SUPPLEMENTARY MATERIALS: SPACE GROUPS P1 AND Cc: HOW ARE THEY DOING?

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TABLE 1S. Space group revisions; original space group, Cc (No. 9)

Refcode	S. G.	Formula Unit	Reference
AXIYUB	C2/c	$C_{32}H_{36}O_6Sn$	Ma *et al.* (2004a)
AZERUS	C2/c	$C_{16}H_{14}Cr_2O_4Se$	Song *et al.* (2004)
BENWIB	Fdd2	$C_{54}H_{68}N_8Ni_3O_8{\cdot}2(PF_6)$	Adams *et al.* (2004)
BIJKIP	P31c	$C_{24}H_{30}N_3P$	Beddie *et al.* (2004)
BIJMIR	C2/c	$C_{44}H_{70}O_2Si_4Zr$	Bradley *et al.* (2004)
DADMEB	C2/c	$C_4H_{10}N_2O_{10}Zn$	Yang *et al.* (2004)
DALNOU	C2/c	$C_{33}H_{52}ClN_7ORu{\cdot}CF_3SO_3$	Jitsukawa *et al.* (2004)
EBUXUV	C2/c	$C_{42}H_{40}N_2O_2$	Shen *et al.* (2004)
EVUQUH	C2/c	$C_{34}H_{55}N_6Rh{\cdot}2(PF_6)$	Mas-Marza *et al.* (2004)
EXATUS	Fdd2	$C_{68}H_{54}Co_4O_8P_4$	Golovko *et al.* (2004)
FAYQUS	C2/c	$C_{14}H_{14}N_2O_4S_2Zn$	Ng *et al.* (2004)
FEJGAD	C2/c	$C_{24}H_{22}Cl_2N_2Sn$	Ma *et al.* (2004b)
IBUSUU	Ama2	$C_{26}H_{26}GaNO_2P_2$	Montiel-Palma *et al.* (2004)
IREFEQ	C2/c	$C_{54}H_{18}F_{20}N_6Ru{\cdot}3(CH_2Cl_2)$	Li *et al.* (2004)
IXUVOM	C2/c	$C_{18}H_{15}NO_4$	Costa *et al.* (2004)
SAGJIU	C2/c	$C_{23}H_{27}BF_2O_4$	Mayoral *et al.* (2004)
SALTUV	C2/c	$C_{10}H_{16}N_{10}S_2Zn$	Du (2004)
WAGRAY	C2/c	$C_{41}H_{45}ClN_4O_4{\cdot}C_{10}H_9N_3O_7$	Oliva *et al.* (2004)
WAJDIV	C2/c	$C_{35}H_{30}FeN_{12}O_3Sr$	RoyChowdhury *et al.* (2004)
XACMOE	C2/c	$C_{22}H_{28}N_4O_4Zn$	Chantarasiri *et al.* (2004)
YACPAU	C2/c	$C_{38}H_{36}FeN_6{\cdot}2(PF_6)$	Brady *et al.* (2004)
YAPZAR	C2/c	$C_{90}H_{172}Li_4NO_{24}Si_{16}Yb$	Lorenz *et al.* (2004)
CEBLUR	C2/c	$C_{12}H_8N_4S_4Zn$	Suen *et al.* (2005)
CEFDOH	C2/c	$C_{104}H_{28}F_{40}N_{10}{\cdot}3(C_7H_{16}){\cdot}1.5(H_2O)\ {\cdot}2(CH_2Cl_2)$	Anand *et al.* (2005)
ECATIM	C2/c	$C_{12}H_{12}O_{15}Tb{\cdot}Na_3{\cdot}8(H_2O)$	Kang *et al.* (2005)
FENWUR	C2/c	$C_{52}H_{52}ZnN_{16}O_2{\cdot}2(NO_3){\cdot}5(H_2O)$	Zhu *et al.* (2005)
