT2 5A 2 T3           NOLN 1 4 5        END
AT3 5A 1 T2           END
AT4 FT 1 99 0         T236 *CONN
AT5 FT 1 99 0         NFRAG -99
BO 1 2 99             COMM eta1-N(C(R)=O)2
BO 2 3 2              LIG E100 X1 D1
BO 2 4 1              AT1 MM 1
BO 3 5 1              AT2 5A 3 T3
END                  AT3 C 2 T3
T65 *CONN             AT4 6A 1 T1
NFRAG -99             AT5 C 2 T3
COMM Carbene          AT6 6A 1 T1
LIG E2 X2 D1          AT7 FN 1 99 0
AT1 MM 1              AT8 FN 1 99 0
AT2 C 3 T3            BO 1 2 99
AT3 FT 1 99 0         BO 2 3 1
AT4 FT 1 99 0         BO 3 4 2
BO 1 2 2              BO 2 5 1
BO 2 3 1              BO 5 6 2
BO 2 4 1              BO 3 7 1
END                  BO 5 8 1
T66 *CONN             END
NFRAG -99             T235 *CONN
COMM Carbene (alpha-OR) NFRAG -99
LIG E2 X2 D1          COMM eta1-N(C(R)=C)C(R)=O
AT1 MM 1              LIG E100 X1 D1
AT2 C 3 T3            AT1 MM 1
AT3 6A 1 T2            AT2 5A 3 T3
AT4 FT 1 99 0          AT3 C 2 T3
AT5 FT 1 99 0          AT4 6A 1 T1
BO 1 2 2              AT5 C 2 T3
BO 2 3 1              AT6 FZ 1 99
BO 2 4 1              AT7 FN 1 99 0
BO 3 5 1              AT8 FN 1 99 0
END                  BO 1 2 99
T67 *CONN             BO 2 3 1,7
NFRAG -99             BO 3 4 2,7
COMM eta4-deloc-butadiene BO 2 5 1
LIG E4 X0 D4          BO 3 6 1
AT1 MM 5              BO 5 7 99
AT2 C 2 T4            BO 5 8 99
AT3 C 3 T4            END
AT4 C 3 T4            T234 *CONN
AT5 C 2 T4            NFRAG -99
AT6 FX 1 99 0          COMM eta1-N(CR3)C(R)=O
AT7 FX 1 99 0          LIG E100 X1 D1
AT8 FX 1 99 0          AT1 MM 1
AT9 FX 1 99 0          AT2 5A 2 T3
BO 1 2 9              AT3 C 2 T3
BO 2 3 7              AT4 6A 1 T1
BO 3 4 7              AT5 C 1 T4
BO 4 5 7              AT6 FN 1 99 0
BO 3 1 9              AT7 FN 1 99 0
BO 4 1 9              AT8 FN 1 99 0
BO 5 1 9              AT9 FN 1 99 0
BO 2 6 1              BO 1 2 99
BO 2 7 1              BO 2 3 1,7
BO 5 8 1              BO 3 4 2,7
BO 5 9 1              BO 2 5 1
NOLN 2 5              BO 3 6 1
END                  BO 5 7 1
T68 *CONN             BO 5 8 1
NFRAG -99             BO 5 9 1
COMM eta1-O=C(R)OR etc. END
LIG E2 X0 D1          T69 *CONN
AT1 MM 1              NFRAG -99
AT2 6A 2 T2           COMM mu2-phosphinidine
AT3 FY 1 T3            etc.
AT4 6A 1 T2 99 0       LIG E100,100,X1,1 D1
AT5 FN 1 99 0          AT1 MM 1
AT6 FX 1               AT2 MM 1
BO 1 2 99              AT3 5A 3 T3
BO 2 3 2               AT4 FT 1
BO 3 4 1               BO 1 3 99

```

AT1 MM 1
 AT2 MM 2
 AT3 6A 2 T2
 AT4 5A 3 T3
 AT5 6A 1 T2
 AT6 6A 1 T1
 BO 1 3 99
 BO 3 4 99
 BO 4 5 99
 BO 4 6 99
 BO 5 2 99
 END
 T75 *CONN
 COMM Carbyne
 NFRAG -99
 LIG E3 X3 D1
 AT1 MM 1
 AT2 C 2 T2
 AT3 FT 1
 BO 1 2 3
 BO 2 3 1
 END
 T76 *CONN
 NFRAG -99
 COMM eta1-N=N-R
 LIG E100 X1 D1
 AT1 MM 1
 AT2 5A 2 T2
 AT3 5A 1 T2
 AT4 FT 1
 BO 1 2 99
 BO 2 3 2,3
 BO 3 4 1
 END
 T77 *CONN
 NFRAG -99
 COMM O-pyridine oxide,
 etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 5A 3
 AT4 C 2
 AT5 CN 2
 AT6 CN 2
 AT7 CN 2
 AT8 C 2
 BO 1 2 99
 BO 2 3 1
 BO 3 4 5
 BO 4 5 5
 BO 5 6 5
 BO 6 7 5
 BO 7 8 5
 BO 8 3 5
 END
 T213 *CONN
 NFRAG -99
 COMM mu3-RC...C
 LIG E0.67,0.67,0.67 X0,0,0
 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 C 4 T5
 AT5 FT 1
 AT6 C 1
 BO 1 4 99
 BO 4 2 99
 BO 4 3 99
 BO 4 5 1
 BO 4 6 99
 END
 T78 *CONN
 NFRAG -99
 COMM Carbene (alpha-NR2)

LIG E2 X2 D1
 AT1 MM 1
 AT2 C 3 T3
 AT3 5A 1 T3
 AT4 FT 1 99 0
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 BO 1 2 2
 BO 2 3 1
 BO 2 4 1
 BO 3 5 1
 BO 3 6 1
 END
 T79 *CONN
 COMM N-nitrite
 NFRAG -99
 LIG E1 X1 D1
 AT1 MM 1
 AT2 N 3 T3
 AT3 6A 1 T1
 AT4 6A 1 T1
 BO 1 2 99
 BO 2 3 99
 BO 2 4 99
 END
 T80 *CONN
 NFRAG -99
 COMM mu2-carbyne etc.
 LIG E1.5,1.5 X1.5,1.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 C 2 T3
 AT4 E 1
 BO 1 3 99
 BO 3 2 99
 BO 3 4 1
 END
 T81 *CONN
 NFRAG -99
 COMM eta1-sulphate etc.
 LIG E2 X2 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 FY 4 T4
 AT4 FY 1 T1
 AT5 FY 1 T1
 AT6 6A 1 T1
 BO 1 2 99
 BO 2 3 99
 BO 3 4 99
 BO 3 5 99
 BO 3 6 99
 END
 T220 *CONN
 COMM eta1-dioxygen
 NFRAG -99
 LIG E99 X99 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 6A 1 T1
 BO 1 2 1
 BO 2 3 99
 END
 T82 *CONN
 COMM eta1-polychalcogen
 etc.
 NFRAG -99
 LIG E1 X1 D1
 AT1 MM 2
 AT2 6A 2 T2
 AT3 6A 2 T2
 AT4 FX 1
 BO 1 2 99
 BO 2 3 1
 BO 3 4 1
 END

T83 *CONN
 NFRAG -99
 COMM mu3-chalcogen
 LIG E1.34,1.34,1.34
 X0.67,0.67,0.67 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 6A 3 T3
 BO 1 4 1
 BO 4 2 1
 BO 4 3 1
 END
 T84 *CONN
 NFRAG -99
 COMM mu4-chalcogen
 LIG E100,100,100,100
 X0.5,0.5,0.5,0.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 MM 1
 AT5 6A 4 T4
 BO 1 5 1
 BO 5 2 1
 BO 5 3 1
 BO 5 4 1
 END
 T85 *CONN
 NFRAG -99
 COMM eta2 ..-/C=-C
 LIG E1,1 X0.5,0.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 C 3 T3
 AT4 C 1
 BO 1 3 1
 BO 3 2 9
 BO 3 4 3
 END
 T86 *CONN
 NFRAG -99
 COMM mu2-pyrazole
 LIG E1.5,1.5 X0.5,0.5 D2
 AT1 MM 1
 AT2 MM 2
 AT3 N 3 T3
 AT4 N 3 T3
 AT5 C 2 T3
 AT6 C 2 T3
 AT7 C 2 T3
 BO 1 3 99
 BO 3 5 5,2
 BO 5 6 5,1
 BO 6 7 5,2
 BO 7 4 5,1
 BO 4 2 99
 BO 4 3 5,1
 END
 T87 *CONN
 NFRAG -99
 COMM eta2-Carbonate,
 Sulphite etc.
