

ELECTRONIC SUPPLEMENTARY INFORMATION

for

Organizing a bis(iminoylnitroxide) diradical into antiferromagnetically coupled chains by co-crystallization with dichloromethane

*Handan Akpınar,^a John A. Schlueter^b and Paul M. Lahti^{*a}*

^aDepartment of Chemistry, University of Massachusetts, Amherst, MA 01003 USA

^bDivision of Materials Research, National Science Foundation, 4201 Wilson Boulevard,
Arlington, VA 2223 USA

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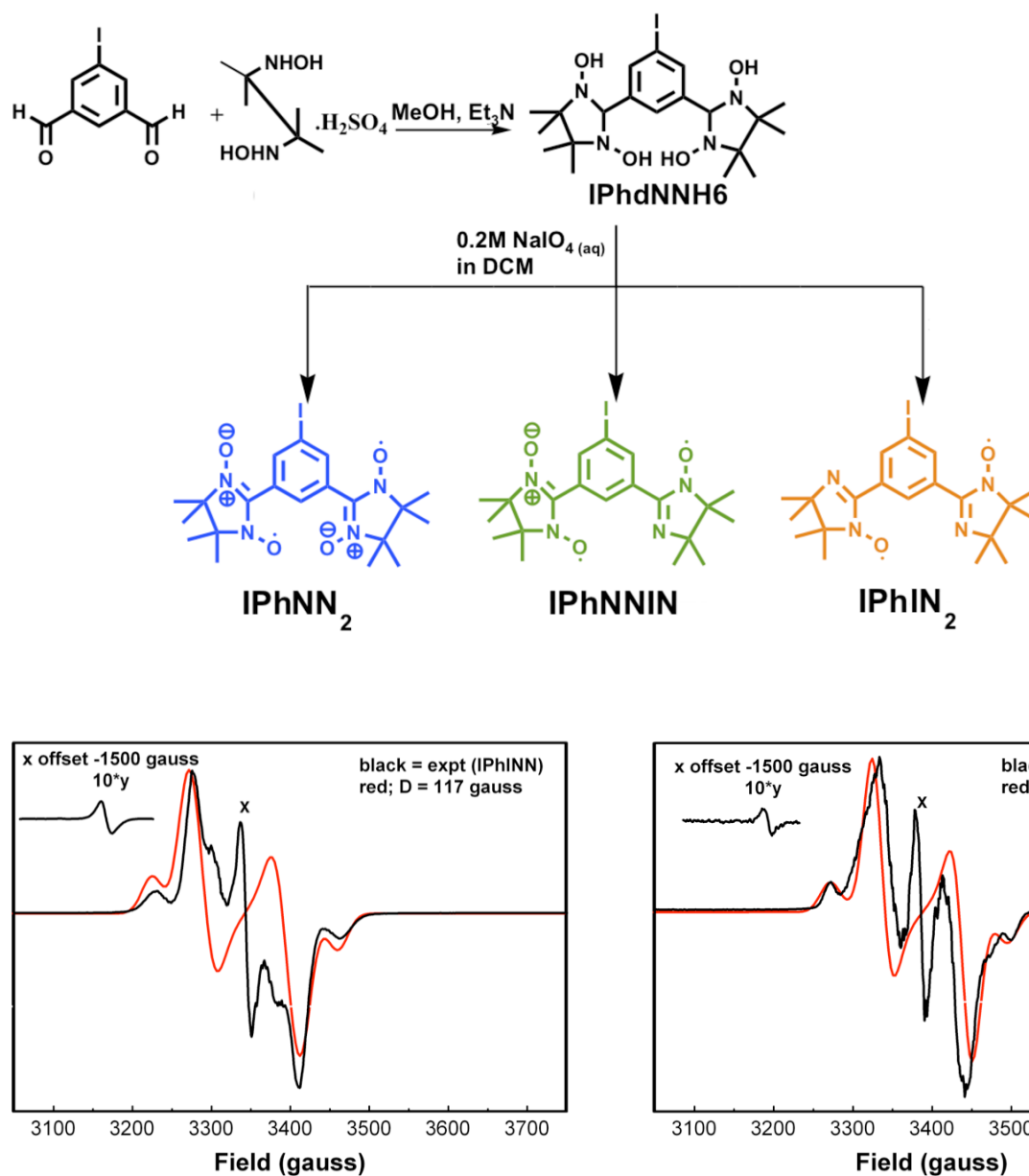


Figure S1. Left -- EPR spectrum of IPhNNN in frozen toluene at 80 K: experimental spectrum at 9.37043 GHz (solid black); simulation with $|D| = 117$ gauss (red dotted). Upper left inset is half-field region with field-offset -1500 gauss, 10× intensity-expanded. "X" experimental peak is not part of diradical spectra.

Figure S2. Right -- EPR spectrum of IPhNN₂ in frozen toluene at 80 K: experimental spectrum at 9.49648 GHz (solid black); simulation with $|D| = 112$ gauss (red dotted). Upper left inset is half-field region with field-offset -1500 gauss, 10× intensity-expanded. "X" experimental peak is not part of diradical spectra.

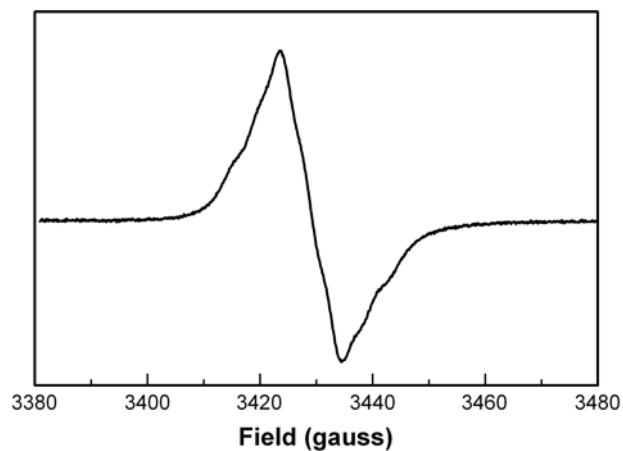


Figure S3. EPR spectrum of IPhIN₂ in toluene at room temperature, at 9.62712 GHz.

Mathematical Expressions Used for Mathematical Analysis.

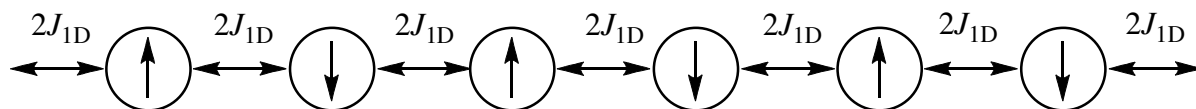
- 1-D linear Heisenberg chain model for $S = 1/2$ spin units

From D. D. Swank, C. P. Landee and R. D. Willet, *Phys. Rev. B*, **1979**, 20, 2154-2162;
based on a Padé approximant.

$$\chi T = \frac{Ng^2\beta^2}{4k} \cdot \frac{T}{T-\theta} \cdot \left[\frac{1 + A \cdot \left(\frac{J_{1D}}{2kT}\right) + B \cdot \left(\frac{J_{1D}}{2kT}\right)^2 + C \cdot \left(\frac{J_{1D}}{2kT}\right)^3 + D \cdot \left(\frac{J_{1D}}{2kT}\right)^4 + E \cdot \left(\frac{J_{1D}}{2kT}\right)^5}{1 + F \cdot \left(\frac{J_{1D}}{2kT}\right) + G \cdot \left(\frac{J_{1D}}{2kT}\right)^2 + H \cdot \left(\frac{J_{1D}}{2kT}\right)^3 + I \cdot \left(\frac{J_{1D}}{2kT}\right)^4} \right]^{\frac{2}{3}}$$

$$H = -2J_{1D} \sum_{N=1}^{\infty} S_1 \cdot S_{1+N}$$

$A = 5.7979916$, $B = 16.902653$, $C = 29.376885$, $D = 29.832959$, $E = 14.036918$
and $F = 2.7979916$, $G = 7.0086780$, $H = 8.6538644$, $I = 4.5743114$



This fit was done for all data; the fitted results were $J/k = (-)21.1 \pm 1.8$ K, $g = 1.93 \pm 0.02$ (uncertainties are standard deviations).

CDS version 5.35 *meta* linked iminoylnitroxides or nitronylnitroxides.

CDS version 5.35 lists 27 structures that have *meta* linked iminoylnitroxides or nitronylnitroxides: Refcodes AJISER, EDEDIB, FUYDUZ, KEHPET, KEHPIX, MILFAP, OLABEL, QUFFIG, QUFFOM, QUSCOS, SUGCAY, SUKBOP, SUKCAC, TICVUX, TICWAE, TICYAG, VIBRIJ, VIBROP, XEQSOB, XEQSOB01, XEQSOB02, XEZWUU, XEZXAB, XEZXE, XEZXI, XEZXOP, XEZXUV

Search Overview

S4

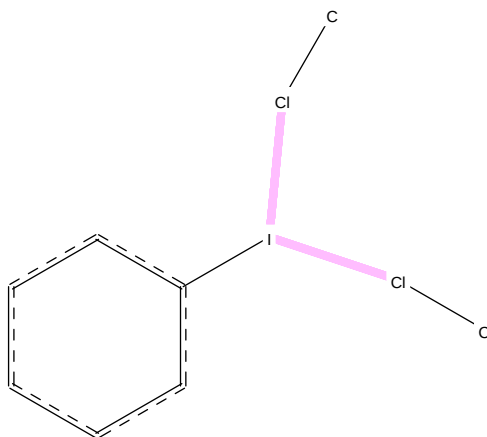
Search: search1
Date/Time done: Wed Jan 22 16:56:37 2014
Database(s): CSD version 5.35 updates (Nov 2013)
CSD version 5.35 (November 2013)
Restriction Info: No refcode restrictions applied
Filters: 3D coordinates determined
Percentage Completed: 100%
Number of Hits: 9

