Table 1. *Structures originally described in space group P*1 *that are more properly described in higher symmetries.* Included are the "Reference Code" (Cambridge Structural Database, 1992) and the revised space group.

Refcode	S. G.	Z	Formula Unit	Reference	Note
ABEGET	P1-bar	4	$C_{18}H_{26}O$	Nakamura *et al.* (2000)	*a*
ACANUN	P1-bar	1	$C_{16}H_{18}N_6O_8Cl_2Pd$	Federov *et al.* (2001)	*b*
ADOVOE	C2	4	$C_{47}H_{67}N_{10}O_{11}I{\cdot}CH_3NO_2$	Schoenholzer *et al.* (2000)	*c*
AGEBIX	P1-bar	1	$C_{20}H_{44}O_4Sn_2$	Boyle *et al.* (2002)	
AGECIY	P1-bar	2	$C_{30}H_{23}N_2OCl_3PSRe$	Gangopadhyay *et al.* (2002)	
BAPDOL	C2	4	$C_{32}H_{42}O_6Ti_2$	Spaether *et al.* (1997)	
BAQDEC	P1-bar	1	$C_{22}H_{40}N_6O_2Ni$	Choi *et al.* (1999b)	
BOYPIO	P1-bar	1	$2(C_9H_{27}N_3O_3Cu){\cdot}C_6H_{16}N_2O_2Cu{\cdot}4(CF_3O_3S)$	Nieuwpoort *et al.* (1983)	
CIBNIK	P1-bar	2	$C_5H_{12}N{\cdot}C_{16}H_{13}N_4OS_3{\cdot}0.5(C_3H_6O)$	Graubaum *et al.* (1993)	*d*
CIJFAC01	P1-bar	1	$C_{32}H_{22}N_2O_4Cl_2Pd{\cdot}4(C_3H_7NO)$	Qin *et al.* (2002)	*e*
COTKEB	P1-bar	1	$C_{32}H_{64}O_2B_2Ga_2$	Anulewicz-Ostrowska *et al.* (1999)	
DAGSEJ	P1-bar	1	$C_{42}H_{58}N_2P_4Ni{\cdot}2(C_{24}H_{20}B)$	Mealli *et al.* (1985)	
DAVLER	P1-bar	1	$C_{12}H_{28}N_2O_4{\cdot}2(C_{14}H_7O_4){\cdot}2H_2O$	Gómez-Lara *et al.* (1999)	*f*
DIQZAE	P1-bar	1	$C_{10}H_{28}O_{16}Nd_2{\cdot}2Cl{\cdot}4H_2O$	Legendziewicz *et al.* (1999)	
DOLZEJ	P1-bar	2	$C_{32}H_{49}SiSm{\cdot}0.5(C_6H_{14})$	Evans *et al.* (1999)	*g*
EDOWUP	P1-bar	2	$C_{42}H_{54}N_4$	Maury *et al.* (2001)	*h*
FESNIA	Cc	4	$C_7H_6N_2O_5$	Nyburg *et al.* (1987)	
FEXCOA	P1-bar	1	$C_{34}H_{52}N_2O_6Cl_2$	Jinling *et al.* (1987)	
FIQDOY	P1-bar	2	$(C_8H_6S_6)_4{\cdot}H_{16}O_{32}Ca_2TeW_6{\cdot}7H_2O$	Boubekeur *et al.* (1998)	
GIXPAE	P1-bar	1	$C_{30}H_{28}N_2O_4{\cdot}2(C_7H_8O)$	Kishikawa *et al.* (1999)	
GIXREK	P1-bar	1	$C_{30}H_{28}N_2O_4{\cdot}2(C_{10}H_8O)$	Kishikawa *et al.* (1999)	
GIXWAL	P1-bar	1	$C_{12}H_{14}N_2{\cdot}Sb_2Cl_8$	Jaschinski *et al.* (1998)	
GOBNOA	P1-bar	1	$C_{18}H_{40}N_{14}FeNi_2{\cdot}NO_3{\cdot}2H_2O$	Kou *al.* (1998)	*i*
GOVSEP	P1-bar	2	$C_{22}H_{20}FeRu{\cdot}PF_6$	Watanabe *et al.* (1998)	
GULPUY	R3	9	$C_{33}H_{33}NSi$	Kawachi *et al.* (1999)	
GUPPOW	P1-bar	1	$C_{36}H_{32}N_4S_4Ag_2 \cdot 2ClO_4$	Zhao *et al.* (2000)	*j*
HIJYII	P1-bar	1	$C_{42}H_{30}O_6F_6Zn{\cdot}2SbCl_6{\cdot}C_7H_5OF$	Müller & Vahrenkamp (1999)	*k*
HITNED	P1-bar	2	$C_{14}H_{16}N_4O_4$	Marek *et al.* (1995)	
HOKCUF	P1-bar	1	$C_{38}H_{30}O_2Cl_2P_2Ru$	De Araujo *et al.* (2001)	
HORLOP	P1-bar	1	$C_{32}H_{50}N_6O_8Ni_2{\cdot}14(H_2O)$	Zhu *et al.* (1999)	*l*
HOZGAE	Cc	4	$C_{56}H_{50}N_2O_2Ti$	Thorn *et al.* (1999)	
ICISES	P1-bar	1	$C_{68}H_{80}P_2S_4Fe_2Pt$	Wong *et al.* (2001)	*m*
IFAGUR	$P2_12_12_1$	4	$C_{18}H_{16}O_4$	Kumagai *et al.* (2001)	
IFEDEC	P1-bar	2	$C_{20}H_{44}N_6Si_2Zr$	Skinner *et al.* (2002)	