 LIG E2 X2 D2
 AT1 MM 2
 AT2 6A 2 T2
 AT3 6A 2 T2
 AT4 FY 3 T3
 AT5 FY 1
 BO 1 2 99
 BO 2 4 1,7
 BO 4 3 1,7
 BO 3 1 1
 BO 4 5 2
 END
 T88 *CONN

NFRAG -99
 COMM O-p-tosyl etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 6A 4 T4
 AT4 6A 1 T1
 AT5 6A 1 T1
 AT6 FT 1
 BO 1 2 1
 BO 2 3 1
 BO 3 4 2
 BO 3 5 2
 BO 3 6 1
 END
 T89 *CONN
 NFRAG -99
 COMM eta1-P(R)2=S etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 P 2 T4
 AT3 6A 1 T1
 AT4 E 1 99 0
 AT5 E 1 99 0
 BO 1 2 99
 BO 2 3 1,2
 BO 2 4 1
 BO 2 5 1
 END
 T90 *CONN
 NFRAG -99
 COMM eta1-cyclobutadiene
 LIG E4 X0 D1
 AT1 MM 1
 AT2 C 3 T4
 AT3 C 2 T3
 AT4 C 2 T3
 AT5 C 2 T3
 AT6 E 1
 AT7 E 1
 AT8 E 1
 AT9 E 1
 BO 1 2 9
 BO 2 3 5,7
 BO 3 4 5,7
 BO 4 5 5,7
 BO 5 2 5,7
 BO 2 6 1
 BO 3 7 1
 BO 4 8 1
 BO 5 9 1
 END
 T216 *CONN
 NFRAG -99
 COMM mu2-imidazole
 LIG E1.5,1.5 X0.5,0.5 D2
 AT1 MM 1
 AT2 MM 2
 AT3 N 3 T3
 AT4 C 2 T3
 AT5 N 3 T3
 AT6 C 2 T3
 AT7 C 2 T3
 AT8 FT 1
 BO 1 3 99
 BO 3 6 5
 BO 6 7 5
 BO 7 5 5
 BO 5 4 5
 BO 5 2 99
 BO 4 3 5
 BO 4 8 1
 END
 T208 *CONN
 NFRAG -99

COMM sigma-pyrazole (non-deloc.)
 LIG E1 X1 D1
 AT1 MM 1
 AT2 N 3 T3
 AT3 C 2 T3
 AT4 N 2
 AT5 C 2 T3
 AT6 C 2 T3
 AT7 FT 1
 BO 1 2 99
 BO 2 5 1 C
 BO 5 6 2 C
 BO 6 4 1 C
 BO 4 3 2 C
 BO 3 2 1 C
 BO 3 7 1
 END
 T91 *CONN
 NFRAG -99
 COMM pi-sigma
 cyclopentadienyl
 LIG E1,5 X1,1 D2
 AT1 MM 1
 AT2 MM 1
 AT3 C 3 T3
 AT4 C 2
 AT5 C 2
 AT6 C 2
 AT7 C 2
 BO 1 3 1
 BO 3 4 5
 BO 4 5 5
 BO 5 6 5
 BO 6 7 5
 BO 7 3 5
 BO 2 7,4,5,6 9
 END
 T231 *CONN
 COMM eta1-cycloheptatriene
 LIG X-1 E7 D1
 NFRAG -99
 AT1 MM 1
 AT2 C 3 T4
 AT3 C 2 T3
 AT4 C 2 T3
 AT5 C 2 T3
 AT6 C 2 T3
 AT7 C 2 T3
 AT8 C 2 T3
 BO 1 2 9
 BO 2 3 99 C
 BO 3 4 99 C
 BO 4 5 99 C
 BO 5 6 99 C
 BO 6 7 99 C
 BO 7 8 99 C
 BO 2 8 99 C
 END
 T92 *CONN
 NFRAG -99
 COMM HMPA etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 5A 4 T4
 AT4 5A 1 T3
 AT5 5A 1 T3
 AT6 5A 1 T3
 BO 1 2 99
 BO 2 3 1,2
 BO 3 4 1
 BO 3 5 1
 BO 3 6 1
 END
 T93 *CONN

NFRAG -99
 COMM mu2-eta2,eta2-dichalcogen
 LIG E3,3 X1,1 D2
 AT1 MM 2
 AT2 MM 2
 AT3 6A 3 T3
 AT4 6A 3 T3
 BO 1 4 1
 BO 4 2 1
 BO 2 3 1
 BO 3 1 1
 BO 3 4 1
 END
 T94 *CONN
 NFRAG -99
 COMM eta2-O~C~NR etc
 LIG E3 X1 D2
 AT1 MM 2
 AT2 6A 2 T2
 AT3 N 2 T3
 AT4 C 2 T3
 AT5 FX 1 99 0
 AT6 FX 1 99 0
 BO 1 2 99
 BO 2 4 99
 BO 4 3 99
 BO 3 1 1
 BO 3 5 1
 BO 4 6 1
 END
 T95 *CONN
 NFRAG -99
 COMM ||-mu2-O=CR
 LIG E1,2 X1,0 D2
 AT1 MM 1
 AT2 MM 1
 AT3 C 2 T3
 AT4 6A 2 T2
 AT5 FT 1 99 0
 BO 1 3 99
 BO 3 4 99
 BO 4 2 99
 BO 3 5 1
 END
 T96 *CONN
 NFRAG -99
 COMM ||-mu2-acetylene
 LIG E1,1 X0,0 D2
 AT1 MM 1
 AT2 MM 1
 AT3 C 2 T3 99 0
 AT4 C 2 T3 99 0
 AT5 FX 1 99 0
 AT6 FX 1 99 0
 BO 1 3 1
 BO 3 4 2
 BO 4 2 1
 BO 3 5 1
 BO 4 6 1
 END
 T238 *CONN
 NFRAG -99
 COMM eta2-N,N-RN~C~C~NR
 LIG E3 X1 D2
 AT1 MM 2
 AT2 N 2 T3
 AT3 N 2 T3
 AT4 C 2
 AT5 C 2
 AT6 C 2
 AT7 FT 1
 AT8 FT 1
 AT9 E 1
 BO 1 2 99
 BO 2 4 7

BO 4 5 7
 BO 5 6 7
 BO 6 3 7
 BO 3 1 99
 BO 2 7 1
 BO 3 8 1
 BO 5 9 1
 END
 T97 *CONN
 NFRAG -99
 COMM eta1=N-NR2
 LIG E101 X1 D1
 AT1 MM 1
 AT2 5A 2 T2
 AT3 5A 1 T3
 AT4 FT 1
 AT5 FT 1
 BO 1 2 99
 BO 2 3 1,2
 BO 3 4 1
 BO 3 5 1
 END
 T98 *CONN
 NFRAG -99
 COMM mu2=carbene etc.
 LIG E1,1 X1,1 D1
 AT1 MM 1
 AT2 MM 1
 AT3 FO 2 T4
 AT4 FX 1
 AT5 FX 1
 BO 1 3 1
 BO 3 2 1
 BO 3 4 1
 BO 3 5 1
 END
 T228 *CONN
 NFRAG -99
 COMM sigma-vinyl(alpha-R)
 LIG E1 X1 D1
 AT1 MM 1
 AT2 C 2 T3
 AT3 C 1 T3
 AT4 FT 1
 AT5 E 1
 AT6 E 1
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 BO 3 5 1
 BO 3 6 1
 END
 T99 *CONN
 NFRAG -99
 COMM mu3=hydride
 LIG E0.34,0.34,0.34
 X0.34,0.34,0.34 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 HD 3 T3
 BO 1 4 1
 BO 4 2 1
 BO 4 3 1
 END
 T100 *CONN
 COMM N(H)aryl
 NFRAG -99
 LIG E1 X1 D1
 AT1 MM 1
 AT2 5A 2 T3
 AT3 HD 1 T1
 AT4 C 3 T3
 AT5 C 1
 AT6 C 1
 BO 1 2 99

BO 2 3 1
 BO 2 4 1
 BO 4 5 5 C
 BO 4 6 5 C
 END
 T101 *CONN
 NFRAG -99
 COMM eta1-cyclo-octatetraene
 LIG E8 X2 D1
 AT1 MM 1
 AT2 C 3 T4
 AT3 C 2 T3
 AT4 C 2 T3
 AT5 C 2 T3
 AT6 C 2 T3
 AT7 C 2 T3
 AT8 C 2 T3
 AT9 C 2 T3
 BO 1 2 9
 BO 2 3 5,7
 BO 3 4 5,7
 BO 4 5 5,7
 BO 5 6 5,7
 BO 6 7 5,7
 BO 7 8 5,7
 BO 8 9 5,7
 BO 9 2 5,7
 NOLN 2 3 4 5 6 7 8 9
 END
 T102 *CONN
 NFRAG -99
 COMM mu3=carbonyl etc.