Single query used. Search found structures that:

match

Query 1

Query 1



Search: search1 (Wed Jan 22^{S5} 16:56:37 2014): Hits 1-4

PEYBUS

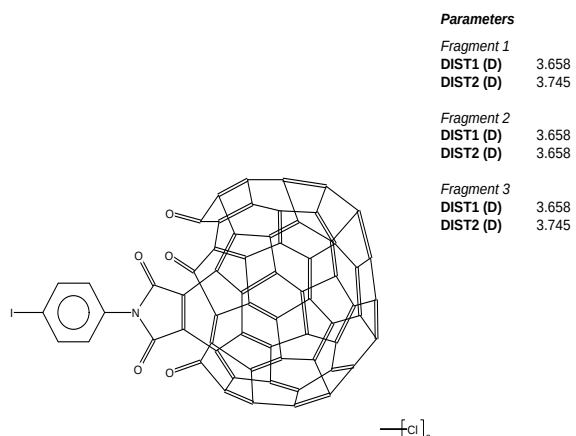
Reference: Yuming Yu, Lijun Shi, Dazhi Yang, Liangbing Gan (2013) *Chemical Science* ,**4**,814

Formula: C₆₅ H₄ I₁ N₁ O₅,2(C₁ H₁ Cl₃)

Compound Name: ((4-iodophenyl)imino)-(open-cage)-C59fullerene-pentaone chloroform solvate

Space Group: P-1 **Cell:** **a** 12.754(3) **b** 12.843(3) **c** 14.630(3)
Space Group No.: 2 **(Å,°)** **α** 78.32(3) **β** 82.27(3) **γ** 68.22(3)

R-Factor (%): 19.14 **Temperature(K):** 173 **Density(g/cm³):** 1.900



BAXYEF

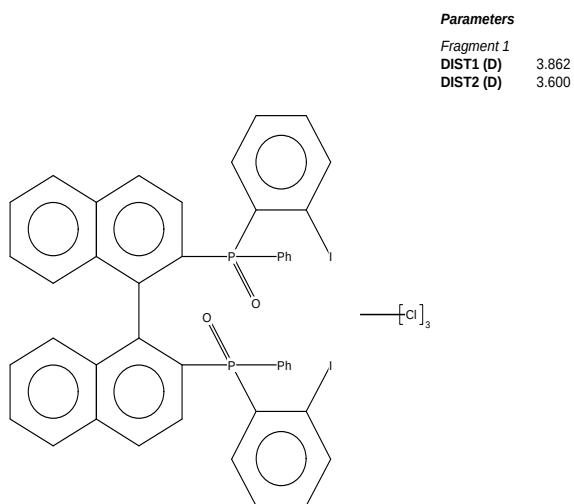
Reference: M.Widhalm, K.Mereiter (2003) *Bull.Chem.Soc.Jpn.* ,**76**, 1233

Formula: C₄₄ H₃₀ I₂ O₂ P₂,2(C₁ H₁ Cl₃)

Compound Name: 2,2'-bis((2-iodophenyl)(phenyl)phosphinoyl)-1,1'-binaphthyl chloroform solvate

Space Group: Pca21 **Cell:** **a** 21.079(4) **b** 12.549(2) **c** 17.566(3)
Space Group No.: 29 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 2.76 **Temperature(K):** 183 **Density(g/cm³):** 1.637



GIZTIT

Reference: D.Schollmeyer, O.V.Shishkin, T.Ruhl, M.O.Vysotsky (2008) *CrystEngComm* ,**10**,715

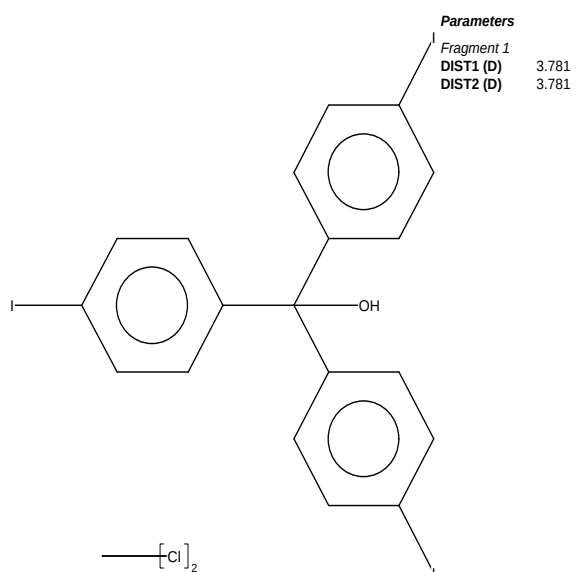
Formula: C₁₉ H₁₃ I₃ O₁,C₁ H₂ Cl₂

Compound Name: tris(4-iodophenyl)methanol dichloromethane solvate

Synonym: tri-iodotriptyl alcohol dichloromethane solvate

Space Group: Abm2 **Cell:** **a** 12.218(0) **b** 20.479(0) **c** 8.594(0)
Space Group No.: 39 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 2.73 **Temperature(K):** 193 **Density(g/cm³):** 2.233



HAMROC

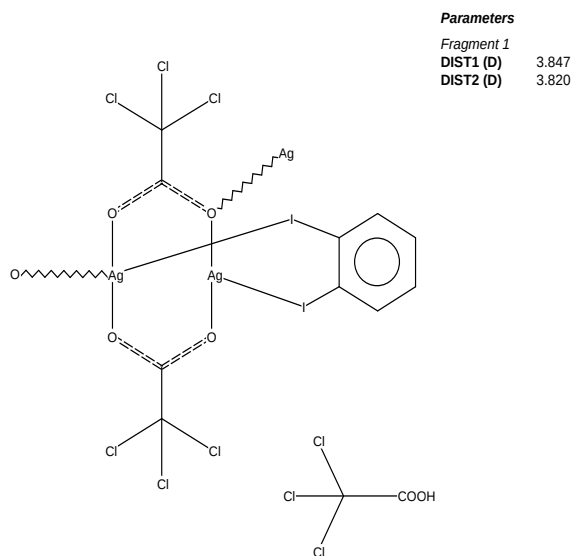
Reference: J.Powell, M.Horvath, A.Lough (1993) *J.Organomet.Chem.* , **456**,C27

Formula: (C₁₀ H₄ Ag₂ Cl₆ I₂ O₄)_n,n(C₂ H₁ Cl₃ O₂)

Compound Name: catena-(bis(μ₃-Trichloroacetato-O,O,O')-(μ₂-1,2-di-iodobenzene-1,1')-di-silver trichloroacetic acid solvate)

Space Group: P21/c **Cell:** **a** 13.755(3) **b** 17.999(2) **c** 11.344(1)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 113.59(5) **γ** 90.00

R-Factor (%): 3.70 **Temperature(K):** 295 **Density(g/cm³):** 2.668



Search: search1 (Wed Jan 22^{S6} 16:56:37 2014): Hits 5-8

HAMROC01

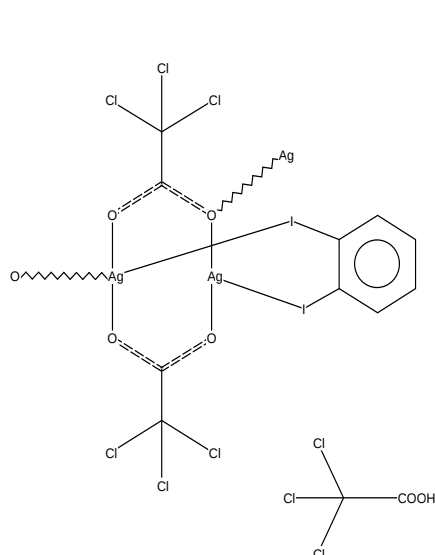
Reference: J.Powell, M.J.Horvath, A.Lough, A.Phillips, J.Brunet (1998) *J.Chem.Soc.,Dalton Trans.* ,637

Formula: (C₁₀ H₄ Ag₂ Cl₆ I₂ O₄)_n·n(C₂ H₁ Cl₃ O₂)

Compound Name: catena-(bis(μ₃-Trichloroacetato-O,O,O')-(μ₂-1,2-di-iodobenzene-1,I')-di-silver trichloroacetic acid solvate)

Space Group: P2₁/c **Cell:** **a** 13.755(3) **b** 17.999(2) **c** 11.344(2)
Space Group No.: 14 **Cell:** **(Å,°)** **α** 90.00 **β** 113.59(5) **γ** 90.00

R-Factor (%): 3.68 **Temperature(K):** 295 **Density(g/cm³):** 2.668



Parameters

Fragment 1
DIST1 (D) 3.850
DIST2 (D) 3.820

HUBBUC

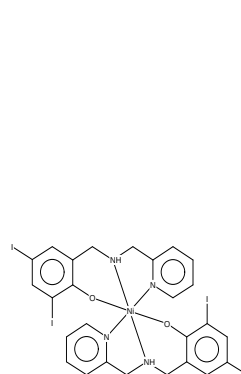
Reference: M.Frezza, S.S.Hindo, D.Tomca, M.M.Allard, Q.C.Cui, M.J.Heeg, Di Chen, Q.P.Dou, C.N.Verani (2009) *Inorg.Chem.* ,48,5928

Formula: C₂₆ H₂₂ I₄ N₄ O₂·3(C₁ H₁ Cl₃)

Compound Name: fac,trans-bis(2,4-Di-iodo-6-(((2-pyridinylmethyl)amino)methyl)phenolato-N,N',O)-nickel(ii) chloroform solvate

Space Group: P2₁/n **Cell:** **a** 18.423(0) **b** 10.180(0) **c** 22.149(0)
Space Group No.: 14 **Cell:** **(Å,°)** **α** 90.00 **β** 92.81(0) **γ** 90.00

R-Factor (%): 3.63 **Temperature(K):** 100 **Density(g/cm³):** 2.156



Parameters

Fragment 1
DIST1 (D) 3.831 **Fragment 9**
DIST2 (D) 3.705 **DIST1 (D)** 3.562
DIST2 (D) 3.816

