

STRUCTURES OF SMALL MOLECULES SOLVED BY THE CRYSTALLISATION FACTORY IN 2009

MOLECULE NAME	DATABASE	REGISTRATION CODE
ethyl-N,N',N''-trialkylbenzene-1,3,5-carboxamide		
propyl-N,N',N''-trialkylbenzene-1,3,5-carboxamide		
[Sm(bpym)(NO ₃) ₂ (H ₂ O) ₃][Fe(bipy)(CN) ₄] · H ₂ O ·	CCDC	696695
[[Gd(bpym)(NO ₃) ₂ (H ₂ O) ₃][Fe(bipy)(CN) ₄] · H ₂ O · CH ₃ CN	CCDC	696696
[Tb(bpym)(NO ₃) ₂ (H ₂ O) ₃][Fe(bipy)(CN) ₄] · H ₂ O · CH ₃ CN	CCDC	696697
[Dy(bpym)(NO ₃) ₂ (H ₂ O) ₃][Fe(bipy)(CN) ₄] · H ₂ O · CH ₃ CN	CCDC	696698
[Ho(bpym)(NO ₃) ₂ (H ₂ O) ₃][Fe(bipy)(CN) ₄] · H ₂ O · CH ₃ CN	CCDC	696699
[Pr(bpym)(NO ₃) ₂ (H ₂ O) ₄][Fe(bipy)(CN) ₄]	CCDC	696700
[Nd(bpym)(NO ₃) ₂ (H ₂ O) ₄][Fe(bipy)(CN) ₄]	CCDC	696701
[Sm(bpym)(NO ₃) ₂ (H ₂ O) ₄][Fe(bipy)(CN) ₄]	CCDC	696702
[Gd(bpym)(NO ₃) ₂ (H ₂ O) ₄][Fe(bipy)(CN) ₄]	CCDC	696703
[Cu(3-lpy)(Memal)(H ₂ O)]	CCDC	705220
[Cu(2,4'-bpy)(Memal)(H ₂ O)] · 3H ₂ O	CCDC	705221
[Cu ₄ (mpba)(Me ₄ en) ₄ (H ₂ O) ₄](ClO ₄) ₄ · 3H ₂ O	CCDC	650175
[Cu ₄ (mpba)(Me ₄ en) ₄ (H ₂ O) ₄](PF ₆) ₄ · 2H ₂ O	CCDC	650176
[Cu ₄ (ppba)(Me ₄ en) ₄ (H ₂ O) ₄](ClO ₄) ₄ · 2H ₂ O	CCDC	711356
[Cu ₄ (mpba)(dipn) ₄](ClO ₄) ₄ · 3H ₂ O	CCDC	711357
[Cu ₄ (ppba)(dipn) ₄](ClO ₄) ₄ · 2H ₂ O	CCDC	711359
[Cu ₂ Ni ₂ (ppba)(dipn) ₄ (H ₂ O) ₂](PF ₆) ₄	CCDC	723126
[Co(H ₂ O) ₂ (phda)] _n	CCDC	723127
[Co(phda)] _n	CCDC	723128
[Co(chda)] _n	CCDC	
Gomerolactone C		692916
Gomerolactone D	CCDC	692917
[Gd ₂ (ac) ₆ (H ₂ O) ₄] · 2H ₂ O	CCDC	721062
[Gd ₂ (ac) ₂ (fum) ₂ (H ₂ O) ₄] _n	CCDC	721063
[Co ₂ (bta)(4,4'-bpy) ₂ (H ₂ O) ₂] _n		
{Hbpe[Co(Hbta)(bpe)(H ₂ O) ₂]} _n		
{[Co(H ₂ bta)(azpy)(H ₂ O) ₂] · azpy} _n		
{[Co ₂ (bta)(bpa) ₂ (H ₂ O) ₄] · 8H ₂ O} _n		