Notes

a Several hydrogen atoms are disordered or missing.

b The hydrogen atoms on one methylene group are missing.

c The hydrogen atoms of the solvent molecule are apparently disordered.

d The acetone solvate is unpaired in space group P1-bar.

e The hydrogen atoms on one solvent methyl group are apparently disordered.

f The hydrogen atoms of the water molecules were apparently misplaced, and have been removed.

g Many hydrogen atoms appear to be disordered; all have been deleted, plus two disordered atoms of the hexane solvent.

h In both molecules in the asymmetric unit, two butyl groups appear to be disordered.

i In P1-bar the nitrate ion lies on a center of symmetry, and must be disordered. Its geometry and U's are peculiar in P1.

j The disordered oxygen atoms of the perchlorate group have been removed.

k In P1-bar the fluorobenzaldehyde molecule lies on a center of symmetry, and must be disordered. It was restrained – and distorted – in P1.

l The hydrogen atoms bonded to nitrogen are missing.

m One methyl group appears to be disordered.

KAHBUQ	P1-bar	1	$C_{32}H_{50}N_6Zn{\cdot}2Cl{\cdot}10H_2O$	Choi *et al.* (1999a)	*n*
KETCAN	P1-bar	2	$C_{12}H_{17}N_3O_2S$	Kovala-Demertzi *et al.* (2000)	
MAPNUM	P1-bar	1	$2(C_{34}H_{72}N){\cdot}Cr_2O_7$	Fosse & Brohan (1999)	*o*
MAYSUA	P1-bar	2	$C_{50}H_{92}P_4Pt_2{\cdot}2(C_6H_6)$	Ficker *et al.* (2000)	
MERYEN	P1-bar	2	$C_{26}H_{32}N_4Cu{\cdot}ClO_4$	Osako *et al.* (2001)	
MEYYEU	P1-bar	2	$C_{34}H_{25}NO_2$	Kohmoto *et al.* (2001)	
MITQUB	P1-bar	2	$C_{23}H_{18}N_2O_2Mo{\cdot}0.5(CH_2Cl_2)$	Pérez *et al.* (2002)	*p*
MIZLAI	P1-bar	1	$C_{44}H_{60}N_{10}O_{24}S_2Nd_2$	Xu *et al.* (2001)	*q*
NAVQAC	P1-bar	1	$2(C_{24}H_{20}P){\cdot}C_6N_6Br_8Mo_6{\cdot}4(H_2O)$	Simsek *et al.* (1997)	
NEQROQ	P1-bar	1	$C_{54}H_{72}N_4O_4Zn_2$	Cheng *et al.* (2001)	*r*
NEQSAD	P1-bar	1	$C_{50}H_{64}N_4O_4Zn_2$	Cheng *et al.* (2001)	*r*
NIBLEP	P1-bar	1	$C_{42}H_{32}S_4Sn_2$	Sato & Sensui (1997)	
NINPOP	P1-bar	2	$C_{20}H_{21}N_2OPd{\cdot}C_{24}H_{20}B{\cdot}2(CH_2Cl_2)$	Kositzyna *et al.* (1996)	