Fragment 2
DIST1 (D) 3.614
DIST2 (D) 3.831

Fragment 3
DIST1 (D) 3.614
DIST2 (D) 3.705

Fragment 4
DIST1 (D) 3.559
DIST2 (D) 3.831

Fragment 5
DIST1 (D) 3.559
DIST2 (D) 3.705

Fragment 6
DIST1 (D) 3.614
DIST2 (D) 3.559

Fragment 7
DIST1 (D) 3.611
DIST2 (D) 3.816

Fragment 8
DIST1 (D) 3.562
DIST2 (D) 3.611

MESMIH

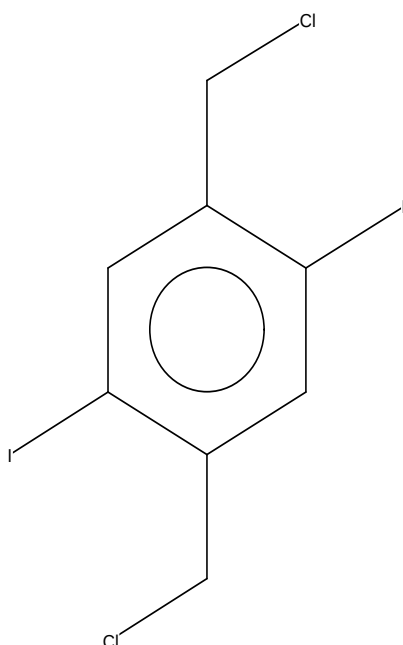
Reference: G.Gaefke, V.Enkelmann, S.Hoger (2006) *Synthesis* ,2971

Formula: C₈ H₆ Cl₂ I₂

Compound Name: 2,5-Diiodo-1,4-bis(chloromethyl)benzene

Space Group: P-1 **Cell:** **a** 4.357(0) **b** 7.292(0) **c** 8.999(0)
Space Group No.: 2 **Cell:** **(Å,°)** **α** 70.89(0) **β** 83.38(0) **γ** 84.97(0)

R-Factor (%): 3.57 **Temperature(K):** 120 **Density(g/cm³):** 2.645



Parameters

Fragment 1
DIST1 (D) 3.868
DIST2 (D) 3.537

SAPCOD

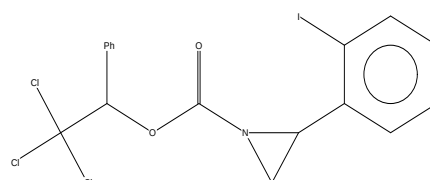
Reference: H.Lebel, C.Spitz, O.Leogane, C.Trudel, M.Parmentier (2011) *Org.Lett.* ,13,5460

Formula: C₁₇ H₁₃ Cl₃ I₁ N₁ O₂

Compound Name: 2,2,2-Trichloro-1-phenylethyl 2-(2-iodophenyl)aziridine-1-carboxylate

Space Group: P2₁ **Cell:** **a** 10.187(0) **b** 10.121(0) **c** 10.385(0)
Space Group No.: 4 **Cell:** **(Å,°)** **α** 90.00 **β** 117.00(0) **γ** 90.00

R-Factor (%): 2.51 **Temperature(K):** 200 **Density(g/cm³):** 1.729



Parameters

Fragment 1
DIST1 (D) 3.613
DIST2 (D) 3.770

Search: search1 (Wed Jan 22^{S7} 16:56:37 2014): Hit 9

YACQAW

Reference: R.Shakya, M.M.Allard, M.Johann, M.J.Heeg,
E.Rentschler, J.M.Shearer, B.McGarvey, C.N.Verani (2011)
Inorg.Chem., **50**,8356

Formula: $C_{26}H_{22}FeI_4N_4O_2 \cdot Cl_1O_4 \cdot 2(C_1H_1Cl_3)$

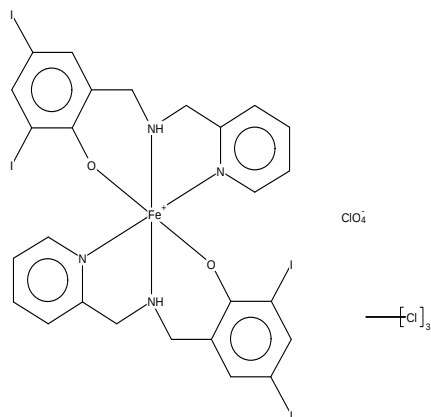
Compound Name: bis(2,4-diiodo-6-(((pyridin-2-yl)methyl)amino)methyl)phenolato)-iron(iii)
perchlorate chloroform solvate

Space Group: P-1 **Cell:** **a** 10.020(0) **b** 13.229(0) **c** 16.160(0)
Space Group No.: 2 ($\text{\AA}$, °) α 103.71(0) β 103.23(0) γ 101.82(0)

R-Factor (%): 4.80 **Temperature(K)**: 100 **Density(g/cm³)**: 2.257

Parameters

Fragment 1
DIST1 (D) 3.886
DIST2 (D) 3.908



Search Overview

S8

Search: search3
Date/Time done: Sun Jan 12 22:45:21 2014
Database(s): CSD version 5.35 updates (Nov 2013)
CSD version 5.35 (November 2013)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 58

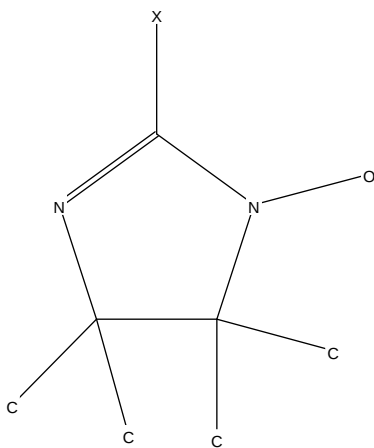
Summary of queries used. Search found structures that:

match

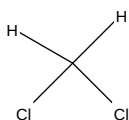
Query 1

Query 2

Query 1



Query 2



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 1-4

FERREB

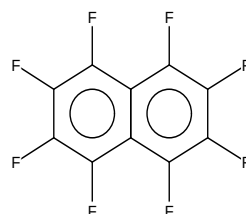
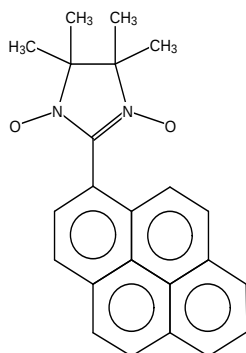
Reference: H.Akpınar, J.T.Mague, P.M.Lahti (2013) *CrystEngComm*, **15**,831

Formula: $C_{23}H_{21}N_2O_2 \cdot 0.5(C_{10}F_8) \cdot C_1H_2Cl_2$

Compound Name: 2-(1-Pyrenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl hemikis(octafluoronaphthalene) dichloromethane solvate

Space Group: P2₁/n **Cell:** a 13.884(0) b 10.104(0) c 18.735(1)
Space Group No.: 14 **Cell:** ($^\circ$) α 90.00 β 107.12(0) γ 90.00

R-Factor (%): 4.42 **Temperature(K):** 100 **Density(g/cm³):** 1.530



APIGIQ

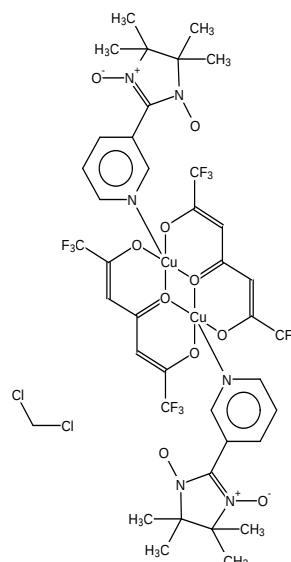
Reference: V.I.Ovcharenko, S.V.Fokin, G.V.Romanenko, A.S.Bogomyakov, D.S.Yachevsky, D.L.Chizhov, V.N.Charushin, O.N.Chupakhin (2010) *Izv.Akad.Nauk SSSR, Ser.Khim.(Russ.)(Russ.Chem.Bull.)*, 1138

Formula: $C_{38}H_{36}Cu_2F_{12}N_6O_{10} \cdot C_1H_2Cl_2$

Compound Name: bis(μ_2 -1,1,1,7,7,7-hexafluorohepta-2,5-diene-2,6-diolato-4-one)-bis(2-(pyridin-3-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl)-di-copper(II) dichloromethane solvate

Space Group: P-1 **Cell:** a 8.910(3) b 10.734(4) c 13.062(5)
Space Group No.: 2 **Cell:** ($^\circ$) α 76.29(0) β 84.14(0) γ 76.86(0)

R-Factor (%): 5.78 **Temperature(K):** 295 **Density(g/cm³):** 1.655



BAMMUZ

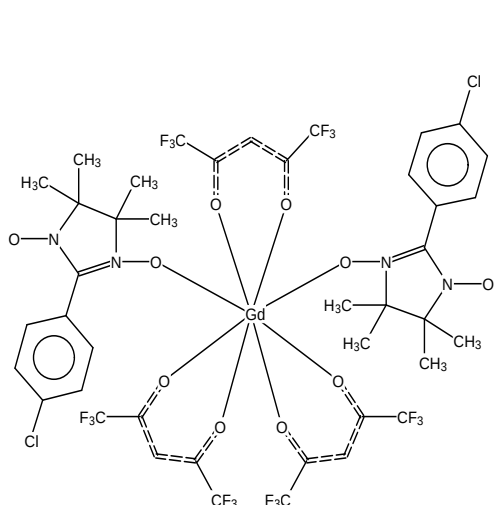
Reference: Chen-xi Zhang, Wen-Min Wang, Xiang-Yu Zhao, Ling-Fang Ji, Yu-Ying Zhang (2011) *Polyhedron*, **30**,3177