[Cu ₃ (dipyatriz) ₂ (H ₂ O) ₃](ClO ₄) ₆ · 2H ₂ O	CCDC	722374
{[Cu ₄ (dipyatriz) ₂ (H ₂ O) ₂ (NO ₃) ₂ (ox) ₂](NO ₃) ₂ · 2H ₂ O} _n	CCDC	722375
[Cu ₆ (dipyatriz) ₂ (H ₂ O)(NO ₃) ₃ (ox) ₃](NO ₃) ₃ · 4H ₂ O	CCDC	722376
Na ₁₂ [Co ₃ (obmpox) ₃] · 33H ₂ O		
Na ₁₁ [Co ₃ (obmpox) ₃] · 30H ₂ O		
[{Mn ^{III} (4-MeO-salen)(H ₂ O) (m-CN)} ₄ Cr ^{III} (CN) ₂] [{Mn ^{III} (4-MeO-salen)- (H ₂ O)(m-CN)} ₂ Cr ^{III} (CN) ₄]. 2H ₂ O	CCDC	693544
[Co ₂ (bta)(H ₂ O) ₆] _n · 2nH ₂ O	CCDC	748199
[Co(phda)(H ₂ O)] _n · nH ₂ O	CCDC	748200
[Co(phda)(H ₂ O)] _n · nH ₂ O	CCDC	729732
[Gd(H ₃ clhex)(H ₂ O) ₄] _n · 3nH ₂ O	CCDC	729733
[Gd(H ₃ clhex)(H ₂ O) ₄] _n · 6nH ₂ O	CCDC	708996
[Cu(tren)(mpda)](ClO ₄) ₂ · 1/2H ₂ O	-	
[Cu ₂ (tren) ₂ (ppda)](ClO ₄) ₄ · 2H ₂ O	CCDC	708997
[Cu ₂ (tren) ₂ (bpda)](ClO ₄) ₄	-	
[Cu ₂ (tren) ₂ (tpda)](ClO ₄) ₄	CCDC	738677
{[Cr ^{III} (phen)(ox) ₂] ₂ Co ^{II} (Me ₂ bpy)} · 1.5H ₂ O	CCDC	742480
[Gd ₂ (pac) ₆ (H ₂ O) ₄]	CCDC	741329
[Gd ₂ (tpac) ₆ (H ₂ O) ₄]	CCDC	741330
K ₄ [Cr ₂ (mal) ₄ (OH) ₂] · 6H ₂ O	-	
{[Cu(tren)] ₄ [Cr ₂ (mal) ₄ (OH) ₂]}(ClO ₄) ₄ · 8H ₂ O	-	
[Ni(Htren) ₂][Cr ₂ (mal) ₄ (OH) ₂] · 8H ₂ O	-	
Cu[(M)-binaba]Co(DMF) ₂ · DMF	-	
[Gd(mta)(H ₂ O) ₃] _n · 4nH ₂ O	-	
[Gd(mta)(H ₂ O) ₃] _n · 2nH ₂ O	-	
[Gd ₂ (mta) ₂ (H ₂ O) ₂] _n · 2nH ₂ O	-	
[Rh(N(CH ₃) ₂) (Ph ₂ P)(C ₃ H ₅)(COD)] (BF ₄)		Fjl20a
[Rh(N(CH ₃) ₂) (Ph ₂ P)(C ₃ H ₅)(TFB)] (BF ₄)		Fjl69a
[Rh(C ₁₇ H ₂₁ O P) ₂] (PF ₆)		Fjl111a
[Ru(C ₁₂ H ₁₅ N ₄ O ₂) Cl (C ₈ H ₁₂)]		Fjl113a
[Rh(Cp*) (P(NMe ₂)(OC ₁₀ H ₆) ₂)OCH ₂ (NC ₅ H ₄)] (SbF ₆) ₂		Fjl114a
[Ir(Cp*) (P(NMe ₂)(OC ₁₀ H ₆) ₂)OCH ₂ (NC ₅ H ₄)] (SbF ₆) ₂		Fjl117a
[Rh(Cp*)(OC ₇ H ₆)] ₂ (SbF ₆) ₂		Fjl119a