NUCFAS	P1-bar	1	$C_{64}H_{68}O_8Ti_2{\cdot}C_7H_8$	Mahrwald *et al.* (1996)	*s*
OMAPBD	P1-bar	1	$C_{12}H_{28}N_4O_2P_2$	Born (1969)	*t*
PAHGAG	P1-bar	1	$5(C_6S_{10}Ni){\cdot}C_{10}H_{26}N_2{\cdot}2(C_2H_3N)$	Cornelissen *et al.* (1992)	
PAPDEP	P1-bar	1	$C_{16}H_{20}O_4F_6Cu{\cdot}C_{12}H_{24}O_6$	Polyanskaya *et al.* (1991)	*u*
PAQYUB	P1-bar	2	$C_8H_{20}O_4Cl_2S_4Ru{\cdot}H_2O$	Yapp *et al.* (1997)	*v*
PHPNCD	P1-bar	1	$C_{52}H_{44}N_4O_4Cd$	Rodesiler *et al.* (1980)	
PIDBEJ	P1-bar	1	$C_{18}H_{42}N_6O_6Fe{\cdot}S_6W_2$	Zhang *et al.* (1992)	
QEKSAA	P1-bar	2	$C_{60}H_{64}O_{10}Cs{\cdot}C_{24}H_{20}B{\cdot}CHCl_3$	Blanda *et al.* (2000)	*w*
QETTEO	P1-bar	2	$C_{16}H_{15}N_3O_2$	Sauro & Workentin (2001)	
QIMRIN	P1-bar	2	$C_{18}H_{32}N_{11}O_{11}Pr$	Kahn *et al.* (2000)	
QOSBOP	I4-bar	2	$C_{40}H_{40}O_8{\cdot}C_6H_6$	Choi & Hiratani (1999)	*x*
QUDQOV	P1-bar	1	$C_{68}H_{94}N_8O_2Si_3$	Sasa *et al.* (1998)	
QUDQUB	P1-bar	1	$C_{52}H_{62}N_8O_2Si_3$	Sasa *et al.* (1998)	
QUJDAA	Cc	4	$C_7H_9N_2O{\cdot}C_6H_5O_4S$	Anwar *et al.* (1999)	
QURGIT	P1-bar	2	$C_{81}H_{102}N_6O_6{\cdot}0.5(CH_3OH){\cdot}0.5(C_2H_3N)$	Sénèque *et al.* (2001)	*y*
RAWKEF	Cc	2	$2(C_9H_{18}Cl_6Te_3){\cdot}C_3H_7NO{\cdot}1.5(H_2O)$	Takaguchi *et al.* (1996)	*z*
ROFTUB	C2	4	$C_{13}H_{21}N_2O_5ClS$	Bregant *et al.* (2001)	
ROQHAG	Cm	2	$C_{38}H_{39}NO_4P_2Mo$	Jacobi *et al.* (1997)	
SEQPOT	P1-bar	6	$C_{16}H_{24}O_2$	Lokanath *et al.* (2000)	
SUYYEQ	P1-bar	1	$C_{30}H_{26}N_{12}F_{18}B_2Cu$	Hu *et al.* (2001)	
TCNICO	P1-bar	1	$C_{14}H_{16}N_6O_4S_2Co$	Tsintsadze *et al.* (1979)	
TIDJOF	P1-bar	1	$C_{48}H_{50}N_2O_6F_6P_2Ag_2$	Brandys & Puddephatt (2001)	
TIRVUL	P1-bar	1	$C_{32}H_{52}P_2Pt$	van der Boom *et al.* (1996)	
TIYYOP	C2	4	$C_{13}H_{24}O_{10}{\cdot}0.5(H_2O)$	Watt *et al.* (1996)	*aa*
TUJGUA	P1-bar	1	$C_{28}H_{16}Cl_2O_2S_2{\cdot}2(C_6H_6)$	Mori *et al.* (1996)	*bb*
TULKIU	P1-bar	1	$C_6N_6O_6Cl_8Mo_6{\cdot}2(C_{16}H_{36}N)$	Simsek & Preetz (1997)	*cc*
TULLAN	P1-bar	1	$C_6N_6Se_6Br_8Mo_6{\cdot}2(C_{16}H_{36}N){\cdot}2(C_3H_6O)$	Simsek & Preetz (1997)	