FIPGOB	C2/c	$C_{38}H_{24}CdN_4O_4{\cdot}2(H_2O)$	Shi *et al.* (2005)
JARNOG	C2/c	$C_{26}H_{28}CdN_{10}O_6{\cdot}CH_2Cl_2$	Yeh *et al.* (2005)
LAMDIN	Fdd2	$C_{12}H_{36}CaO_6S_6{\cdot}2(ClO_4)$	Ullstrom *et al.* (2005)
LARTII	C2/c	$C_{19}H_{30}N_3O_2P$	Gholivand *et al.* (2005)
LEBWAR	Fdd2	$C_{11}H_{16}NS{\cdot}C_2HO_4$	Ananikov *et al.* (2005)
NATLAW	C2/c	$C_{27}H_{36}AuClN_2{\cdot}C_7H_8$	Fructos *et al.* (2005)
NAVTUA	C2/c	$C_{20}H_{28}AuN_8O_8{\cdot}Na_3{\cdot}2(C_5H_7N_2O_2){\cdot}8(H_2O)$	Oyaizu *et al.* (2005)
NICJEP	C2/c	$C_{13}H_{12}O_3$	Wang *et al.* (2005)
TASDUN	Fdd2	$C_{21}H_{18}O_3$	Muthusamy *et al.* (2005)
TAVDAW	C2/c	$C_{25}H_{45}N_3O_5$	Hanessian *et al.* (2005)
TAWFIH	C2/c	$C_{24}H_{18}FeN_{12}$	Gaspar *et al.* (2005)
WARTEP	C2/c	$C_{36}H_{24}N_6Ni{\cdot}2(C_9H_{12}NO_5S_2){\cdot}H_2O$	Lan *et al.* (2005)
YAJXIR	C2/c	$C_{21}H_{24}N_3O_2{\cdot}C_6H_2N_3O_7$	Voskressensky *et al.* (2005)
DEJCOL	C2/c	$C_{43}H_{49}N_5{\cdot}CH_2Cl_2$	Champouret *et al.* (2006)
DELJAG	C2/c	$C_{26}H_{24}FeN_6Se_2$	Morita *et al.* (2006)
DIFBUQ	C2/c	$C_{32}H_{40}F_{12}HfO_8$	Zherikova *et al.* (2006)
GEFYEW	C2/c	$C_{42}H_{46}Co_2N_{14}O_{12}{\cdot}2(H_2O)$	Fernandez-Fernandez *et al.* (2006a)
HEBZUK	C2/c	$C_{24}H_{32}B_2BiN_{12}S_6{\cdot}NO_2(?){\cdot}2.5(C_3H_7NO)$	Dodds *et al.* (2006)
KIBFUX	C2/c	$C_6H_{24}MnN_6{\cdot}C_{10}H_6S_2{\cdot}H_2O$	Yu *et al.* (2006)
KIBGAE	C2/c	$C_6H_{24}CoN_6{\cdot}C_{10}H_6S_2{\cdot}H_2O$	Yu *et al.* (2006)
KIBGEI	C2/c	$C_6H_{24}NiN_6{\cdot}C_{10}H_6S_2{\cdot}H_2O$	Yu *et al.* (2006)
NEJTOM	C2/c	$C_{58}H_{58}CuN_{10}O_4{\cdot}2(ClO_4){\cdot}0.5(C_6H_6){\cdot}\ 2.5(C_2H_3N)$	Plante & Glass (2006)
NEKFEP	Fdd2	$C_{42}H_{48}$	Muller *et al.* (2006)
NIMPIJ	C2/c	$C_{34}H_{28}Cu_2N_4O_8$	Tao *et al.* (2006)
SERXOD	C2/c	$C_{86}H_{110}N_4O_{22}{\cdot}2(CH_4O)$	Zhang *et al.* (2006)
XEFCUH	C2/c	$C_{30}H_{38}Ag_2N_{10}{\cdot}2(ClO_4){\cdot}2(C_2H_3N)$	Fernandez-Fernandez *et al.* (2006b)