[Ru(O ₂ C ₇ H ₁₅ N ₄)(NCCH ₃) ₃]BF ₄		Fjl123a

[Ir(Cp*) Cl ₂ (P(NMe ₂)(OC ₁₀ H ₆) ₂)		Fjl124a
[Rh(Cp*) Cl ₂ (P(NMe ₂)(OC ₁₀ H ₆) ₂)		Fjl125a
[Ir(CO) (SB ₉ H ₁₀) (PMe ₃) ₂]		Fjl126a
[(h ₅ :h ₂ -C ₅ Me ₄ CH ₂ CH=CH ₂)Re(CO) ₂]		Fjl128a
[IrBrH (C ₁₄ H ₁₃ N ₂ O) (NCCH ₃)(C ₈ H ₁₂)] BF ₄		Fjl133a
[Rh ₃ (μ-H) (μ ₃ -S) ₂ (CO) ₂ (PPh ₃) ₂ (NBD)]		Fjl134a
C ₁₁ H ₁₃ O ₂ ReS		Fjl135a
[Rh (C ₈ H ₁₂) (OPC ₁₇ H ₂₁)] BF ₄		Fjl138a
[Ir(dppp)(PN-iPr)(H)Cl] SbF ₆		Fjl141a
[Rh (POC ₁₉ H ₂₆) ₂] PF ₆		Fjl143a
[Rh ₂ Pt (C ₈ H ₁₂) (P(OPh) ₃) ₄]		Fjl145a
C ₅₄ H ₂₆ Cl F ₂₀ Ir N O P, Sb F ₆		Fjl147a
[Ir(Cp*)(P _{Bn})(C ₄ H ₇ O)] (SbF ₆) ₂		Fjl148a
[RhSB ₉ H ₁₀ (PPh ₃) ₂ (4-pic)]		Fjl151a
[RhSB ₉ H ₁₀ (PPh ₃)(3-pic)]		Fjl154a
[Rh Cl ₂ (N ₄ C ₅₈ (H ₈₀)]		Fjl155a
(p-cimeno) RuC ₁₆ H ₂₁ Cl ₂ NO ₂ , SbF ₆		Fjl163a
[{p-cimeno}Ru(NO)] ₂ (SbF ₆) ₂		Fjl167a
C ₁₉ H ₁₀ N ₂ O ₃ Re		Fjl03e
{Rh(PPh ₃)(PMe)} {Ir(PMe ₃) ₂ }		Fjl06e
[Rh ₂ Pt(μ ₃ -S) ₂ (CO) ₂ (PPh ₃) ₂ (COD)]		Fjl07e
[RhSB ₉ H ₁₀ (PMePh ₂) ₂ (Py)]		Fjl10e
[RuCl ₂ (PPh ₃)(C ₁₂ H ₁₅ N ₄ O ₂)]		Fjl14e
Piv-Ala-2(S)-BnAze-NHMe	CSD	CCDC-723375
[Sc ₂ (nds)(OH) ₄] _n	CCDC	623276
[Y(1,5-nds)(OH)(H ₂ O)] _n	CCDC	623277
[Sc ₂ (2,6-nds)(OH) ₄] _n	CCDC	718897
α-[Yb(C ₄ H ₄ O ₄) _{1,5}]-296	CCDC	706459
α-[Yb(C ₄ H ₄ O ₄) _{1,5}]-374	CCDC	706460
β-[Yb(C ₄ H ₄ O ₄) _{1,5}]-408	CCDC	706461
β-[Yb(C ₄ H ₄ O ₄) _{1,5}]-429	CCDC	706462
α-[Yb(C ₄ H ₄ O ₄) _{1,5}]-293	CCDC	706463
C ₉₇ H ₁₁₃ Cl ₂ N ₃	CCDC	728466

C112 H125 N9 O5	CCDC	728467
C27 H21 N3	CCDC	670066
β -Ln ₂ (hfipbb) ₃	CCDC	690458
γ -Ln ₂ (hfipbb) ₃	CCDC	690459
[cis-Pd-2(C ₆ H ₄ PPh ₂)(₂)(NCCH ₃)(₄)]	CCDC	714216
Sc ₂ (C ₄ O ₄) ₃	CCDC	706458