Formula: $C_{41}H_{35}Cl_2F_{18}Gd_1N_4O_{10} \cdot 0.25(C_1H_2Cl_2)$

Compound Name: tris(1,1,1,5,5,5-hexafluoropentane-2,4-dione)-bis(2-(4-chlorophenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-3 λ^5 -imidazole-1,3-diol)-gadolinium dichloromethane solvate

Space Group: P-1 **Cell:** a 11.439(2) b 12.794(3) c 19.269(4)
Space Group No.: 2 **Cell:** ($^\circ$) α 91.20(3) β 105.50(3) γ 95.18(3)

R-Factor (%): 5.61 **Temperature(K):** 113 **Density(g/cm³):** 1.640



BEBMOK

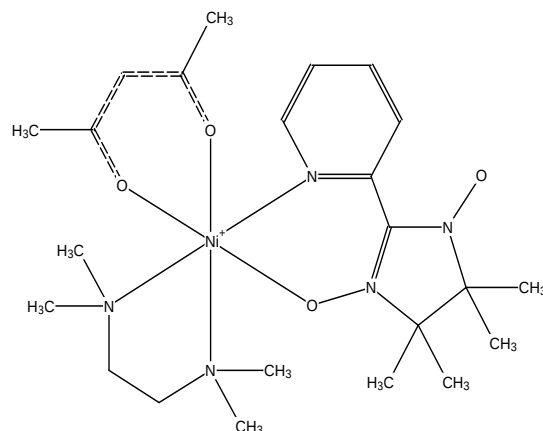
Reference: T.Yoshida, T.Suzuki, K.Kanamori, S.Kaizaki (1999) *Inorg.Chem.*, **38**,1059

Formula: $C_{23}H_{39}N_5Ni_1O_4 \cdot 1^+ \cdot 0.33(C_1H_2Cl_2)$

Compound Name: mer-(Acetylacetonato-O,O')-(2-(2-pyridyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-oxyl-3-oxide-N,O)-(N,N,N',N'-tetramethylethylenediamine-N,N')-nickel(II) hexafluorophosphate dichloromethane solvate

Space Group: R-3 **Cell:** a 33.299(5) b 33.299(5) c 15.007(9)
Space Group No.: 148 **Cell:** ($^\circ$) α 90.00 β 90.00 γ 120.00

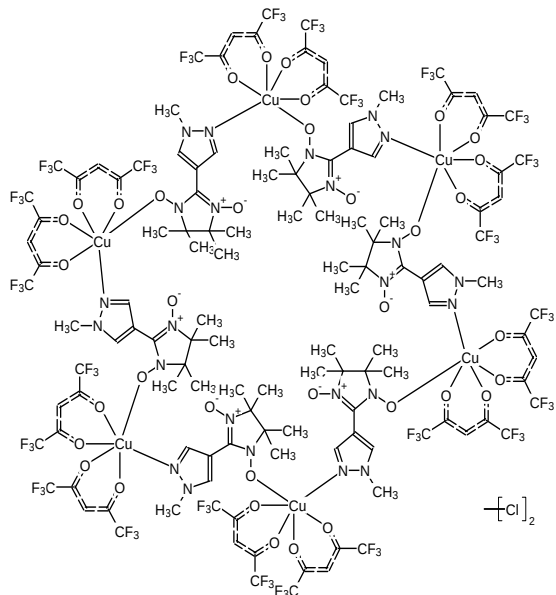
R-Factor (%): 6.15 **Temperature(K):** 295 **Density(g/cm³):** 1.413



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 5-8

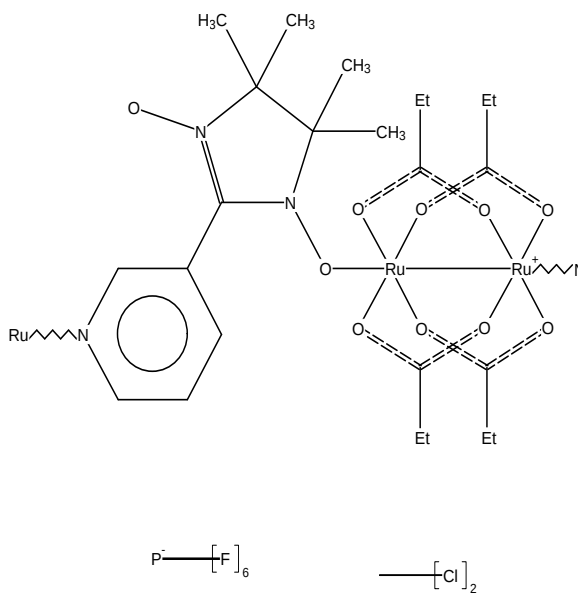
BEMTET

Reference:	S.Fokin, V.Ovcharenko, G.Romanenko, V.Ikorski (2004) <i>Inorg.Chem.</i> , 43 ,969					
Formula:	C ₁₂₆ H ₁₁₄ Cu ₆ F ₇₂ N ₂₄ O ₃₆ 6(C ₁ H ₂ Cl ₂)					
Compound Name:	hexakis(μ ₂ -2-(1-Methylpyrazol-4-yl)-4,4,5,5-tetramethylimidazoline-3-oxide-1-oxyl-N',O')-dodecakis(hexafluoroacetylacetonato-O,O')-hexa-copper(ii) dichloromethane solvate					
Space Group:	R-3c	Cell:	a 22.581(3)	b 22.581(3)	c 64.185(13)	
Space Group No.:	167	(Å,°)	α 90.00	β 90.00	γ 120.00	
R-Factor (%) :	8.45	Temperature(K) :	293	Density(g/cm³) :	1.687	



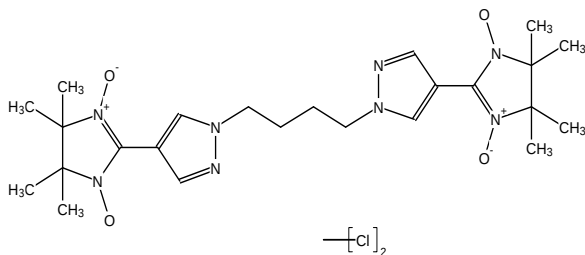
CEBTEJ

Reference:	M.Mikuriya, K.Tanaka, M.Handa, I.Hiromitsu, D.Yoshioka, D.Luneau (2005) <i>Polyhedron</i> , 24 ,2658					
Formula:	(C ₂₄ H ₃₆ N ₃ O ₁₀ Ru ₂ 1 ⁺) _n (F ₆ P ₁ 1 ⁻) _n (C ₁ H ₂ Cl ₂)					
Compound Name:	catena-(tetrakis(μ ₂ -Propionato-O,O')-(μ ₂ -2-(3'-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide-N,O)-ruthenium(ii)-ruthenium(iii) hexafluorophosphate dichloromethane solvate)					
Space Group:	P21/c	Cell:	a 13.419(4)	b 12.637(2)	c 22.441(6)	
Space Group No.:	14	(Å,°)	α 90.00	β 97.79(1)	γ 90.00	
R-Factor (%) :	5.30	Temperature(K) :	298	Density(g/cm³) :	1.689	



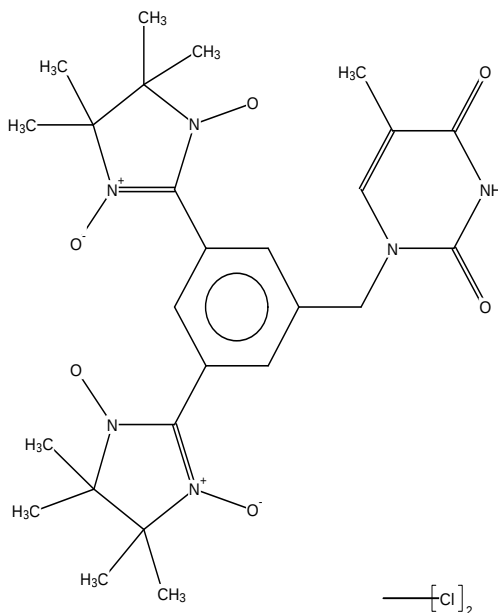
CEJYUM

Reference:	E.Tretyakov, S.Fokin, G.Romanenko, V.Ikorski, S.Vasilevsky, V.Ovcharenko (2006) <i>Inorg.Chem.</i> , 45 ,3671					
Formula:	C ₂₄ H ₃₆ N ₈ O ₄ C ₁ H ₂ Cl ₂					
Compound Name:	1,4-bis(4-(4,4,5,5-Tetramethyl-3-oxide-1-oxyl-4,5-dihydro-1H-imidazol-2-yl)pyrazol-1-yl)butane dichloromethane solvate					
Space Group:	P21/n	Cell:	a 11.708(1)	b 10.076(1)	c 24.904(4)	
Space Group No.:	14	(Å,°)	α 90.00	β 98.02(0)	γ 90.00	
R-Factor (%) :	6.74	Temperature(K) :	240	Density(g/cm³) :	1.337	



EDEDIB

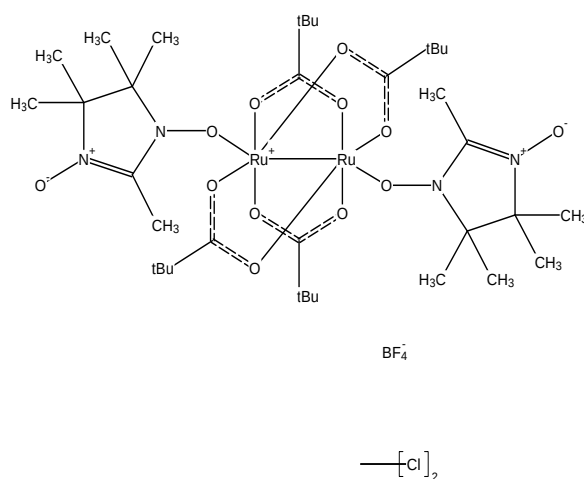
Reference:	H.Tanaka, D.Shiomi, T.Ise, K.Sato, T.Takui (2007) <i>Polyhedron</i> , 26 ,2230					
Formula:	C ₂₆ H ₃₄ N ₆ O ₆ C ₁ H ₂ Cl ₂					
Compound Name:	1-(3,5-bis(1-Oxyl-3-oxido-4,4,5,5-tetramethylimidazolidin-2-yl)benzyl)-5-methyl-1H-pyrimidin-2,4-dione dichloromethane solvate					
Space Group:	P-1	Cell:	a 10.786(1)	b 12.118(3)	c 12.522(2)	
Space Group No.:	2	(Å,°)	α 78.15(1)	β 69.17(1)	γ 75.16(1)	
R-Factor (%) :	6.79	Temperature(K) :	293	Density(g/cm³) :	1.385	