TABLE 1S. Space group revisions; original space group, Cc (No. 9) – Continued

Refcode	S. G.	Formula Unit	Reference
CIBJED	C2/c	$C_{22}H_{34}N_2O_4Ti$	Boyle *et al.* (2007)
HIWMAC	C2/c	$2(C_{12}H_{28}N)\cdot C_{35}H_{65}Co_2N_{13}O_5\cdot C_4H_9NO$	Zinn *et al.* (2007)
KIJCOW	C2/c	$C_{30}H_{20}MoN_2O_4$	Sakakura *et al.* (2007)
SICNAU	C2/c	$2(C_{40}H_{38}N_4O_8)\cdot 3(CHCl_3)\cdot 6(H_2O)$	Chawla *et al.* (2007)
TICZAH	C2/c	$C_{24}H_{52}O_2Si_2$	Yamada *et al.* (2007)
TIZZIM	C2/c	$C_7H_{14}N_2$	Morozova *et al.* (2007)
YIDGAU	C2/c	$C_{44}H_{34}IrN_6\cdot 3(PF_6)\cdot 2(C_2H_3N)$	Yoshikawa *et al.* (2007)
BOJWUT	C2/c	$C_{10}H_{18}CdN_4O_4S_2$	Zhu *et al.* (2008)
CIRZUZ	C2/c	$C_{54}H_{76}CuN_4\cdot PF_6$	Diez-Gonzales *et al.* (2008)
DELWEX01	C2/c	$C_{23}H_{24}CuN_2O_2$	Sarkar *et al.* (2008)
JIYGAA	C2/c	$C_{22}H_{22}N_4S$	Zheng *et al.* (2008)
NIYXID	C2/c	$Na\cdot C_{16}H_{24}GaN_4O_8\cdot 5(H_2O)$	Heppeler *et al.* (2008)
QOBJAT	C2/c	$C_{44}H_{32}N_8Ni_2O_{12}\cdot 2(H_2O)$	Wang *et al.* (2008)
RIWNER	C2/c	$C_{31}H_{57}FeN_2O_2ScSi_2$	Carver *et al.* (2008)
VIZHIW01	C2/c	$C_{16}H_{22}O_4$	Liskin & Valente (2008)

Revisions to space groups other than P1 or Cc

Refcode	Old	New	Formula Unit	Reference
BENWOH	$P2_1$	$C222_1$	$C_{62}H_{80}N_8NaNi_4O_{16}\cdot ClO_4$	Adams *et al.* (2004)
BENWUN	C2	$C222_1$	$C_{62}H_{80}N_8NaNi_4O_{16}\cdot PF_6$	Adams *et al.* (2004)
DALNAG	$P2_1$	$P2_1/m$	$C_{28}H_{40}Cl_2N_6Ru\cdot PF_6\cdot 2(H_2O)$	Jitsukawa *et al.* (2004)
FENXOM	C2	C2/c	$C_{26}H_{24}CuN_8O_4S\cdot 8.5(H_2O)$	Zhu *et al.* (2005)
FENXUS	$P\overline{1}$	C2/c	$C_{26}H_{24}CoN_8O_4S\cdot 8.25(H_2O)$	Zhu *et al.* (2005)
LARTOO	$P\overline{1}$	C2/c	$C_{17}H_{26}N_3O_2P$	Gholivand *et al.* (2005)
DELJEK	$P2_1/a$	Pbam	$C_{26}H_{24}FeN_6Se_2\cdot 2(C_2H_6O)$	Morita *et al.* (2006)
DIFGIJ	$P\overline{1}$	$P2_1/c$	$C_{10}H_8F_6O_4Pt$	Zharkova *et al.* (2006).
NIMPOP	Pc	$P2_1/c$	$C_{35}H_{32}Cu_2MgN_4O_{10}\cdot CH_4O$	Tao *et al.* (2006)
CIBKAA	$P\overline{1}$	C2/c	$C_{44}H_{50}N_2O_4Ti$	Boyle *et al.* (2007)
TIZZAE	Pnc2	Pbcn	$C_{14}H_{26}N_4Cu$	Morozova *et al.* (2007)

TABLE 2S. Space group revisions; original space group, P1 (No. 1)