[Yb ₄ (OH) ₁₀ (H ₂ O) ₄] [2,6-AQDS]	CCDC	604277
[Yb(OH)(2,6-AQDS)(H ₂ O)]	CCDC	653646
[Zn(C ₅ Me ₄ SiMe ₃) ₂]	CCDC	720029
C ₉ H ₁₆ Er O ₈	CCDC	763862
C ₉ H ₁₅ Er O ₈	CCDC	763863
C ₁₈ H ₂₆ Er ₂ O ₁₃	CCDC	763864
C ₂₀ H ₁₈ O ₂	CCDC	750177
C ₂₂ H ₂₄ O ₄	CCDC	750178
C ₂₄ H ₁₈ O ₂	CCDC	750179
C ₂₆ H ₂₄ O ₄	CCDC	750180
C ₂₂ H ₂₀ O ₄	CCDC	750181
C ₂₂ H ₁₆ F ₆ O ₂ S ₂	CCDC	750182
C ₂₄ H ₂₂ F ₆ O ₄ S ₂	CCDC	750183
C ₂ H ₄ MnN ₄ O ₄	CCDC	717035
C ₄ H ₂₀ Mn ₂ N ₈ O ₁₄	CCDC	717036
C ₄ H ₁₆ Cu ₂ N ₈ O ₁₂	CCDC	717037
C ₁₂ H ₁₉ NniO ₇	CCDC	732816
C ₁₂ H ₂₁ NniO ₉	CCDC	732817
C ₄₂ H ₅₈ N ₁₄ Ni ₂ O ₁₂	CCDC	732818
C ₄₂ H ₅₈ N ₁₄ Ni ₂ O ₁₄	CCDC	732819
C ₁₇ H ₁₆ CuN ₄ O ₄	CCDC	730725
C ₁₃ H ₁₇ CuN ₃ O ₅	CCDC	730726
C ₁₈ H ₁₉ CuN ₃ O ₅	CCDC	730727
C ₁₄ H ₁₆ CuN ₄ O ₆ S	CCDC	730728
C ₅₅ H ₃₆ N ₁₂ O ₂₁ F ₃ SNi ₂ Tb	CCDC	750065
High Temperatura C ₁₀ H ₁₉ O ₂ H	CCDC	738369
High Temperatura C ₁₂ H ₂₃ O ₂ H	CCDC	738617

High Temperatura C14H27O2H	CCDC	738618
High Temperatura C16H31O2H	CCDC	738619
High Temperatura C18H35O2H	CCDC	738620
High Temperatura C20H39O2H	CCDC	738621
C36H35ClBN5F4Pd	CCDC	708273
C14H21NO5S	CCDC	707178
C20H31NO8S	CCDC	707179
C17H16N2O4	CCDC	705916
C29H30N2OCl2SPtFe	CCDC	
C23H14Cl2F10N2Pt	CCDC	
C38H25BrClF5NPt	CCDC	
C15H27NS2O2	CCDC	713599
[Pd(SCN)(l-med)]2 0.5CH3CN Hmed = N-(2-mercaptoethyl)-3,5-dimethylpyrazole	CCDC	690118
[Pd(N3)(l-med)]2H med = N-(2-mercaptoethyl)-3,5-dimethylpyrazole	CCDC	690119
(BF4)2, [Pd(CN)(bdtp)](BF4)	CCDC	714291
trans-[Pd(SCN)2(bddo)] bddo = 1,8-bis(3,5-dimethyl-1-pyrazolyl)-3,6-dithiaoctane)	CCDC	723189
[Pd(bedp)][Pd2Cl4(l-SMe)2] (bedp = 1,4-bis[2-(3,5-dimethyl-1-pyrazolyl)ethyl]piperazine)	CCDC	714291