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 9-12

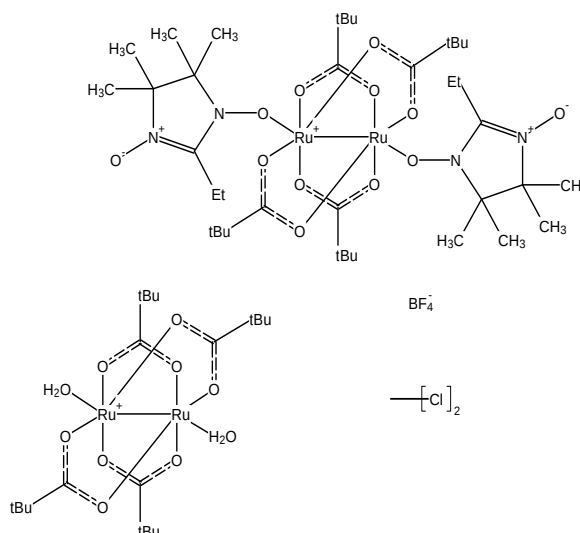
ENIKOB

Reference:	Y.Sayama, M.Handa, M.Mikuriya, I.Hiromitsu, K.Kasuga (2003) <i>Bull.Chem.Soc.Jpn.</i> , 76 ,769				
Formula:	C ₃₆ H ₆₆ N ₄ O ₁₂ Ru ₂ ¹⁺ , B ₁ F ₄ ¹⁻ , 2(C ₁ H ₂ Cl ₂)				
Compound Name:	tetrakis(μ ₂ -2,2-Dimethylpropanoato)-bis(2,4,4,5,5-pentamethyl-4,5-dihydro-1H-imidazol-1-oxyl-3-oxide)-di-ruthenium(ii,iii) tetrafluoroborate dichloromethane solvate				
Space Group:	Pbcn	Cell:	a 18.370(1)	b 16.464(1)	c 18.191(1)
Space Group No.:	60	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%) :	4.50	Temperature(K) :	298	Density(g/cm³) :	1.456



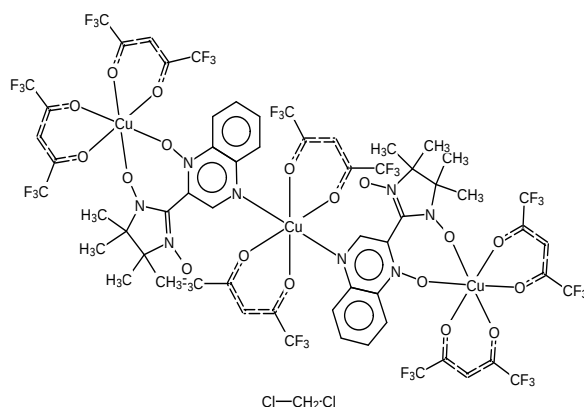
ENILAO

Reference:	Y.Sayama, M.Handa, M.Mikuriya, I.Hiromitsu, K.Kasuga (2003) <i>Bull.Chem.Soc.Jpn.</i> , 76 ,769				
Formula:	C ₃₈ H ₇₀ N ₄ O ₁₂ Ru ₂ ¹⁺ , C ₂₀ H ₄₀ O ₁₀ Ru ₂ ¹⁺ , 2(B ₁ F ₄ ¹⁻), 2(C ₁ H ₂ Cl ₂)				
Compound Name:	tetrakis(μ ₂ -2,2-Dimethylpropanoato)-bis(2-ethyl-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-oxyl-3-oxide)-di-ruthenium(ii,iii) tetrakis(μ ₂ -2,2-dimethylpropanoato)-diaqua-di-ruthenium(ii,iii) bis(tetrafluoroborate) dichloromethane solvate				
Space Group:	C2/c	Cell:	a 46.705(19)	b 10.413(1)	c 18.940(5)
Space Group No.:	15	(Å, °)	α 90.00	β 105.71(1)	γ 90.00
R-Factor (%) :	5.50	Temperature(K) :	298	Density(g/cm³) :	1.471



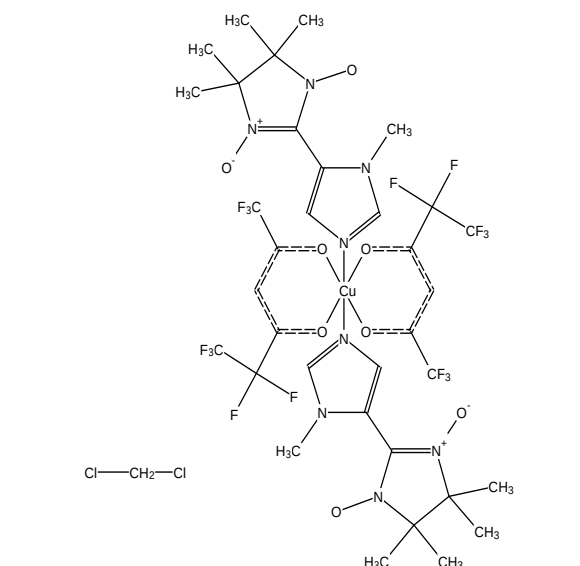
EPUFIF

Reference:	O.N.Chupakhin, E.V.Tretyakov, I.A.Utepova, M.V.Varaksin, G.V.Romanenko, A.S.Bogomyakov, S.L.Veber, V.I.Ovcharenko (2011) <i>Polyhedron</i> , 30 ,647				
Formula:	C ₆₀ H ₄₀ Cu ₃ F ₃₆ N ₈ O ₁₈ , 2(C ₁ H ₂ Cl ₂)				
Compound Name:	bis(μ ₂ -4,4,5,5-tetramethyl-2-(1-oxidoquinoxalin-2-yl)-4,5-dihydro-1H-imidazol-1-olato 3-oxide)-hexakis(1,1,1,5,5,5-hexafluoropentane-2,4-dionato)-tri-copper dichloromethane solvate				
Space Group:	P-1	Cell:	a 12.643(1)	b 12.994(1)	c 13.866(1)
Space Group No.:	2	(Å, °)	α 70.26(0)	β 82.10(0)	γ 88.66(0)
R-Factor (%) :	4.93	Temperature(K) :	240	Density(g/cm³) :	1.725



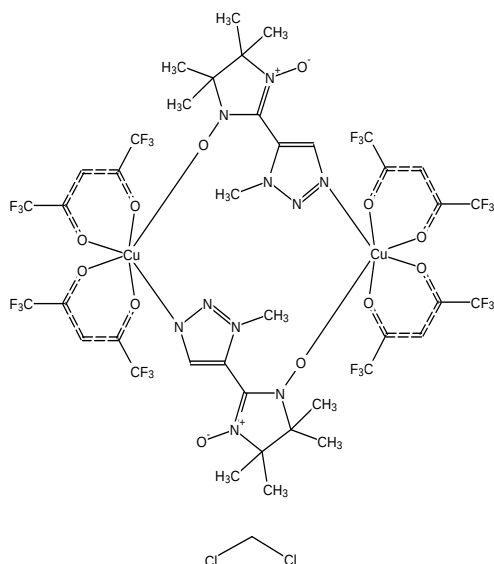
GELQAR

Reference:	V.I.Ovcharenko, E.V.Tretyakov, S.V.Fokin, E.Yu.Fursova, O.V.Kuznetsova, S.E.Tolstikov, G.V.Romanenko, A.S.Bogomyakov, R.Z.Sagdeev (2011) <i>Izv.Akad.Nauk SSSR, Ser.Khim.(Russ.)(Russ.Chem.Bull.)</i> , 2411				
Formula:	C ₃₄ H ₃₆ Cu ₁ F ₁₆ N ₈ O ₈ , 0.5(C ₁ H ₂ Cl ₂)				
Compound Name:	bis(1,1,1,2,2,6,6,6-Octafluorohexane-3,5-dionato-O,O')-bis(2-(1-methyl-1H-imidazol-5-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl-3-oxide-N)-copper(ii) dichloromethane solvate				
Space Group:	P-1	Cell:	a 9.838(0)	b 14.385(0)	c 17.725(0)
Space Group No.:	2	(Å, °)	α 95.23(0)	β 92.56(0)	γ 106.80(0)
R-Factor (%) :	7.68	Temperature(K) :	240	Density(g/cm³) :	1.524