Refcode	S. G.	Formula Unit	Reference
CEGJUU	Cc	$C_{14}H_{23}NO_7Sn_2 \cdot C_{12}H_8N_2$	Ma *et al.* (2006)
CEPKOY	Cc	$C_{22}H_{14}O_3$	Zhu *et al.* (2006)
DELHUY	$P\bar{1}$	$C_{26}H_{24}FeN_6S_2 \cdot C_2H_6O$	Morita *et al.* (2006)
DERMET	$P\bar{1}$	$C_{38}H_{46}N_2NiS$	Malyshev *et al.* (2006)
DESNUL	$P\bar{1}$	$C_{24}H_{44}O_2$	Wang *et al.* (2006)
DIDTIU	$P\bar{1}$	$C_{10}H_8F_6O_4Pt$	Zharkova *et al.* (2006)
ECEHAW	$P2_1$	$C_{26}H_{16}N_4OS$	Ogura *et al.* (2006)
HEQZAF	$P\bar{1}$	$2(C_{10}H_{21}N_2) \cdot C_6NiS_{10}$	Onozaki & Miyamura (2006)
JECROZ	$P2_1$	$C_{36}H_{48}Cl_4Cu_2N_4O_4$	Hatano *et al.* (2006)
KEVKIG	$P\bar{1}$	$C_{14}H_{16}Fe_2O_9S_2$	Song *et al.* (2006)
PEDSUN	$P\bar{1}$	$C_{16}H_{14}N_6Ni_2O_2S_4$	Shi *et al.* (2006)
SEWXUO	$P\bar{4}n2$	$C_{32}H_{30}Co_2CrLaN_8O_{12}$	Shiga *et al.* (2006)
SEWYAV	$P\bar{4}n2$	$C_{32}H_{30}Co_2CrGdN_8O_{12}$	Shiga *et al.* (2006)
TEJCAN	$P2_1$	$C_{40}H_{40}FeN_2PPd \cdot SbF_6 \cdot CH_2Cl_2$	Hintermann *et al.* (2006)
UCUNOW	$P\bar{1}$	$C_{24}H_{20}As \cdot C_6H_{12}Cl_8N_3O_3Pt_2 \cdot 0.5(C_5H_{12})$	Pellicani *et al.* (2006)
VENPOU	$P2_12_12_1$	$C_{23}H_{14}F_6O_5S_2$	Hasegawa *et al.* (2006)
VIMBID	$P\bar{1}$	$C_{28}H_{48}N_2O_4$	Uncuta *et al.* (2006)
ZENVAP01	$P\bar{1}$	$C_{13}H_{12}O$	Babkov *et al.* (2006)
CIBLOP	$P\bar{1}$	$C_{24}H_{22}N_2O_4S_2Ti$	Boyle *et al.* (2007)
CIWFEU	$P\bar{1}$	$C_{32}H_{18}F_4$	Ie *et al.* (2007)
CIWGAR	$P\bar{1}$	$C_{36}H_{16}F_{10}O_2$	Ie *et al.* (2007)
DICREN	$P\bar{1}$	$C_{21}H_{31}N_5O_6$	Comelles *et al.* (2007)
DIHXUO	$P\bar{1}$	$2(C_{12}H_{16}N_8Zn) \cdot C_6H_8Mo_8N_4O_{26} \cdot 6(H_2O)$	Tian *et al.* (2007a)
GIJQUM	$P\bar{1}$	$C_{34}H_{52}CoP \cdot 2PF_6$	Yu *et al.* (2007)
HEYHEZ	$P\bar{1}$	$C_{28}H_{34}Cl_2Cu_2N_6 \cdot 2(ClO_4)$	Liang *et al.* (2007)
HEZJIG	$P\bar{1}$	$2(C_{19}H_{14}Cl_2N_2O_2) \cdot CH_2Cl_2$	Cheng & Cheng (2007)
HIDJUA	$P\bar{1}$	$C_{11}H_{14}N_2O_2S$	Lin *et al.* (2007)
HIGHAH	$P\bar{1}$	$C_{19}H_{14}O_2$	Kavala *et al.* (2007)
KEYSAJ	$P\bar{1}$	$2(C_3H_{10}N) \cdot C_{12}H_8O_6S_2 \cdot C_4H_8O_2$	Mizobe *et al.* (2007)
KEYSIR	$P\bar{1}$	$2(C_3H_{10}N) \cdot C_{12}H_8O_6S_2 \cdot C_4H_8O_2$	Mizobe *et al.* (2007)
KICDEG	$P\bar{1}$	$C_{18}H_{24}CoN_{12} \cdot 2(C_7H_4NO_4) \cdot 2(H_2O)$	Shi *et al.* (2007)
KIDYOM	$P\bar{1}$	$C_{32}H_{36}Ag_2N_8O_4 \cdot 2(ClO_4) \cdot 2(C_2H_3N)$	Chen *et al.* (2007)
KIDZIH	$P\bar{1}$	$C_{32}H_{36}Ag_2N_8O_4 \cdot 2(BF_4) \cdot C(_2H_3N) \cdot H_2O$	Chen *et al.* (2007)
LEZLEI	$P2_1$	$C_{35}H_{32}O_5$	Shimasaki *et al.* (2007)
MILDUH	$P2_1$	$C_{18}H_{28}C_{12}Cl_2N_2P_2Pd \cdot CH_2Cl_2$	Imamoto *et al.* (2007)
ODUWEQ	$P\bar{1}$	$C_6H_8N \cdot C_6H_7N \cdot H_4B_5O_{10}$	Beckett *et al.* (2007)
RIFSEF	Fdd2	$C_{12}H_{24}Br_3FeN_4O_2$	Lundberg *et al.* (2007)
TIDXAG	$P\bar{1}$	$C_{62}H_{40}Br_6N_4O_{12}Tb_2 \cdot 2(C_7H_5BrO_2) \cdot 2(H_2O)$	Li *et al.* (2007a)
TIDXEK	$P\bar{1}$	$C_{52}H_{38}Br_4N_4O_{12}Tb_2$	Li *et al.* (2007a)
TILDUO	$P\bar{1}$	$C_{56}H_{34}Eu_2N_4O_{20}$	Tian *et al.* (2007b)
TILROW	$P\bar{1}$	$C_{62}H_{40}Cl_6Dy_2N_4O_{12}$	Li *et al.* (2007b)
VICVUZ	$P\bar{1}$	$C_{16}H_{21}ClCuN_3O \cdot ClO_4$	Mikata *et al.* (2007)
WEWZII	$P\bar{1}$	$C_{34}H_{28}O_{14} \cdot C_3H_6O \cdot CHCl_3$	Tatsuta *et al.* (2007)
WEZBAF	C2	$C_{14}H_{21}NO_7$	Metta-Magana *et al.* (2007)
XIJPUC	$P\bar{1}$	$C_{45}H_{31}F_8N_2NiO_2 \cdot C_{24}BF_{20} \cdot CH_2Cl_2$	Meinhard *et al.* (2007)
XIKCOK	$P\bar{1}$	$C_{17}H_{23}Cl_4IrN_2 \cdot PF_6 \cdot 0.5(CH_4O)$	Corberan *et al.* (2007)