C16H26Cl2N4O2Zn	CCDC	725389
C16H26Cl2N4O2Cd	CCDC	725390
C36H62Cl4N8O5Pd2	CCDC	725391
C20H34Cl2N4O3Pt	CCDC	725392
C16H30Cl2N4O4Ni	CCDC	725393
[PtCl2{NH2CH(CH3)C6H5}{SOMe2}]	CCDC	713902
[Pt(4-MeC6H4){4-ClC6H3CHNCH2CH2NMe2}]	CCDC	
[PtCl{(MeC6H3)(ClC6H3CHNCH2CH2NMe2)}]	CCDC	
[PtCl{(MeC6H3)(ClC6H3)CHNCH2(4-ClC6H4)}SEt2]	CCDC	
[PtCl{(MeC6H3)(ClC6H3)CHNCH2(4-ClC6H4)}PPH3]	CCDC	
tert-Butyl rac-N-((1R,3S,4R,5S,7R,8S,9S)-8-hydroxy-4,9-dimethyl-2,6-dioxatricyclo[3.3.1.0 ^{3,7}]non-1-yl)-carbamate	CCDC	731404
tert-Butyl rac-N-((1R,2R,4R,5S,6S,7S,8S)-7-hydroxy-6,8-dimethyl-3,9-dioxatricyclo[3.3.1.0 ^{2,4}]non-1-yl)-carbamate	CCDC	720950
tert-Butyl rac-N-((1R,2S,4S,5S,6S,7S,8S)-7-hydroxy-6,8-dimethyl-3,9-	CCDC	720951

dioxatricyclo[3.3.1.0 ^{2,4}]non-1-yl}-carbamate		
CdCl ₂ 1-[(2-(tert-butylamino)ethyl)]-3,5-dimethylpyrazole	CCDC	694165
CdCl ₂ bis-[(3,5-dimethylpyrazolyl)-methyl]ethylamine	CCDC	694166
5-[2-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl] ethyl]-6-chloro-1,3-dihydro-2H-indol-2-one	CCDC	694162
[PtMe ₂ {j ₂ -(C,N)-4-ClC ₆ H ₃ CH=NCH(CH ₂ C ₆ H ₅)CO ₂ Me}(PPh ₃)]	CCDC	723579
[PtMe ₂ {j ₂ -(C,N)-4-ClC ₆ H ₃ CH=NCH(CH ₂ C ₆ H ₄ -(4'-OH))CO ₂ Me}(PPh ₃)]	CCDC	723580
[PtMe ₂ {j ₂ -(C,N)-4-ClC ₆ H ₃ CH=NCH(CH ₂ C ₆ H ₅)CO ₂ Me}(PPh ₃)]	CCDC	723581
cis-[PdCl ₂ ((3,5-dimethyl-1H-pyrazol-1-yl)methyldiphenylphosphinite)]	CCDC	686189
trans-III-[CrCl ₂ L ₁₅](ClO ₄) ₂	CCDC	736218
trans-III-[CrCl(HL ₁₄)(H ₂ O)](ClO ₄) ₃ · 2H ₂ O	CCDC	736219
[Pd(Me ₂ NCH ₂ (CH ₂) _n -NCH(2-C,4-ClC ₅ H ₃))Cl]	CCDC	699234
[j ₂ -N,C ₁ -g ₂ -C ₃ ,C ₄ -Pd{(PhC=CPh) ₂ -C ₁₀ H ₆ -CH ₂ -N=CH-(2,6-Cl ₂ C ₆ H ₃)}Cl]·CH ₂ Cl ₂	CCDC	717397