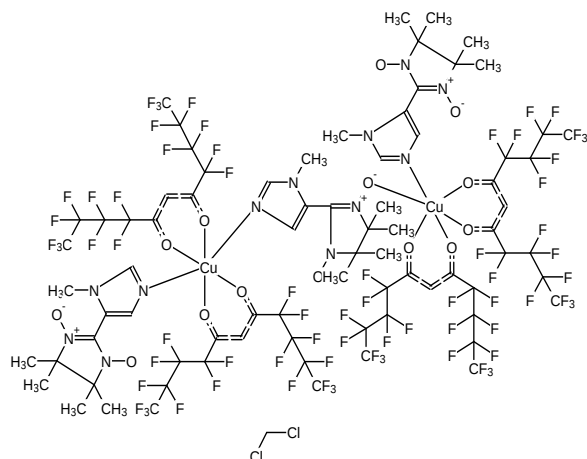
GELQEV

Reference:	V.I.Ovcharenko, E.V.Tretyakov, S.V.Fokin, E.Yu.Fursova, O.V.Kuznetsova, S.E.Tolstikov, G.V.Romanenko, A.S.Bogomyakov, R.Z.Sagdeev (2011) <i>Izv.Akad.Nauk SSSR,Ser.Khim.(Russ.)(Russ.Chem.Bull.)</i> ,2411					
Formula:	C ₄₀ H ₃₆ Cu ₂ F ₂₄ N ₁₀ O ₁₂ , C ₁ H ₂ Cl ₂					
Compound Name:	bis(μ ₂ -2-(1-methyl-1,2,3-triazol-5-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl-3-oxide-N,O)-tetrakis(1,1,1,5,5,5-hexafluoropentane-2,4-dionato-O,O')-di-copper(II) dichloromethane solvate					
Space Group:	C2/c	Cell:	a	b	c	
Space Group No.:	15	(Å, °)	29.205(1) α 90.00	10.552(0) β 105.25(0)	20.741(1) γ 90.00	
R-Factor (%) :	5.46	Temperature(K):	240	Density(g/cm³):	1.634	



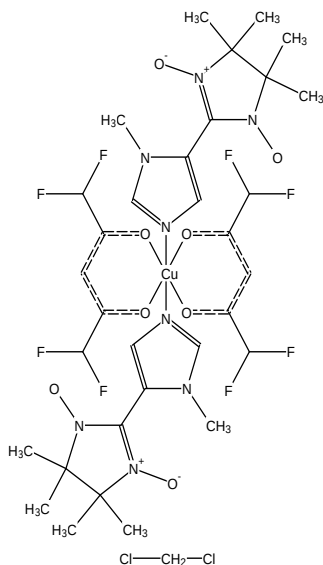
GELREW

Reference:	V.I.Ovcharenko, E.V.Tretyakov, S.V.Fokin, E.Yu.Fursova, O.V.Kuznetsova, S.E.Tolstikov, G.V.Romanenko, A.S.Bogomyakov, R.Z.Sagdeev (2011) <i>Izv.Akad.Nauk SSSR,Ser.Khim.(Russ.)(Russ.Chem.Bull.)</i> ,2411					
Formula:	C ₇₇ H ₅₅ Cu ₂ F ₇₂ N ₁₂ O ₁₄ , 0.5(C ₁ H ₂ Cl ₂)					
Compound Name:	(μ ₂ -2-(1-methyl-1H-imidazol-5-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl-3-oxide-N,O)-tetrakis(1,1,1,2,2,3,3,4,4,8,8,9,9,10,10,11,11,11-octadecafluoroundecane-5,7-dionato-O,O')-bis(2-(1-methyl-1H-imidazol-5-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl-3-oxide-N)-di-copper(II) dichloromethane solvate					
Space Group:	P-1	Cell:	a	b	c	
Space Group No.:	2	(Å, °)	13.724(0) α 95.47(0)	15.714(0) β 93.29(0)	27.578(1) γ 105.45(0)	
R-Factor (%) :	8.66	Temperature(K):	240	Density(g/cm³):	1.700	



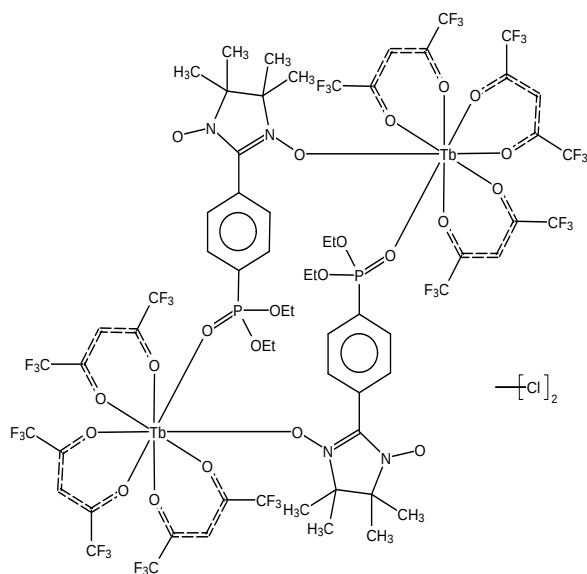
GEMSUO

Reference:	V.I.Ovcharenko, E.V.Tretyakov, S.V.Fokin, E.Yu.Fursova, O.V.Kuznetsova, S.E.Tolstikov, G.V.Romanenko, A.S.Bogomyakov, R.Z.Sagdeev (2011) <i>Izv.Akad.Nauk SSSR,Ser.Khim.(Russ.)(Russ.Chem.Bull.)</i> ,2411					
Formula:	C ₃₂ H ₄₀ Cu ₁ F ₈ N ₈ O ₈ , 2(C ₁ H ₂ Cl ₂)					
Compound Name:	bis(1,1,1,5,5-Tetrafluoropentane-2,4-dionato-O,O')-bis(2-(1-methyl-1H-imidazol-5-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl-3-oxide-N)-copper(II) dichloromethane solvate					
Space Group:	P-1	Cell:	a	b	c	
Space Group No.:	2	(Å, °)	7.130(0) α 86.68(0)	12.222(0) β 74.83(0)	13.207(0) γ 85.18(0)	
R-Factor (%) :	7.57	Temperature(K):	295	Density(g/cm³):	1.576	



GENDOU

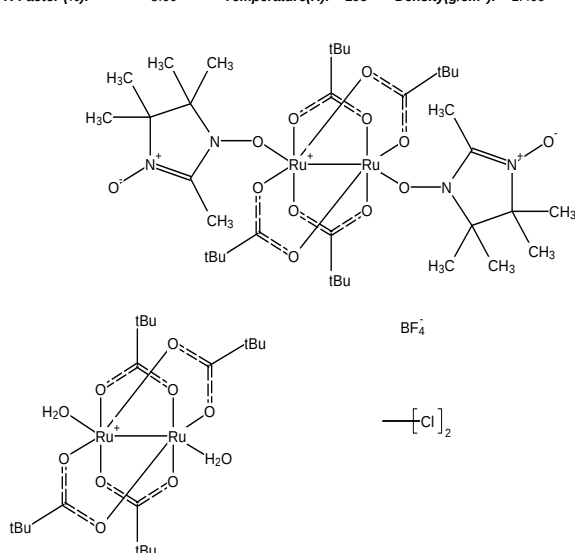
Reference:	F.Pointillart, K.Bernot, G.Poneti, R.Sessoli (2012) <i>Inorg.Chem.</i> ,51,12218					
Formula:	C ₆₄ H ₅₈ F ₃₆ N ₄ O ₂₂ P ₂ Tb ₂ , 2(C ₁ H ₂ Cl ₂)					
Compound Name:	bis(μ ₂ -(2-(4-(Diethoxyphosphoryl)phenyl)-4,4,5,5-tetramethyl-3-oxido-4,5-dihydro-1H-imidazol-1-yl)oxidanil) radical)-hexakis(hexafluoroacetylacetonato-O,O')-di-terbium(III) dichloromethane solvate					
Space Group:	P21/n	Cell:	a	b	c	
Space Group No.:	14	(Å, °)	12.169(0) α 90.00	22.730(1) β 90.65(0)	16.450(1) γ 90.00	
R-Factor (%) :	6.58	Temperature(K):	150	Density(g/cm³):	1.802	



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 17-20

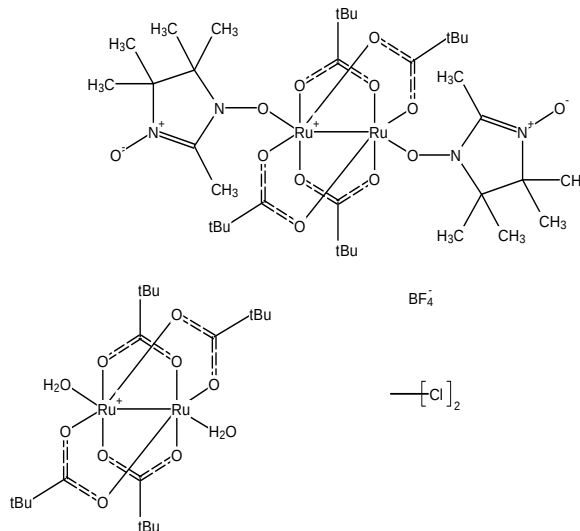
GOBQUJ

Reference:	Y.Sayama, M.Handa, M.Mikuriya, I.Hiromitsu, K.Kasuga (1999) <i>Chem.Lett.</i> ,453				
Formula:	$C_{36}H_{66}N_4O_{12}Ru_2^{1+}, C_{20}H_{40}O_{10}Ru_2^{1+}, 2(B_1F_4^{1-}), 2(C_1H_2Cl_2)$				
Compound Name:	tetrakis(μ_2 -2,2-Dimethylpropanoato)-bis(nitronyl nitroxide)-di-ruthenium(ii,iii) tetrakis(μ_2 -2,2-dimethylpropanoato)-diaqua-di-ruthenium(ii,iii) bis(tetrafluoroborate) dichloromethane solvate				
Synonym:	tetrakis(μ_2 -2,2-Dimethylpropanoato)-bis(2,4,4,5,5-pentamethyl-4,5-dihydro-1H-imidazolyl-1-oxyl 3-oxide)-di-ruthenium(ii,iii) tetrakis(μ_2 -2,2-dimethylpropanoato)-diaqua-di-ruthenium(ii,iii) bis(tetrafluoroborate) dichloromethane solvate				
Space Group:	C2/c	Cell:	a 46.695(14)	b 10.404(2)	c 18.273(5)
Space Group No.:	15	(Å,°)	α 90.00	β 105.03(1)	γ 90.00
R-Factor (%) :	5.60	Temperature(K):	295	Density(g/cm³):	1.499