TABLE 2S. Space group revisions; original space group, P1 (No. 1) - Continued

Refcode	S. G.	Formula Unit	Reference
BOHCOR	$P\bar{1}$	$C_{21}H_{26}N_2$	Iglesias *et al.* (2008)
CIZBOD	$P\bar{1}$	$C_{19}H_{18}N_2O_2S$	Cho & Chang (2008)
CONKAS	$P\bar{1}$	$C_{74}H_{94}N_6O_{12}\cdot 2(CHCl_3)$	Lin *et al.* (2008)
DISHIX	$P\bar{1}$	$C_{18}H_{20}O_4$	Cacciapaglia *et al.* (2008)
DISHOD	$P\bar{1}$	$C_{18}H_{20}O_4$	Cacciapaglia *et al.* (2008)
DOCFOR	$P\bar{1}$	$C_{30}H_{30}N_{10}Ni_2O_6$	Xing *et al.* (2008)
DOCFUX	$P\bar{1}$	$C_{15}H_{15}N_5O_3Zn$	Xing *et al.* (2008)
DOCXID	$P\bar{1}$	$C_{62}H_{40}Cl_6N_4O_{12}Tb_2$	Li *et al.* (2008)
KIYRAM	C2/c	$C_{22}H_{20}N_8O_4$	Shawali *et al.* (2008)
KOMYAN	$P\bar{1}$	$C_{24}H_{16}Cu_2N_4O_8\cdot 4(H_2O)$	Csonka *et al.* (2008)
NOMXUJ	$P\bar{1}$	$C_{36}H_{48}N_6Zn$	Zheng *et al.* (2008)
PIXMOZ	$P\bar{1}$	$C_6H_{10}N_2\cdot 2(ClO_4)$	Kapoor *et al.* (2008)
POCMUQ	$P\bar{1}$	$C_{76}H_{48}F_{12}N_4O_8Pb_2$	Marandi *et al.* (2008)
POKLEH	Cc	$C_{21}H_{25}MnN_5O\cdot 2(C_{24}H_{20}B)$	Hureau *et al.* (2008)
QOFTAH	$P\bar{1}$	$C_{26}H_{46}F_2N_2O_2Sn_2\cdot\ 2(CF_3O_3S)$	Svec *et al.* (2008)
QQQWPO02	$P\bar{1}$	$C_{10}H_8CuF_6O_4$	Baidina *et al.* (2008)
ROJTIA	$P\bar{1}$	$C_{54}H_{50}Eu_2)_{22}$	Yan *et al.* (2008)
YOKPUK	$P\bar{1}$	$C_{24}H_{36}Ag_2Cl_2N_{12}O_8$	Luo *et al.* (2008)
YOMKER	$P2_1$	$C_{12}H_{13}NO_2$	Chmielewski *et al.* (2008)
XIXCOX	$P\bar{1}$	$C_{128}H_{146}N_{14}Zn_2\cdot 4(C_6H_6)\cdot 8(C_2H_3N)$	Maeda *et al.* (2008)

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