 LIG E0.67,0.67,0.67 X0,0,0
 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 C 4 T4
 AT5 6A 1 T1
 BO 1 4 99
 BO 4 2 99
 BO 4 3 99
 BO 4 5 99
 END
 T103 *CONN
 NFRAG -99
 COMM O,O eta2-ON(R)C(R)O
 LIG E3 X1 D2
 AT1 MM 1
 AT2 6A 2 T2
 AT3 N 2 T3
 AT4 C 2 T3
 AT5 6A 2 T2
 AT6 FT 1
 AT7 FT 1
 BO 1 2 99
 BO 2 3 99
 BO 3 4 99
 BO 4 5 99
 BO 5 1 99
 BO 3 6 1,5
 BO 4 7 1,5
 END
 T104 *CONN
 COMM =Cumulene
 NFRAG -99
 LIG E2 X2 D1
 AT1 MM 1
 AT2 C 2 T2
 AT3 C 2
 BO 1 2 2
 BO 2 3 2
 END
 T105 *CONN
 COMM eta1-dinitrogen

NFRAG -99
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 2 T2
 AT3 5A 1 T1
 BO 1 2 1,2
 BO 2 3 2,3
 END
 T106 *CONN
 NFRAG -99
 COMM eta2-sigma,sigma-RNCNR.
 LIG E3 X1 D2
 AT1 MM 2
 AT2 5A 2 T3
 AT3 5A 2 T3
 AT4 C 2 T3
 AT5 E 1
 AT6 E 1
 AT7 E 1
 BO 1 2 1
 BO 2 4 99
 BO 4 3 99
 BO 3 1 1
 BO 2 5 1
 BO 3 6 1
 BO 4 7 1
 END
 T107 *CONN
 NFRAG -99
 COMM eta1-C-(R2C)PR3
 LIG E2 X0 D1
 AT1 MM 2
 AT2 C 2 T4
 AT3 5A 2 T4
 AT4 FT 1
 AT5 FT 1
 AT6 FT 1
 AT7 FT 1 99 0
 AT8 FT 1 99 0
 BO 1 2 1 A
 BO 2 3 1 A
 BO 3 4 1
 BO 3 5 1
 BO 3 6 1
 BO 2 7 1
 BO 2 8 1
 END
 T108 *CONN
 NFRAG -99
 COMM mu2-C,C'-(CR2)2PR2
 etc.
 LIG E1.5,1.5 X0.5,0.5 D2
 AT1 MM 1
 AT2 MM 1
 AT3 C 2 T4
 AT4 5A 4 T4
 AT5 C 2 T4
 AT6 FT 1 99 0
 AT7 FT 1 99 0
 AT8 FT 1 99 0
 AT9 FT 1 99 0
 AT10 FT 1 99 0
 AT11 FT 1 99 0
 BO 1 3 1
 BO 3 4 1
 BO 4 5 1
 BO 5 2 1
 BO 4 6 1
 BO 4 7 1
 BO 3 8 1
 BO 3 9 1
 BO 5 10 1
 BO 5 11 1
 END
 T109 *CONN

NFRAG -99
 COMM N,O-eta2-R2N-O etc.
 LIG E2 X0 D2
 AT1 MM 2
 AT2 5A 2 T4
 AT3 6A 2 T2
 AT4 FT 1 99 0
 AT5 FT 1 99 0
 BO 1 2 99
 BO 2 3 1,2
 BO 3 1 99
 BO 2 4 1
 BO 2 5 1
 END
 T110 *CONN
 NFRAG -99
 COMM eta2-R2N-CR2 etc.
 LIG E3 X1 D2
 AT1 MM 2
 AT2 5A 2 T4
 AT3 C 2 T4
 AT4 FT 1 99 0
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 AT7 FT 1 99 0
 BO 1 2 1
 BO 2 3 1
 BO 3 1 1
 BO 2 4 1
 BO 2 5 1
 BO 3 6 1
 BO 3 7 1
 END
 T111 *CONN
 NFRAG -99
 COMM ||-mu2-O-N=CR2
 LIG E2,1 X0,1 D2
 AT1 MM 1
 AT2 MM 1
 AT3 5A 2 T3
 AT4 6A 2 T2
 AT5 C 1 T3
 AT6 FT 1 99 0
 AT7 FT 1 99 0
 BO 1 3 1
 BO 3 4 99
 BO 4 2 1
 BO 3 5 99
 BO 5 6 1
 BO 5 7 1
 END
 T112 *CONN
 NFRAG -99
 COMM eta2-sulphate etc.
 LIG E2 X2 D2
 AT1 MM 2
 AT2 6A 2 T2
 AT3 6A 4 T4
 AT4 6A 2 T2
 AT5 FY 1
 AT6 FY 1
 BO 1 2 99
 BO 2 4 1
 BO 4 3 1
 BO 3 1 1
 BO 3 5 2
 BO 3 6 2
 NOCR 1
 END
 T217 *CONN
 NFRAG -99
 COMM mu1,mu2-carboxylate
 LIG E1.67,1.67,1.67
 X0.34,0.34,0.34 D2
 AT1 MM 1
 AT2 MM 1

AT3 MM 1
 AT4 6A 3 T3
 AT5 6A 2 T2
 AT6 C 2 T3
 AT7 FT 1 99 0
 BO 1 4 99
 BO 4 2 99
 BO 4 6 99
 BO 6 5 99
 BO 5 3 99
 BO 6 7 1
 END
 T113 *CONN
 NFRAG -99
 COMM mu2-carbamate etc.
 LIG E1.5,1.5 X0.5,0.5 D2
 AT1 MM 1
 AT2 MM 1
 AT3 6A 2 T2
 AT4 6A 2 T2
 AT5 C 3 T3
 AT6 5A 1 T3 99 0
 AT7 E 1 99 0
 AT8 E 1 99 0
 BO 1 3 99
 BO 3 5 99
 BO 5 4 99
 BO 4 2 99
 BO 5 6 99
 BO 6 7 1
 BO 6 8 1
 END
 T114 *CONN
 NFRAG -99
 COMM eta2-O,N-RN~C~C~C~O
 LIG E3 X1 D2
 AT1 MM 2
 AT2 N 2 T3
 AT3 6A 2 T2
 AT4 C 2
 AT5 C 2
 AT6 C 2
 AT7 E
 BO 1 2 99
 BO 2 4 7
 BO 4 5 7
 BO 5 6 7
 BO 6 3 7
 BO 3 1 99
 BO 2 7 1
 END
 T222 *CONN
 NFRAG -99
 COMM eta5-pentadienyl-cy6
 LIG E5 X0 D5
 AT1 MM 5
 AT2 C 2 T4
 AT3 C 3 T4
 AT4 C 3 T4
 AT5 C 3 T4
 AT6 C 3 T4
 AT7 C 2 T4
 AT8 FX 1
 AT9 FX 1
 BO 1 2 9
 BO 2 3 7 C
 BO 3 4 7 C
 BO 4 5 7 C
 BO 5 6 7 C
 BO 6 7 7 C
 BO 7 2 7 C
 BO 3 1 9
 BO 4 1 9
 BO 5 1 9
 BO 6 1 9
 BO 7 8 1

BO 7 9 1
 END
 T115 *CONN
 NFRAG -99
 COMM eta2-borohydride
 LIG E1 X1 D2
 AT1 MM 2
 AT2 HD 2 T2
 AT3 HD 2 T2
 AT4 B 0
 AT5 HD 1 T1
 AT6 HD 1 T1
 BO 1 2 1
 BO 2 4 1
 BO 4 3 1
 BO 3 1 1
 BO 4 5 1
 BO 4 6 1
 END
 T116 *CONN
 NFRAG -99
 COMM -O(-)
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 1 T1 99 -1
 BO 1 2 1
 END
 T117 *CONN
 NFRAG -99
 COMM etal-azide
 LIG E100 X1 D1
 AT1 MM 1
 AT2 5A 2 T2
 AT3 5A 2 T2
 AT4 5A 1 T1
 BO 1 2 99
 BO 2 3 99
 BO 3 4 99
 END
 T118 *CONN
 NFRAG -99
 COMM ||-mu2-RN=CR
 LIG E1,2 X1,0 D2
 AT1 MM 1
 AT2 MM 1
 AT3 C 2 T3
 AT4 5A 2 T3
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 BO 1 3 1
 BO 3 4 2
 BO 4 2 1
 BO 3 5 1
 BO 4 6 1
 END
 T119 *CONN
 NFRAG -99
 COMM mu3-P etc.
 LIG E1,1,1 X1,1,1 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 3
 AT4 5A 3 T3
 BO 1 4 1
 BO 4 2 1
 BO 4 3 1
 END
 T120 *CONN
 NFRAG -99
 COMM Nitride, Phosphide etc.