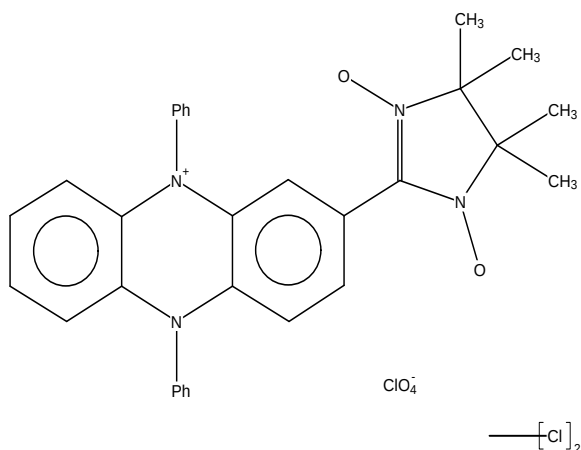
GOBQUJ01

Reference:	Y.Sayama, M.Handa, M.Mikuriya, I.Hiromitsu, K.Kasuga (2003) <i>Bull.Chem.Soc.Jpn.</i> ,76,769				
Formula:	$C_{36}H_{66}N_4O_{12}Ru_2^{1+}, C_{20}H_{40}O_{10}Ru_2^{1+}, 2(B_1F_4^{1-}), 2(C_1H_2Cl_2)$				
Compound Name:	tetrakis(μ_2 -2,2-Dimethylpropanoato)-bis(2,4,4,5,5-pentamethyl-4,5-dihydro-1H-imidazolyl-1-oxyl-3-oxide)-di-ruthenium(ii,iii) tetrakis(μ_2 -2,2-dimethylpropanoato)-diaqua-di-ruthenium(ii,iii) bis(tetrafluoroborate) dichloromethane solvate				
Space Group:	C2/c	Cell:	a 46.695(14)	b 10.404(2)	c 18.273(5)
Space Group No.:	15	(Å,°)	α 90.00	β 105.03(1)	γ 90.00
R-Factor (%) :	5.60	Temperature(K):	298	Density(g/cm³):	1.499



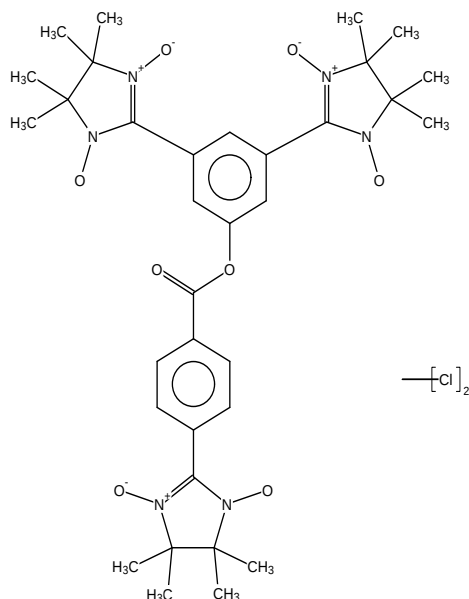
IQEXUX

Reference:	S.Hiraoka, T.Okamoto, M.Kozaki, D.Shiomi, K.Sato, T.Takui, K.Okada (2004) <i>J.Am.Chem.Soc.</i> ,126,58				
Formula:	$C_{31}H_{29}N_4O_2^{1+}, Cl_1O_4^{1-}, C_1H_2Cl_2$				
Compound Name:	2-(4,4,5,5-Tetramethyl-4,5-dihydro-1H-imidazolyl 1-oxyl 3-oxide)-5,10-diphenyl-5,10-dihydrophenazinium perchlorate dichloromethane solvate				
Space Group:	P-1	Cell:	a 10.282(1)	b 11.232(1)	c 15.539(2)
Space Group No.:	2	(Å,°)	α 80.70(1)	β 77.67(1)	γ 64.48(0)
R-Factor (%) :	4.50	Temperature(K):	113	Density(g/cm³):	1.419



KEHPET

Reference:	Y.Kanzaki, D.Shiomi, C.Kaneda, T.Ise, K.Sato, T.Takui (2006) <i>J.Mater.Chem.</i> ,16,2064				
Formula:	$C_{34}H_{43}N_6O_8, 0.5(C_1H_2Cl_2)$				
Compound Name:	4-(1',3'-Oxyl-4',4',5',5'-tetramethylimidazolin-2'-yl)-benzoic acid 3,5-bis-(1",3"-oxyl-4",4",5",5"-tetramethylimidazolin-2"-yl)phenyl ester dichloromethane solvate				
Space Group:	P-1	Cell:	a 11.390(1)	b 12.091(2)	c 14.386(3)
Space Group No.:	2	(Å,°)	α 74.85(2)	β 78.45(2)	γ 68.70(2)
R-Factor (%) :	7.20	Temperature(K):	173	Density(g/cm³):	1.325



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 21-24

KEHPIX

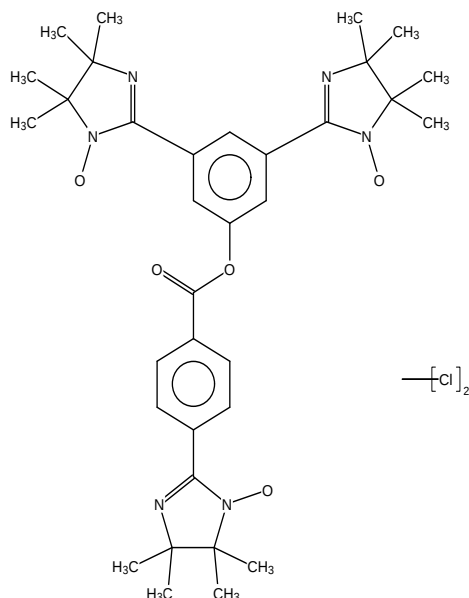
Reference: Y.Kanzaki, D.Shiomi, C.Kaneda, T.Ise, K.Sato, T.Takui (2006) *J.Mater.Chem.* ,**16**,2064

Formula: C₃₄ H₄₃ N₆ O₅.0.5(C₁ H₂ Cl₂)

Compound Name: 4-(1'-Oxyl-4',4',5',5'-tetramethylimidazolin-2'-yl)-benzoic acid 3,5-bis-(1'-oxyl-4'',4'',5'',5''-tetramethylimidazolin-2''-yl)-phenyl ester dichloromethane solvate

Space Group: P-1 **Cell:** **a** 11.280(7) **b** 11.995(7) **c** 14.345(9)
Space Group No.: 2 **Cell:** **(Å, °)** **α** 74.99(2) **β** 78.72(3) **γ** 69.63(2)

R-Factor (%): 9.90 **Temperature(K)**: 293 **Density(g/cm³)**: 1.252



KEPSOP

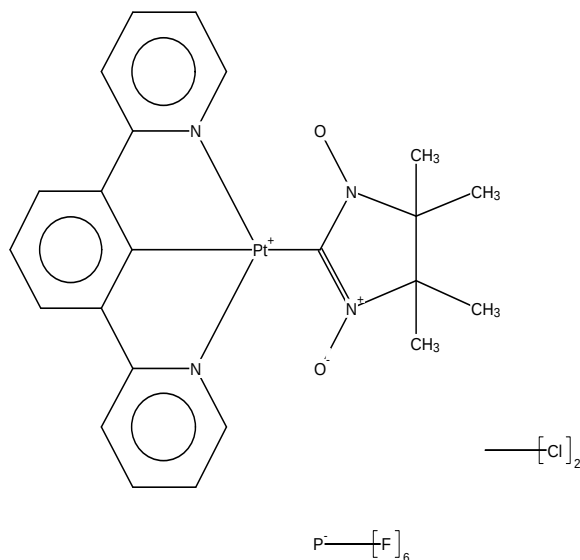
Reference: Xun Zhang, S.Suzuki, M.Kozaki, K.Okada (2012) *J.Am.Chem.Soc.* ,**134**,17866

Formula: C₂₃ H₂₃ N₄ O₂ Pt₁¹⁺.F₆ P₁¹⁻.0.5(C₁ H₂ Cl₂)

Compound Name: (2,6-bis(2-Pyridyl)phenyl)-(1,3-oxy-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-3-ium-2-yl)-platinum hexafluorophosphate dichloromethane solvate

Space Group: Pna21 **Cell:** **a** 29.796(1) **b** 8.408(0) **c** 21.744(1)
Space Group No.: 33 **Cell:** **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 6.57 **Temperature(K)**: 150 **Density(g/cm³)**: 1.878



KEPSUV

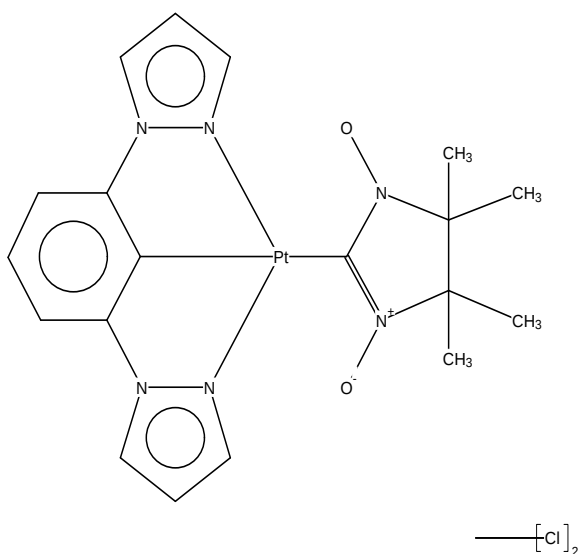
Reference: Xun Zhang, S.Suzuki, M.Kozaki, K.Okada (2012) *J.Am.Chem.Soc.* ,**134**,17866

Formula: C₁₉ H₂₁ N₆ O₂ Pt₁.2(C₁ H₂ Cl₂)

Compound Name: (2,6-bis(Pyrazolyl)phenyl)-(1,3-oxy-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-3-ium-2-yl)-platinum dichloromethane solvate

Space Group: P21/n **Cell:** **a** 8.970(1) **b** 18.360(4) **c** 15.800(3)
Space Group No.: 14 **Cell:** **(Å, °)** **α** 90.00 **β** 91.34(0) **γ** 90.00