Notes

n Isostructural with the Ni compound (KAGVOD).
o The dichromate ion is disordered.
p The dichloromethane solvent is disordered; it lies near a symmetry center in P1-bar.
q A disordered S atom has been removed.
r The H atoms of one methyl group have been removed.
s In P1-bar the toluene solvent lies on a symmetry center, and must be disordered.
t Structure was re-refined, in space group P1-bar; see text.
u The methyl groups, and perhaps the F atoms as well, are disordered.
v The H atoms of the water molecules have been removed.
w Many H atoms are missing or misplaced. All have been removed.
x The benzene molecule is disordered in either space group.
y There is considerable disorder.
z The disordered DMF and water molecules have been removed.
aa The water molecule is disordered between two sites, both lying on the 2-fold axis.
bb The bridging S and C-O atoms are disordered in either space group.
cc One terminal methyl group of the t-butyl ammonium ion appears to be disordered.

VIMTEQ	P1-bar	2	$C_{23}H_{19}NO_3$	Allouchi *et al.* (1999)	*dd*
WEDSED	C2	4	$C_{20}H_{29}NO_4$	Gees *et al.* (1993)	
WEQHEF	P1-bar	2	$C_{17}H_{14}N_2O_3$	Hernandez-Quiroz *et al.* (1998)	
WOKMUE	P1-bar	2	$C_{10}H_{10}N_3I{\cdot}H_2O$	Verardo *et al.* (2000)	
WOSZEJ	P1-bar	2	$C_{25}H_{42}N_9Rh$	Wehlan *et al.* (2000)	
XEJNUV	P1-bar	2	$C_{12}H_6N_2$	Janczak & Kubiak (2000)	
XIWBOU	P1-bar	2	$C_{22}H_{32}N_6O_8S_2Cd$	Yilmaz *et al.* (2002)	
YAGHAP	P1-bar	1	$C_{54}H_{50}N_2O_{10}Cu_2{\cdot}2(C_3H_7)NO{\cdot}H_2O$	Jiang & Yu (1992)	*ee*
YEQKAG	P1-bar	1	$2(C_{24}H_{20}P){\cdot}C_{12}H_8N_4O_4P_2S_4$	Aasen *et al.* (2001)	
AJIRAM	P1-bar	1	$C_{30}H_{26}N_4O_4Cu$	Li *et al.* (2003c)	
AJISAN	P1-bar	2	$C_{26}H_{32}N_4O_4Cu$	Tanaka *et al.* (2003)	
AJORIA	P1-bar	2	$C_{17}H_{20}N_2O_2$	Nagao *et al.* (2002)	
EKOKOE	P1-bar	2	$C_{21}H_{30}O_3$	Li *et al.* (2003a)	*ff*
IHINAO	P1-bar	2	$C_{63}H_{49}N_3O_2SClP_2Ru{\cdot}PF_6$	Panda *et al.* (2003)	
IHIQUL	P1-bar	2	$C_{45}H_{30}OPFeAu$	Wong *et al.* (2003)	
IJAKUZ	P1-bar	1	$C_{41}H_{34}O_5ClP_2Rh$	Dutta *et al.* (2003)	*gg*
IKAJAF	P1-bar	2	$C_{26}H_{25}N_2Fe{\cdot}C_8H_5O_4{\cdot}H_2O$	Lee *et al.* (2003)	
IKETEX	P1-bar	1	$C_{46}H_{38}N_2P_2I_2Cu_2$	Li *et al.* (2003b)	
JABRUA	P1-bar	1	$C_{26}H_{28}N_4Ag_2{\cdot}2ClO_4$	Shin *et al.* (2003b)	
JACNUX	P1-bar	1	$2(C_{35}H_{41}NClPRh){\cdot}NO_2{\cdot}NO_3{\cdot}2H_2O$	Han & Lee (2003)	*hh*
JACPIN	P1-bar	1	$C_{54}H_{48}N_2P_2Rh{\cdot}NO_3{\cdot}H_2O$	Han & Lee (2003)	*hh*
KADXUJ	P1-bar	1	$C_{30}H_{26}N_8O_4F_6Mo_2$	Weng *et al.* (2003)	*ii*