 LIG E3 X3 D1
 AT1 MM 1
 AT2 5A 1 T1
 BO 1 2 3
 END

T121 *CONN
 NFRAG -99
 COMM O-PR3 etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 5A 1 T4
 AT4 FT 1 99 0
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 BO 1 2 99
 BO 2 3 1,2
 BO 3 4 1
 BO 3 5 1
 BO 3 6 1
 NOLN 1 4 5 6
 END
 T122 *CONN
 NFRAG -99
 COMM N-Pyrazine,etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT3 N 3
 AT4 C 2
 AT5 C 2
 AT6 N 2 T2
 AT7 C 2
 AT8 C 2
 BO 1 3 99
 BO 3 4 5 C
 BO 4 5 5 C
 BO 5 6 5 C
 BO 6 7 5 C
 BO 7 8 5 C
 BO 8 3 5 C
 END
 T123 *CONN
 NFRAG -99
 COMM N-Pyrimidine,etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT3 N 3
 AT4 C 2 T3
 AT5 N 2 T2
 AT6 C 2
 AT7 C 2
 AT8 C 2 T3
 AT9 FT 1
 AT10 FT 1
 BO 1 3 99
 BO 3 4 5 C
 BO 4 5 5 C
 BO 5 6 5 C
 BO 6 7 5 C
 BO 7 8 5 C
 BO 8 3 5 C
 BO 4 9 1
 BO 8 10 1
 END
 T124 *CONN
 NFRAG -99
 COMM O,C-eta2-O=CR
 LIG E3 X1 D2
 AT1 MM 1
 AT2 C 2 T3
 AT3 O 2 T2
 AT4 FT 1 99 0
 BO 1 2 1,9
 BO 2 3 1,2
 BO 3 1 1,9
 BO 2 4 1
 END
 T125 *CONN
 NFRAG -99
 COMM mu3-alkoxymethylidene
 LIG E1,1,1 X1,1,1 D1

AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 FO 3 T4
 AT5 6A 1 T2
 AT6 FT 1
 BO 1 4 99
 BO 4 2 1
 BO 4 3 1
 BO 4 5 1
 BO 5 6 1
 END
 T126 *CONN
 NFRAG -99
 COMM etal ... (C=)C(=C)
 LIG E1 X0 D1
 AT1 MM 1
 AT2 C 3 T3
 AT3 C 1
 AT4 C 1
 BO 1 2 9
 BO 2 3 2
 BO 2 4 2
 END
 T127 *CONN
 NFRAG -99
 COMM sigma-vinyl(alpha OR)
 LIG E1 X1 D1
 AT1 MM 1
 AT2 C 2 T3
 AT3 C 1 T3
 AT4 6A 1 T2
 AT5 E 1
 AT6 E 1
 AT7 FT 1
 BO 1 2 1
 BO 2 3 2
 BO 2 4 1
 BO 3 5 1
 BO 3 6 1
 BO 4 7 1
 END
 T128 *CONN
 NFRAG -99
 COMM C(NR2)=NR2
 LIG E2 X0 D1
 AT1 MM 1
 AT2 C 3 T3
 AT3 5A 1 T3
 AT4 5A 1 T3
 AT5 FT 1
 AT6 FT 1
 AT7 FT 1
 AT8 FT 1
 BO 1 2 99
 BO 2 3 99
 BO 2 4 1,5,7
 BO 3 5 1
 BO 3 6 1
 BO 4 7 1
 BO 4 8 1
 END
 T129 *CONN
 NFRAG -99
 COMM etal-N(R)=O
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 2 T3
 AT3 6A 1 T1
 AT4 FT 1 99 0
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 END
 T130 *CONN
 NFRAG -99

COMM mu2-Pyridazine,etc.
 LIG E2,2 X0,0 D2
 AT1 MM 1
 AT2 MM 1
 AT3 N 3
 AT4 N 3
 AT5 C 2
 AT6 C 2
 AT7 C 2
 AT8 C 2
 BO 1 3 99
 BO 3 4 5 C
 BO 4 2 99
 BO 4 5 5 C
 BO 5 6 5 C
 BO 6 7 5 C
 BO 7 8 5 C
 BO 8 3 5 C
 END
 T132 *CONN
 NFRAG -99
 COMM N-Pyridazine,etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT3 N 3
 AT4 N 2 T2
 AT5 C 2
 AT6 C 2
 AT7 C 2
 AT8 C 2
 BO 1 3 99
 BO 3 4 5 C
 BO 4 5 5 C
 BO 5 6 5 C
 BO 6 7 5 C
 BO 7 8 5 C
 BO 8 3 5 C
 END
 T133 *CONN
 NFRAG -99
 COMM mu2-cyanide etc.
 LIG E1,2 X1,0 D2
 AT1 MM 1
 AT2 MM 1
 AT3 C 2 T2
 AT4 5A 2 T2
 BO 1 3 99
 BO 3 4 2,3
 BO 4 2 99
 END
 T134 *CONN
 NFRAG -99
 COMM mu2-dinitrogen
 LIG E2,2 X0,0 D2
 AT1 MM 1
 AT2 MM 1
 AT3 5A 2 T2
 AT4 5A 2 T2
 BO 1 3 99
 BO 3 4 2,3
 BO 4 2 99
 END
 T135 *CONN
 NFRAG -99
 COMM mu3-sigma,mu2-
 phosphinidine etc.
 LIG E2,1,1 X0,1,1 D1
 AT1 MM 1
 AT2 MM 2
 AT3 MM 2
 AT4 5A 3 T4
 AT5 FT 1
 BO 1 4 1
 BO 4 2 1
 BO 2 3 99
 BO 3 4 1

BO 4 5 1
 NOLN 1 2 3
 END
 T136 *CONN
 NFRAG -99
 COMM eta1-OC(NR2)=CR2 etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 C 2 T3
 AT4 C 1 T3 99 0
 AT5 5A 1 T3 99 0
 AT6 FT 1 99 0
 AT7 FT 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 3 4 2
 BO 3 5 1
 BO 5 6 1
 BO 5 7 1
 END
 T137 *CONN
 NFRAG -99
 COMM eta1-ON(R)=0
 LIG E2 X0 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 N 2 T3
 AT4 6A 1 T1
 AT5 FT 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 3 4 2
 BO 3 5 1
 END
 T138 *CONN
 NFRAG -99
 COMM [5]-int/sint-carbide
 LIG E0.8,0.8,0.8,0.8,0.8
 X0,0,0,0,0 D1
 AT1 MM 4
 AT2 MM 4
 AT3 MM 4
 AT4 MM 4
 AT5 MM 4
 AT6 C 5 T5
 BO 1 6 1
 BO 6 2 1
 BO 6 3 1
 BO 6 4 1
 BO 6 5 1
 END
 T139 *CONN
 NFRAG -99
 COMM [6]-int/sint-carbide
 LIG
 E0.67,0.67,0.67,0.67,0.67,
 0.67 X0,0,0,0,0,0 D1
 AT1 MM 5
 AT2 MM 5
 AT3 MM 5
 AT4 MM 5
 AT5 MM 5
 AT6 MM 5
 AT7 C 6 T6
 BO 1 7 1
 BO 7 2 1
 BO 7 3 1
 BO 7 4 1
 BO 7 5 1
 BO 7 6 1
 END
 T140 *CONN
 NFRAG -99
 COMM mu2-nitrosyl etc.
 LIG E1.5,1.5 X0.5,0.5 D1

AT1 MM 1
 AT2 MM 1
 AT3 5A 3 T3
 AT4 6A 1 T1
 BO 1 3 99
 BO 3 2 99
 BO 3 4 2
 END
 T141 *CONN
 NFRAG -99
 COMM eta1,eta2-mu2-
 carbamate etc.
 LIG E3.5,1.5 X0.5,0.5 D2
 AT1 MM 1
 AT2 MM 1
 AT3 6A 3 T3
 AT4 6A 2 T2
 AT5 C 3 T3
 AT6 5A 1 T3 99 0
 AT7 E 1 99 0
 AT8 E 1 99 0
 BO 1 3 99
 BO 3 2 99
 BO 3 5 99
 BO 5 4 99
 BO 4 2 1
 BO 5 6 99
 BO 6 7 1
 BO 6 8 1
 END
 T142 *CONN
 NFRAG -99
 COMM eta1,eta2-mu2-
 carboxylate
 LIG E3.5,1.5 X0.5,0.5 D2
 AT1 MM 2
 AT2 MM 1
 AT3 6A 3 T3
 AT4 6A 2 T2
 AT5 C 2 T3
 AT6 FT 1 99 0
 BO 1 3 99
 BO 3 2 99
 BO 3 5 99
 BO 5 4 99
 BO 4 1 1
 END
 T143 *CONN
 NFRAG -99
 COMM N-mu2-azide
 LIG E1.5,1.5 X0.5,0.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 N 3 T3
 AT4 N 2 T2
 AT5 N 1 T1
 BO 1 3 99
 BO 3 2 99
 BO 3 4 2
 BO 4 5 1
 BO 4 6 1
 END
 T144 *CONN
 NFRAG -99
 COMM mu3-methylidene etc.
 LIG E1,1,1 X1,1,1 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 FO 3 T4
 AT5 FT 1
 BO 1 4 99
 BO 4 2 99
 BO 4 3 99
 BO 4 5 1
 END
 T196 *CONN
 NFRAG -99
 COMM mu4-methylidene etc.
 LIG E0.75,0.75,0.75,0.75
 X0.75,0.75,0.75,0.75 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 MM 1
 AT5 FO 4 T5
 AT6 FT 1 T1
 BO 1 5 1
 BO 5 2 1
 BO 5 3 1
 BO 5 4 1
 BO 5 6 1
 END
 T145 *CONN
 NFRAG -99
 COMM mu3-halogen
 LIG E1.67,1.67,1.67
 X0.34,0.34,0.34 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 7A 3 T3
 BO 1 4 99
 BO 4 2 99
 BO 4 3 99
 END
 T146 *CONN
 NFRAG -99
 COMM O,O eta2-nitrite
 LIG E3 X1 D2
 AT1 MM 2
 AT2 6A 2 T2
 AT3 5A 2 T2
 AT4 6A 2 T2
 BO 1 2 99
 BO 2 3 99
 BO 3 4 99
 BO 4 1 1
 END
 T147 *CONN
 NFRAG -99
 COMM mu2-N=CR2 etc.
 LIG E1.5,1.5 X0.5,0.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 5A 3 T3
 AT4 C 1 T3
 AT5 E 1
 AT6 E 1
 BO 1 3 99
 BO 3 2 99
 BO 3 4 2
 BO 4 5 1
 BO 4 6 1
 END
 T148 *CONN
 NFRAG -99
 COMM N-mu2-isocyanate etc.
 LIG E1.5,1.5 X0.5,0.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 5A 3 T3
 AT4 C 2 T2
 AT5 6A 1 T1
 BO 1 3 99
 BO 3 2 99
 BO 3 4 2
 BO 4 5 2
 END
 T149 *CONN
 NFRAG -99
 COMM eta2-R2B(N~N)2

LIG E3 X1 D2
 AT1 MM 3
 AT2 N 3 T3
 AT3 N 3 T3
 AT4 B 2 T4
 AT5 N 3 T3
 AT6 N 3 T3
 AT7 FN 1
 AT8 FN 1
 BO 1 2 99
 BO 2 5 99 C
 BO 5 4 1
 BO 4 6 1
 BO 6 3 99 C
 BO 3 1 99
 BO 4 7 1
 BO 4 8 1
 NOCR 1 4
 END
 T150 *CONN
 NFRAG -99
 COMM N,S-mu2-thiocyanate
 LIG E2,1 X0,1 D2
 AT1 MM 1
 AT2 MM 1
 AT3 5A 2 T2
 AT4 C 2 T2
 AT5 6A 2 T2
 BO 1 3 99
 BO 3 4 99
 BO 4 5 99
 BO 5 2 99
 END
 T151 *CONN
 NFRAG -99
 COMM O-eta1-nitrite
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 5A 2 T2
 AT4 6A 1 T1
 BO 1 2 99
 BO 2 3 99
 BO 3 4 99
 END
 T152 *CONN
 NFRAG -99
 COMM (sigma-2) eta2-
 acetylene
 LIG E2 X0 D2
 AT1 MM 1
 AT2 C 2 T3 99 0
 AT3 C 2 T3 99 0
 AT4 FX 1 99 0
 AT5 FX 1 99 0
 BO 1 2 1
 BO 2 3 2,3
 BO 3 1 1
 BO 2 4 1
 BO 3 5 1
 END
 T153 *CONN
 NFRAG -99
 COMM mu2-O-Pyridine,etc.
 LIG E1,1 X0,0 D1
 AT1 MM 1
 AT2 MM 1
 AT3 6A 3 T3
 AT4 5A 3
 AT5 C 2
 AT6 C 2
 AT7 C 2
 AT8 C 2
 AT9 C 2
 BO 1 3 99
 BO 3 2 99

BO 3 4 1
 BO 4 5 5
 BO 5 6 5
 BO 6 7 5
 BO 7 8 5
 BO 8 9 5
 BO 9 4 5
 END
 T218 *CONN
 NFRAG -99
 COMM mu2-RC(./[T5])
 LIG E0.5,0.5 X0,0 D1
 AT1 MM 1
 AT2 MM 1
 AT3 C 4 T5
 AT4 FT 1
 AT5 C 1 T5
 AT6 C 1 T5
 BO 1 3 99
 BO 3 2 99
 BO 3 4 1
 BO 3 5 99
 BO 3 6 99
 END
 T154 *CONN
 NFRAG -99
 COMM eta2-
 tetrahaloaluminate
 LIG E3 X1 D2
 AT1 MM 2
 AT2 7A 2 T2
 AT3 3A 4 T4
 AT4 7A 2 T2
 AT5 7A 1 T1
 AT6 7A 1 T1
 BO 1 2 1
 BO 2 3 1
 BO 3 4 1
 BO 4 1 1
 BO 3 5 1
 BO 3 6 1
 END
 T155 *CONN
 NFRAG -99
 COMM mu2-C,0,0 carbonyl
 LIG E2,2 X0,0 D2
 AT1 MM 1
 AT2 MM 1
 AT3 C 3 T3
 AT4 O 2 T2
 BO 1 3 99
 BO 3 2 9
 BO 3 4 99
 BO 4 2 9
 END
 T156 *CONN
 COMM =C=NR2 etc.
 NFRAG -99
 LIG E3 X3 D1
 AT1 MM 1
 AT2 C 2 T2
 AT3 5A 1 T3
 AT4 FT 1
 AT5 FT 1
 BO 1 2 99
 BO 2 3 99
 BO 3 4 1
 BO 3 5 1
 END
 T157 *CONN
 NFRAG -99
 COMM eta2 ... (C=)C(=C)
 LIG E1,1 X0,0 D1
 AT1 MM 2
 AT2 MM 2
 AT3 C 4 T4

AT4 C 1
 AT5 C 1
 BO 1 3 9
 BO 3 2 9
 BO 3 4 2
 BO 3 5 2
 END
 T158 *CONN
 NFRAG -99
 COMM mu2-carbonate,
 sulphite etc.
 LIG E1,1 X1,1 D2
 AT1 MM 1
 AT2 MM 2
 AT3 6A 2 T2
 AT4 6A 2 T2
 AT5 FY 3 T3
 AT6 6A 1 T1 99 0
 BO 1 3 99
 BO 3 5 1,2,7
 BO 5 4 1,7
 BO 4 2 99
 BO 5 6 2,7
 END
 T219 *CONN
 NFRAG -99
 COMM mu2-eta3-allyl
 LIG E1.5,1.5 X0.5,0.5 D3
 AT1 MM 2
 AT2 MM 2
 AT3 C 2 T4
 AT4 C 4 T5
 AT5 C 2 T4
 AT6 FX 1
 AT7 FX 1
 AT8 FX 1
 AT9 FX 1
 AT10 FX 1
 BO 1 3 9
 BO 3 4 99
 BO 4 5 99
 BO 4 1 9
 BO 4 2 9
 BO 5 2 9
 BO 3 6 1
 BO 3 7 1
 BO 4 8 1
 BO 5 9 1
 BO 5 10 1
 END
 T159 *CONN
 NFRAG -99
 COMM sigma-vinyl(alpha
 NR2)
 LIG E1 X1 D1
 AT1 MM 1
 AT2 C 2 T3
 AT3 C 1 T3
 AT4 5A 1 T3
 AT5 E 1
 AT6 E 1
 AT7 E 1
 AT8 E 1
 BO 1 2 1
 BO 2 3 2
 BO 2 4 1
 BO 3 5 1
 BO 3 6 1
 BO 4 7 1
 BO 4 8 1
 END
 T160 *CONN
 NFRAG -99
 COMM O,C/S-eta2-
 carbon/sulphur dioxide
 etc.