OHUGED	P2(1)	2	$C_6H_8N_2O_6SMn$	Song *et al.* (2003)	
OKEKEU	P1-bar	2	$C_8H_{25}N_5ClCo{\cdot}ZnCl_4$	Tao *et al.* (2003)	
TAFROI	P1-bar	1	$C_6H_{18}N_2{\cdot}H_{12}O_{26}B_{12}Zn{\cdot}2(H_2O)$	Natarajan *et al.* (2003)	*jj*
VAHCEN	P1-bar	2	$C_{24}H_{34}N_3O_2S_3Re$	Liu *et al.* (2002)	
VAJPUS	P1-bar	1	$C_{42}H_{26}N_4O_{14}Co_3$	Hao *et al.* (2003)	
VAJZIQ	P1-bar	2	$C_{24}H_{29}NO_5S$	Sun *et al.* (2003)	*kk*
AKOXIH	P2(1)/c	4	$C_{29}H_{30}O_3S$	Carreño *et al.* (2003)	
AMAQAG	P1-bar	1	$C_{38}H_{34}N_6O_8Ni_2{\cdot}2(C_5H_5N)$	Ohmura *et al.* (2003)	*ll*
AMEJUX	P1-bar	2	$C_{11}H_{16}N_4Cl_2Hg$	del Hierro *et al.* (2003)	
BAZCAH	P1-bar	1	$C_{42}H_{36}N_{12}O_4Cu_2{\cdot}2ClO_4{\cdot}3H_2O$	Youngme *et al.* (2003)	*mm*
BAZCEL	P1-bar	1	$C_{42}H_{36}N_{12}O_4Cu_2{\cdot}2BF_4{\cdot}3H_2O$	Youngme *et al.* (2003)	*nn*
BAZHAM	Pna2(1)	8	C_2H_8OSi	Mitzel (2003)	
UKOROB	P1-bar	1	$C_{36}H_{37}O_2F_{12}Co$	Buzzeo *et al.* (2003)	*oo*
ARAQUF	P1-bar	2	$C_{40}H_{38}N_4O_4Ni{\cdot}0.5(C_3H_6O)$	Eilmes *et al.* (2003)	*pp*
ARARAM	P1-bar	1	$C_{34}H_{34}N_8Cl_2S_2Cu_2$	Sreekanth & Kurup (2003)	*qq*
EQOXIR	P1-bar	1	$C_{40}H_{36}N_{10}O_2O_2S_2Co$	Shin *et al.* (2003a)	
ESAHOV	P1-bar	2	$C_{18}H_{22}N_4O_7ClFe{\cdot}C_2H_3N$	Velusamy *et al.* (2003)	
IQACIM01	P1-bar	2	$C_{24}H_{30}N_4{\cdot}2(C_{12}H_4N_4)$	Nishimura *et al.* (2002)	
IQOYIW	P1-bar	2	$C_{11}H_{10}N_3O_2ClCu$	Youngme (2004)	

Notes

dd The central ethylene grouping is disordered over two orientations.

ee The water molecule is misplaced, and has been removed.

ff In the same paper, EKOKIY should be revised from Pc to P2(1)/c).

gg The CO and Cl ligands are disordered in P1-bar, and have been removed; they were restrained in P1.

hh The anions and the water molecules are disordered, and have been removed.

ii The F atoms are disordered equally between two sets of positions.

jj The H atoms of the water molecules have been deleted.

kk The propyl group is disordered; those H atoms have been removed.

ll In the same paper, the entry AMAQEK should be revised from Cc to C2/c.

mm Several disordered oxygen and hydrogen atoms have been removed.

nn The disordered BF(4) anions and water molecules have been removed.

oo The two trifluoromethyl groups and three methyl groups are disordered. The O–H–O bond is very short (2.43 Å) and centrosymmetric.

pp The acetone solvent is disordered across a center of inversion.

qq Several H atoms of the pyrrolidine ring were misplaced, and have been removed.