LIG X0 E2 D2
 AT1 MM 2
 AT2 6A 2 T2
 AT3 FY 3 T3
 AT4 6A 1 T1
 BO 1 2 99
 BO 2 3 99
 BO 3 1 99
 BO 3 4 2
 END
 T161 *CONN
 NFRAG -99
 COMM S,C eta2-S=C-NR2
 LIG E3 X1 D2
 AT1 MM 2
 AT2 6A 2 T2
 AT3 C 3 T3
 AT4 5A 1 T3
 AT5 FT 1
 AT6 FT 1
 BO 1 2 99
 BO 2 3 99
 BO 3 1 99
 BO 3 4 99
 BO 4 5 1
 BO 4 6 1
 END
 T162 *CONN
 NFRAG -99
 COMM O,C-eta2-O-C=CR2
 LIG E2 X0 D2
 AT1 MM 1
 AT2 C 2 T3
 AT3 C 1 T3
 AT4 6A 2 T2
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 BO 1 2 99
 BO 2 4 99
 BO 4 1 99
 BO 2 3 99
 BO 3 5 1
 BO 3 6 1
 END
 T163 *CONN
 COMM pi-etal-pyrrolyl
 NFRAG -99
 LIG E5 X1 D1
 AT1 MM 1
 AT2 5A 2 T3
 AT3 C 2 T3
 AT4 C 2 T3
 AT5 C 2 T3
 AT6 C 2 T3
 BO 1 2 9
 BO 2 3 99 C
 BO 3 4 99 C
 BO 4 5 99 C
 BO 5 6 99 C
 BO 6 2 99 C
 END
 T164 *CONN
 NFRAG -99
 COMM eta2-C,C-(R2C)2PR2
 LIG E3 X1 D2
 AT1 MM 2
 AT2 C 2 T4
 AT3 5A 2 T4
 AT4 C 2 T4
 AT5 FT 1
 AT6 FT 1
 AT7 FT 1 99 0
 AT8 FT 1 99 0
 AT9 FT 1 99 0
 AT10 FT 1 99 0
 BO 1 2 1

BO 2 3 1
 BO 3 4 1
 BO 4 1 1
 BO 3 5 1
 BO 3 6 1
 BO 2 7 1
 BO 2 8 1
 BO 4 9 1
 BO 4 10 1
 END
 T165 *CONN
 COMM mu2-sigma,sigma-
 RN=NR,etc.
 NFRAG -99
 LIG E2,2 X0,0 D1
 AT1 MM 1
 AT2 MM 1
 AT3 5A 2 T3
 AT4 5A 2 T3
 AT5 E 1
 AT6 E 1
 BO 1 3 1
 BO 3 4 2
 BO 4 1 1
 BO 3 5 1
 BO 4 6 1
 NOCR 5 6
 END
 T166 *CONN
 NFRAG -99
 COMM mu2-eta2-RNNR
 LIG E3,3 X0,0 D2
 AT1 MM 1
 AT2 MM 1
 AT3 5A 3 T4
 AT4 5A 3 T4
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 BO 1 3 99
 BO 3 2 99
 BO 3 4 1,2
 BO 4 1 99
 BO 4 2 99
 BO 3 5 1
 BO 4 6 1
 END
 T167 *CONN
 NFRAG -99
 COMM [4]-carbide
 LIG E1,1,1,1 X0,0,0,0 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 MM 1
 AT5 C 4 T4
 BO 1 5 1
 BO 5 2 1
 BO 5 3 1
 BO 5 4 1
 END
 T168 *CONN
 NFRAG -99
 COMM N,N-mu2-azide
 LIG E1.5,1.5 X0.5,0.5 D2
 AT1 MM 1
 AT2 MM 1
 AT3 N 2 T2
 AT4 N 2 T2
 AT5 N 2 T2
 BO 1 3 99
 BO 3 4 2
 BO 4 5 2
 BO 5 2 1
 END
 T169 *CONN
 NFRAG -99

COMM Carbene (di-alpha-OR)
 LIG E2 X0 D1
 AT1 MM 1
 AT2 C 3 T3
 AT3 6A 1 T2
 AT4 6A 1 T2
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 BO 1 2 2
 BO 2 3 1
 BO 2 4 1
 BO 3 5 1
 BO 4 6 1
 END
 T170 *CONN
 NFRAG -99
 COMM eta3-mul-mul1-mu2-
 carbonate
 LIG E3,3 X1,1 D3
 AT1 MM 1
 AT2 MM 2
 AT3 6A 2 T2
 AT4 6A 2 T2
 AT5 FY 3 T3
 AT6 6A 1 T3
 BO 1 3 99
 BO 3 5 99
 BO 5 4 99
 BO 4 2 99
 BO 5 6 99
 BO 6 1 99
 BO 6 2 99
 END
 T171 *CONN
 NFRAG -99
 COMM mul-O,mu2-O deloc-
 diketonate
 LIG E3.5,1.5 X0.5,0.5 D2
 AT1 MM 1
 AT2 MM 1
 AT3 6A 3 T3
 AT4 6A 2 T2
 AT5 C 2 T3
 AT6 C 2 T3
 AT7 C 2 T3
 AT8 FX 1
 BO 1 3 99 C
 BO 3 2 99
 BO 3 5 7 C
 BO 5 6 7 C
 BO 6 7 7 C
 BO 7 4 7 C
 BO 4 1 99 C
 BO 5 8 1
 END
 T221 *CONN
 NFRAG -99
 COMM mu2-etal-etal-
 dichalcogen
 AT1 MM 1
 AT2 MM 1
 AT3 6A 2 T2
 AT4 6A 2 T2
 BO 1 3 1
 BO 3 4 1
 BO 4 2 1
 END
 T172 *CONN
 NFRAG -99
 COMM mu2-sulphate etc.
 LIG X1,1 E1,1 D2
 AT1 MM 1
 AT2 MM 1
 AT3 6A 2 T2
 AT4 6A 2 T2
 AT5 6A 4 T4

AT6 6A 1 T1	AT6 E 1 99 0	LIG E2 X0 D1
AT7 6A 1 T1	BO 1 2 99	AT1 MM 1
BO 1 3 99	BO 3 2 1	AT2 6A 4 T4
BO 3 5 99	BO 3 4 2	AT3 6A 1 T1
BO 5 4 99	BO 4 5 1	AT4 FT 1
BO 4 2 99	BO 3 6 1	AT5 FT 1
BO 5 6 99	END	BO 1 2 99
BO 5 7 99	T178 *CONN	BO 2 3 2
END	NFRAG -99	BO 2 4 1
T173 *CONN	COMM O-P(R2)=S etc.	BO 2 5 1
NFRAG -99	LIG E1 X1 D1	END
COMM eta1=N-N=CR2	AT1 MM 1	T184 *CONN
LIG E101 X2 D1	AT2 6A 2 T2	COMM 1-eta1-3-R-triazole
AT1 MM 1	AT3 5A 4 T4	NFRAG -99
AT2 5A 2 T2	AT4 FX 1	AT1 MM 1
AT3 5A 2 T2	AT5 FX 1	AT2 N 2 T3
AT4 C 1 T3	AT6 6A 1 T1	AT3 N 2 T2
AT5 FT 1	BO 1 2 99	AT4 N 2 T3
AT6 FT 1	BO 2 3 1	AT5 C 2
BO 1 2 99	BO 3 4 1	AT6 C 2
BO 2 3 1,2	BO 3 5 1	AT7 FT 1
BO 3 4 2	BO 3 6 2	BO 2 3 99 C
BO 4 5 1	NOLN 1 4 5 6	BO 3 4 99 C
BO 4 6 1	END	BO 4 5 99 C
END	T179 *CONN	BO 5 6 99 C
T174 *CONN	NFRAG -99	BO 6 2 99 C
NFRAG -99	COMM eta2-S2PR2 etc.	BO 1 2 99
COMM O-NR2 etc.	LIG E3 X1 D2	BO 4 7 1
LIG E2 X0 D1	AT1 MM 1	END
AT1 MM 1	AT2 6A 2 T2	T210 *CONN
AT2 6A 2 T2	AT3 5A 4 T4	NFRAG -99
AT3 5A 3 T3	AT4 6A 2 T2	COMM mu2-C(R)PR3
AT4 FT 1	AT5 FX 1	LIG E1.5,1.5 X0.5,0.5 D1
AT5 FT 1	AT6 FX 1	AT1 MM 2
BO 1 2 99	BO 1 2 99	AT2 MM 2
BO 2 3 99	BO 2 3 99	AT3 FO 3 T4
BO 3 4 1	BO 3 4 99	AT4 5A 1 T4
BO 3 5 1	BO 4 1 99	AT5 FT 1
END	BO 3 5 1	AT6 FT 1
T175 *CONN	BO 3 6 1	AT7 FT 1
NFRAG -99	END	AT8 FT 1
COMM O=NR etc.	T180 *CONN	BO 1 3 99
LIG E2 X0 D1	NFRAG -99	BO 3 2 99
AT1 MM 1	COMM mu2-S-P(R2)-S etc.	BO 3 4 1
AT2 6A 2 T2	LIG E1.5,1.5 X0.5,0.5 D2	BO 3 5 1
AT3 5A 2 T2	AT1 MM 1	BO 4 6 1
AT4 FT 1	AT2 MM 1	BO 4 7 1
BO 1 2 99	AT3 6A 2 T2	BO 4 8 1
BO 2 3 99	AT4 6A 2 T2	END
BO 3 4 1	AT5 5A 4 T4	T185 *CONN
END	AT6 FX 2 99 0	NFRAG -99
T176 *CONN	AT7 FX 2 99 0	COMM pi-cyclopropenyl
NFRAG -99	BO 1 3 99	LIG E3 X0 D1
COMM mu2-S=CR2 etc.	BO 3 5 99	AT1 MM 1
LIG E2,2 X0,0 D1	BO 5 4 99	AT2 C 3 T4
AT1 MM 1	BO 4 2 99	AT3 C 2 T3
AT2 MM 2	BO 5 6 1	AT4 C 2 T3
AT3 6A 3 T3	BO 5 7 1	AT5 FX 1 99 0
AT4 FY 1 T3	END	AT6 FX 1 99 0
AT5 FZ 99 0	T181 *CONN	AT7 FX 1 99 0
AT6 FZ 99 0	NFRAG -99	BO 1 2 9
BO 1 3 99	COMM S-etal-RSO2 etc.	BO 2 3 5,7
BO 3 2 99	LIG E1 X1 D1	BO 3 4 5,7
BO 3 4 2	AT1 MM 1	BO 4 2 5,7
BO 4 5 1,7	AT2 6A 4 T4	BO 2 5 1
BO 4 6 1	AT3 6A 1 T1	BO 3 6 1
END	AT4 6A 1 T1	BO 4 7 1
T177 *CONN	AT5 FT 1	END
NFRAG -99	BO 1 2 99	T186 *CONN
COMM eta1-OC(R)=NR	BO 2 3 2	NFRAG -99
LIG E1 X1 D1	BO 2 4 2	COMM eta1-NR2-N=CR2 etc.
AT1 MM 1	BO 2 5 1	LIG E2 X0 D1
AT2 6A 2 T2	END	AT1 MM 2
AT3 C 3 T3	T182 *CONN	AT2 5A 2 T4
AT4 5A 2 T2	NFRAG -99	AT3 5A 1 T2
AT5 E 1 99 0	COMM S-etal-R2S=O etc.	AT4 FT 1 99 0

AT5 FT 1 99 0
 AT6 C 1 T3 99 0
 AT7 FX 1
 AT8 FX 1
 BO 1 2 99
 BO 2 3 1
 BO 2 4 1
 BO 2 5 1
 BO 3 6 2
 BO 6 7 1
 BO 6 8 1
 END
 T187 *CONN
 NFRAG -99
 COMM eta3-borohydride
 LIG E1 X1 D3
 AT1 MM 3
 AT2 HD 2 T2
 AT3 B 0
 AT4 HD 2 T2
 AT5 HD 2 T2
 AT6 FT 1 T1
 BO 1 2 1
 BO 2 3 1
 BO 3 4 1
 BO 4 1 1
 BO 1 5 1
 BO 5 3 1
 BO 3 6 1
 NOLN 1 6
 END
 T188 *CONN
 NFRAG -99
 COMM eta1-borohydride
 LIG E1 X1 D1
 AT1 MM 1
 AT2 HD 2 T2
 AT3 B 0
 AT4 FT 1 T1
 AT5 FT 1 T1
 AT6 FT 1 T1
 BO 1 2 1
 BO 2 3 1
 BO 3 4 1
 BO 3 5 1
 BO 3 6 1
 NOLN 1 4 5 6
 END
 T215 *CONN
 NFRAG -99
 COMM S-mu2-thiocyanate
 etc.
 LIG E1.5,1.5 X0.5,0.5 D1
 AT1 MM 1
 AT2 MM 1
 AT3 6A 3 T3
 AT4 C 2 T2
 AT5 5A 1 T1
 BO 1 3 99
 BO 3 2 99
 BO 3 4 99
 BO 4 5 99
 END
 T189 *CONN
 NFRAG -99
 COMM pi-P=-X
 LIG E1 X0 D1
 AT1 MM 1
 AT2 5A 2 T2
 AT3 E 1
 BO 1 2 9
 BO 2 3 3
 END
 T190 *CONN
 COMM 1-eta1-triazole etc
 LIG E1 X1 D1

NFRAG -99
 AT1 MM 1
 AT2 N 2 T3
 AT3 N 2 T2
 AT4 N 2 T2
 AT5 C 2
 AT6 C 2
 BO 2 3 99 C
 BO 3 4 99 C
 BO 4 5 99 C
 BO 5 6 99 C
 BO 6 2 99 C
 BO 1 2 99
 END
 T191 *CONN
 NFRAG -99
 COMM eta3-nitrosyl
 LIG E1,1,1 X0,0,0 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 5A 4 T4
 AT5 6A 1 T1
 BO 1 4 99
 BO 4 2 99
 BO 4 3 99
 BO 4 5 99
 END
 T192 *CONN
 NFRAG -99
 COMM mu4-alkoxy etc.
 LIG E1.25,1.25,1.25,1.25
 X0.25,0.25,0.25,0.25 D1
 AT1 MM 1
 AT2 MM 1
 AT3 MM 1
 AT4 MM 1
 AT5 6A 4 T5
 AT6 FT 1
 BO 1 5 99
 BO 5 2 99
 BO 5 3 99
 BO 5 4 99
 BO 5 6 1
 END
 T193 *CONN
 NFRAG -99
 COMM eta1-S/C-
 sulphur/carbon dioxide
 etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 FY 3 T3
 AT3 6A 1 T1
 BO 1 2 99
 BO 2 3 99
 BO 2 4 99
 END
 T195 *CONN
 NFRAG -99
 COMM eta1-O=S(R2)=O etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 6A 2 T2
 AT3 6A 4 T4
 AT4 6A 1 T1
 AT5 FT 1
 AT6 FT 1
 BO 1 2 99
 BO 2 3 2
 BO 3 4 2
 BO 3 5 1
 BO 3 6 1
 END
 T202 *CONN

NFRAG -99
 COMM N-triazine,etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT3 N 3
 AT4 C 2
 AT5 N 2 T2
 AT6 C 2
 AT7 N 2 T2
 AT8 C 2
 BO 1 3 99
 BO 3 4 5 C
 BO 4 5 5 C
 BO 5 6 5 C
 BO 6 7 5 C
 BO 7 8 5 C
 BO 8 3 5 C
 END
 T201 *CONN
 NFRAG -99
 COMM S-etal-ROSO2 etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 6A 4 T4
 AT3 6A 1 T1
 AT4 6A 1 T1
 AT5 6A 1 T2
 AT6 FT 1
 BO 1 2 99
 BO 2 3 99
 BO 2 4 99
 BO 2 5 1
 BO 5 6 1
 END
 T211 *CONN
 NFRAG -99
 COMM eta2-S2CPR3 etc.
 LIG E4 X2 D2
 AT1 MM 2
 AT2 6A 2 T2
 AT3 C 3 T3
 AT4 6A 2 T2
 AT5 5A 1 T4 99 0
 AT6 E 1 99 0
 AT7 E 1 99 0
 AT8 E 1 99 0
 BO 1 2 99
 BO 2 3 99
 BO 3 4 99
 BO 4 1 99
 BO 3 5 99
 BO 5 6 1
 BO 5 7 1
 BO 5 8 1
 END
 T203 *CONN
 NFRAG -99
 COMM eta1 RC=NR etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 C 3 T3
 AT3 5A 1 T2
 AT4 E 1 99 0
 AT5 E 1 99 0
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 BO 3 5 1
 END
 T204 *CONN
 NFRAG -99
 COMM mu2-OPR3 etc.
 LIG E1,1 X0,0 D1
 AT1 MM 1
 AT2 MM 1
 AT3 6A 3 T3

AT4 5A 1 T4
 AT5 FT 1
 AT6 FT 1
 AT7 FT 1
 BO 1 3 99
 BO 3 2 99
 BO 3 4 1,2
 BO 4 5 1
 BO 4 6 1
 BO 4 7 1
 END
 T214 *CONN
 NFRAG -99
 COMM eta1-N=C=CR2 etc.
 LIG E100 X1 D1
 AT1 MM 1
 AT2 5A 2 T2
 AT3 C 1 T2
 AT4 C 1 T3
 AT5 FX 1 99 0
 AT6 FX 1 99 0
 BO 1 2 99
 BO 2 3 2
 BO 3 4 2
 BO 4 5 1
 BO 4 6 1
 END
 T223 *CONN
 NFRAG -99
 COMM eta4-cyclobutadiene
 LIG E4 X0 D4
 AT1 MM 1
 AT2 C 3 T4
 AT3 C 3 T4
 AT4 C 3 T4
 AT5 C 3 T4
 AT6 E 1
 AT7 E 1
 AT8 E 1
 AT9 E 1
 BO 1 2 9
 BO 2 3 99 C
 BO 3 4 99 C
 BO 4 5 99 C
 BO 5 2 99 C
 BO 3 1 9
 BO 4 1 9
 BO 5 1 9
 BO 2 6 1
 BO 3 7 1
 BO 4 8 1
 BO 5 9 1
 END
 T212 *CONN
 NFRAG -99
 COMM Carbene (alpha-PR3)
 LIG E3 X1 D1
 AT1 MM 1
 AT2 C 3 T3
 AT3 5A 1 T4
 AT4 FT 1 99 0
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 AT7 FT 1 99 0
 BO 1 2 2
 BO 2 3 1
 BO 2 4 1
 BO 3 5 1
 BO 3 6 1
 BO 3 7 1
 END
 T205 *CONN
 NFRAG -99
 COMM eta1 RC=N=N etc.
 LIG E1 X1 D1
 AT1 MM 1

AT2 C 3 T3
 AT3 5A 2
 AT4 E 1 99 0
 AT5 5A 1
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 BO 3 5 2
 NOCR 1
 END
 T206 *CONN
 NFRAG -99
 COMM eta1 RC=N=CR2 etc.
 LIG E2 X0 D1
 AT1 MM 1
 AT2 C 3 T3
 AT3 5A 2
 AT4 E 1 99 0
 AT5 FY 1
 BO 1 2 99
 BO 2 3 2
 BO 2 4 1
 BO 3 5 2
 NOCR 1
 END
 T224 *CONN
 NFRAG -99
 COMM N(NR2)=NR
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 3 T3
 AT3 5A 1 T2
 AT4 5A 1 T3
 AT5 FT 1
 AT6 FT 1
 AT7 FT 1
 BO 1 2 99
 BO 2 3 2,5,7
 BO 2 4 1,5,7
 BO 3 5 1
 BO 4 6 1
 BO 4 7 1
 END
 T225 *CONN
 NFRAG -99
 COMM eta2-hydrazine etc.
 LIG E4 X0 D2
 AT1 MM 2
 AT2 5A 2 T4
 AT3 5A 2 T4
 AT4 FT 1 99 0
 AT5 FT 1 99 0
 AT6 FT 1 99 0
 AT7 FT 1 99 0
 BO 1 2 99
 BO 2 3 99
 BO 3 1 99
 BO 2 4 1
 BO 2 5 1
 BO 3 6 1
 BO 3 7 1
 END
 T226 *CONN
 NFRAG -99
 COMM mu2-isocarbonyl etc.
 LIG E100,100 X0,0 D1
 AT1 MM 1
 AT2 MM 1
 AT3 C 2 T2
 AT4 6A 2 T2
 BO 1 3 99
 BO 3 4 2,3
 BO 4 2 99
 END
 T230 *CONN
 COMM N=-CBH3

NFRAG -99
 LIG E1 X1 D1
 AT1 MM 1
 AT2 N 2 T2
 AT3 C 2 T2
 AT4 B 1 T4
 AT5 HD 1 T1
 AT6 HD 1 T1
 AT7 HD 1 T1
 BO 1 2 1
 BO 2 3 3
 BO 3 4 1
 BO 4 5 1
 BO 4 6 1
 BO 4 7 1
 END
 T227 *CONN
 COMM N=S=S etc.
 NFRAG -99
 LIG E100 X1 D1
 AT1 MM 1
 AT2 5A 2 T2
 AT3 6A 2 T2
 AT4 6A 1 T1
 BO 1 2 99
 BO 2 3 99
 BO 3 4 99
 END
 T207 *CONN
 NFRAG -99
 COMM eta1-SO3 etc.
 LIG E99 X99 D1
 AT1 MM 1
 AT2 6A 4 T4
 AT3 6A 1 T1
 AT4 6A 1 T1
 AT5 6A 1 T1
 BO 1 2 99
 BO 2 3 2
 BO 2 4 2
 BO 2 5 2
 END
 T209 *CONN
 NFRAG -99
 COMM eta2-RNNNR.
 LIG E3 X1 D2
 AT1 MM 3
 AT2 5A 2 T3
 AT3 5A 2 T2
 AT4 5A 3 T3
 AT5 E 1
 AT6 E 1
 BO 1 2 1
 BO 2 3 99
 BO 3 4 99
 BO 4 1 1
 BO 2 5 1
 BO 4 6 1
 END
 T239 *CONN
 COMM sigma-eta1-pyrrolyl
 NFRAG -99
 LIG E1 X1 D1
 AT1 MM 1
 AT2 5A 2 T3
 AT3 C 2 T3
 AT4 C 2 T3
 AT5 C 2 T3
 AT6 C 2 T3
 BO 1 2 99
 BO 2 3 5 C
 BO 3 4 5 C
 BO 4 5 5 C
 BO 5 6 5 C
 BO 6 2 5 C
 END

T183 *CONN
 NFRAG -99
 COMM eta1-N(H)C(R)=O
 LIG E100 X1 D1
 AT1 MM 1
 AT2 5A 2 T3
 AT3 C 3 T3
 AT4 6A 1 T1
 AT5 HS 1 T1
 AT6 FN 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 3 4 2
 BO 2 5 1
 BO 3 6 1
 END
 T200 *CONN
 NFRAG -99
 COMM eta1-N(R)=C(R)(OR)
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 2 T3
 AT3 FN 1
 AT4 C 1 T3
 AT5 FN 1 99 0
 AT6 6A 1 T2 99 0
 AT7 FZ 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 2 4 2
 BO 4 5 1
 BO 4 6 1
 BO 6 7 1
 NOLN 1 3 5 6
 END
 T232 *CONN
 NFRAG -99
 COMM N(C(R)=C)(CR3) etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 5A 1 T3
 AT3 C 1 T3
 AT4 C 1 T4
 AT5 C 1 T3 99 0
 AT6 FZ 1 99 0
 AT7 FN 1 99 0
 AT8 FN 1 99 0
 AT9 FN 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 2 4 1
 BO 3 5 99
 BO 3 6 1,5
 BO 4 7 1
 BO 4 8 1
 BO 4 9 1
 END
 T233 *CONN
 NFRAG -99
 COMM N(C(R)=C)(H) etc.
 LIG E1 X1 D1
 AT1 MM 1
 AT2 5A 1 T3
 AT3 C 1 T3
 AT4 HS 1 T1
 AT5 C 1 T3 99 0
 AT6 FZ 1 99 0
 BO 1 2 99
 BO 2 3 1
 BO 2 4 1
 BO 3 5 99
 BO 3 6 1,5
 END
 T194 *CONN
 NFRAG -99
 COMM eta2-O~C(SR)~O etc.

LIG E3 X1 D2
 AT1 MM 2
 AT2 6A 2 T2
 AT3 C 3 T3
 AT4 6A 2 T2
 AT5 6A 1 T2 99 0
 AT6 FZ 1 99 0
 BO 1 2 99
 BO 2 3 99
 BO 3 4 99
 BO 4 1 99
 BO 3 5 99
 BO 5 6 1
 END
 T241 *CONN
 NFRAG -99
 COMM eta2-O~N~N(R)~O
 LIG E3 X1 D2
 AT1 MM 1
 AT2 6A 2 T2
 AT3 6A 2 T2
 AT4 5A 2 T2
 AT5 5A 2 T3
 AT6 FZ 1 99 0
 BO 1 2 99
 BO 2 4 99
 BO 4 5 99
 BO 5 3 99
 BO 3 1 99
 BO 5 6 1
 END
 T242 *CONN
 NFRAG -99
 COMM mul-eta1-pyrazole
 LIG E2 X0 D1
 AT1 MM 1
 AT2 5A 3 T3
 AT3 5A 2 T3
 AT4 C 2 T3
 AT5 C 2 T3
 AT6 C 2 T3
 AT7 FT 1 99 0
 AT8 FX 1 99 0
 AT9 FZ 1 99 0
 AT10 FZ 1 99 0
 BO 1 2 99
 BO 2 3 1,5,7
 BO 3 4 99
 BO 4 5 99
 BO 5 6 99
 BO 6 2 99
 BO 3 7 1
 BO 4 8 1
 BO 5 9 99
 BO 6 10 99
 END
 T243 *CONN
 NFRAG -99
 COMM mul-eta1-pyrazolyl
 LIG E1 X1 D1
 AT1 MM 1
 AT2 5A 3 T3
 AT3 5A 2 T2
 AT4 C 2 T3
 AT5 C 2 T3
 AT6 C 2 T3
 AT7 FX 1 99 0
 AT8 FZ 1 99 0
 AT9 FZ 1 99 0
 BO 1 2 99
 BO 2 3 1,5,7
 BO 3 4 99
 BO 4 5 99
 BO 5 6 99
 BO 6 2 99
 BO 3 7 1
 BO 4 8 1
 BO 5 9 99
 BO 6 10 99
 END
 BO 4 7 1
 BO 4 11 1
 BO 5 8 1
 BO 5 9 1
 END
 T248 *CONN
 NFRAG -99
 LIG E1 X1 D1
 COMM N(R)NO2 etc.
 AT1 MM 1
 AT2 5A 2 T3
 AT3 5A 3 T3
 AT4 6A 1 T1
 AT5 6A 1 T1
 AT6 FT 1 99 0
 BO 1 2 1
 BO 2 3 99
 BO 3 4 99
 BO 3 5 99
 BO 2 6 1
 END
 SAVE REFC