R-Factor (%): 4.76 **Temperature(K)**: 150 **Density(g/cm³)**: 1.865



LOXCUW

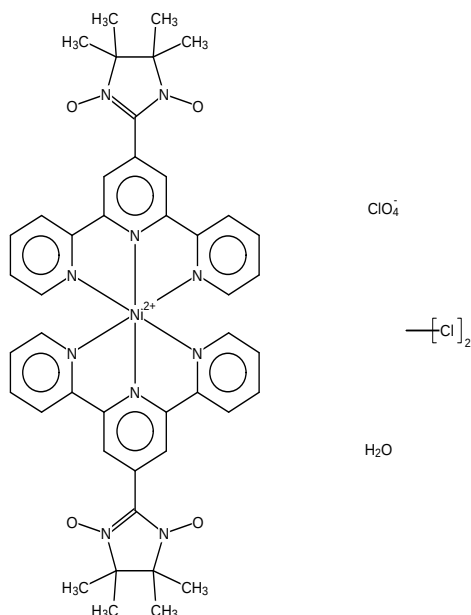
Reference: C.Stroh, P.Turek, P.Rabu, R.Ziessel (2001) *Inorg.Chem.* ,**40**,5334

Formula: C₄₄ H₄₄ N₁₀ O₄²⁺.2(Cl₁ O₄¹⁻).C₁ H₂ Cl₂.H₂ O₁

Compound Name: bis(2-[4'-(2,2',6',2''-terpyridyl)]-(4,4,5,5-tetramethylimidazolyl-3-oxide-1-oxyl))-nickel(ii) diperchlorate dichloromethane solvate monohydrate

Space Group: Pna21 **Cell:** **a** 23.637(0) **b** 8.784(0) **c** 24.275(0)
Space Group No.: 33 **Cell:** **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 6.70 **Temperature(K)**: 173 **Density(g/cm³)**: 1.499



S15 Search: search3 (Sun Jan 12 22:45:21 2014): Hits 25-28

LOXDAD

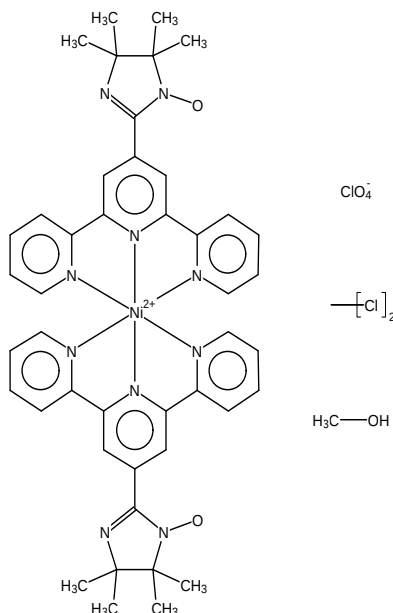
Reference: C.Stroh, P.Turek, P.Rabu, R.Ziessel (2001) *Inorg.Chem.* , **40**,5334

Formula: $2(\text{C}_{44}\text{H}_{44}\text{N}_{10}\text{O}_2\text{Zn}^{2+}) \cdot 4(\text{Cl}_1\text{O}_4^{1-}) \cdot 2(\text{C}_1\text{H}_2\text{Cl}_2) \cdot \text{C}_1\text{H}_4\text{O}_1$

Compound Name: bis(2-[4'-(2,2':6',2''-terpyridyl)]-(4,4,5,5-tetramethylimidazolyl-1-oxyl))-nickel(ii) diperchlorate dichloromethane methanol solvate

Space Group: P21 **Cell:** a 8.738(1) b 25.010(1) c 11.704(1)
Space Group No.: 4 **Cell:** ($\text{\AA}$, $^\circ$) α 90.00 β 102.85(0) γ 90.00

R-Factor (%): 5.00 **Temperature(K)**: 173 **Density(g/cm³)**: 1.470



LOXDEH

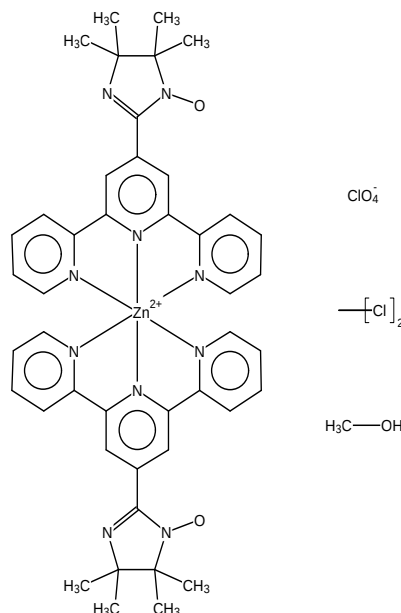
Reference: C.Stroh, P.Turek, P.Rabu, R.Ziessel (2001) *Inorg.Chem.* , **40**,5334

Formula: $2(\text{C}_{44}\text{H}_{44}\text{N}_{10}\text{O}_2\text{Zn}^{2+}) \cdot 4(\text{Cl}_1\text{O}_4^{1-}) \cdot 2(\text{C}_1\text{H}_2\text{Cl}_2) \cdot \text{C}_1\text{H}_4\text{O}_1$

Compound Name: bis(2-[4'-(2,2':6',2''-terpyridyl)]-(4,4,5,5-tetramethylimidazolyl-1-oxyl))-zinc(ii) diperchlorate dichloromethane methanol solvate

Space Group: P21 **Cell:** a 8.746(0) b 25.083(0) c 11.817(0)
Space Group No.: 4 **Cell:** ($\text{\AA}$, $^\circ$) α 90.00 β 102.76(0) γ 90.00

R-Factor (%): 4.90 **Temperature(K)**: 173 **Density(g/cm³)**: 1.458



LUTKER

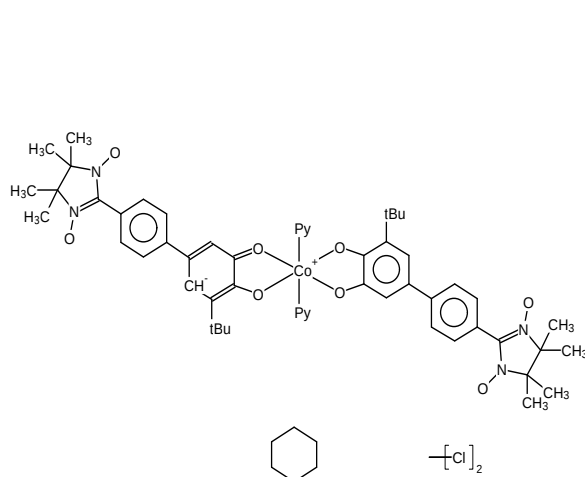
Reference: M.L.Kirk, D.A.Schultz, R.D.Schmidt, D.Habel-Rodriguez, Hyoyoung Lee, Junghyun Lee (2009) *J.Am.Chem.Soc.* , **131**,18304

Formula: $\text{C}_{56}\text{H}_{64}\text{Co}_1\text{N}_6\text{O}_8\text{C}_6\text{H}_{12} \cdot 2.32(\text{C}_1\text{H}_2\text{Cl}_2)$

Compound Name: (3-t-Butyl-5-(4-(4,4,5,5-tetramethylimidazolin-1-oxyl-3-oxide)phenyl)catecholato)-(3-t-butyl-5-(4-(4,4,5,5-tetramethylimidazolin-1-oxyl-3-oxide)phenyl)semiquinonato)-bis(pyridine)-cobalt(iii) cyclohexane dichloromethane solvate

Space Group: P-1 **Cell:** a 8.589(1) b 13.334(1) c 15.195(1)
Space Group No.: 2 **Cell:** ($\text{\AA}$, $^\circ$) α 83.79(0) β 84.08(0) γ 81.53(0)

R-Factor (%): 7.98 **Temperature(K)**: 85 **Density(g/cm³)**: 1.256



MEXQUB

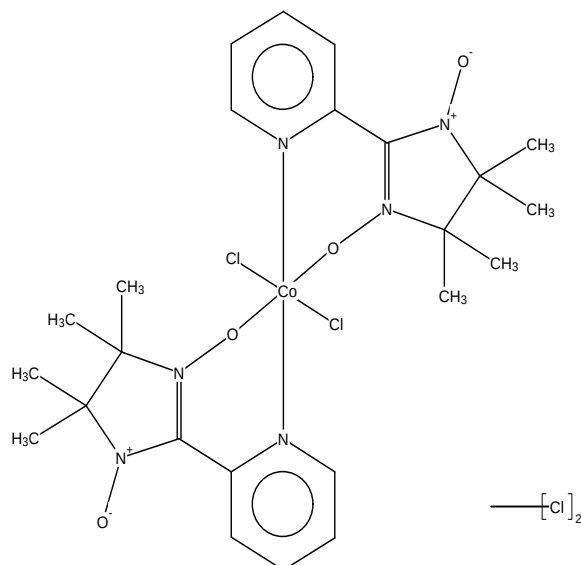
Reference: Y.Yamamoto, T.Yoshida, T.Suzuki, S.Kaizaki (2001) *Inorg.Chim.Acta* , **325**,187

Formula: $\text{C}_{24}\text{H}_{32}\text{Cl}_2\text{Co}_1\text{N}_6\text{O}_4 \cdot 2(\text{C}_1\text{H}_2\text{Cl}_2)$

Compound Name: Dichloro-bis(2-(2-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide)-cobalt(ii) dichloromethane solvate

Space Group: P21/c **Cell:** a 8.937(3) b 14.066(1) c 13.804(1)
Space Group No.: 14 **Cell:** ($\text{\AA}$, $^\circ$) α 90.00 β 103.04(1) γ 90.00

R-Factor (%): 4.64 **Temperature(K)**: 296 **Density(g/cm³)**: 1.509



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 29-32

MEXRAI

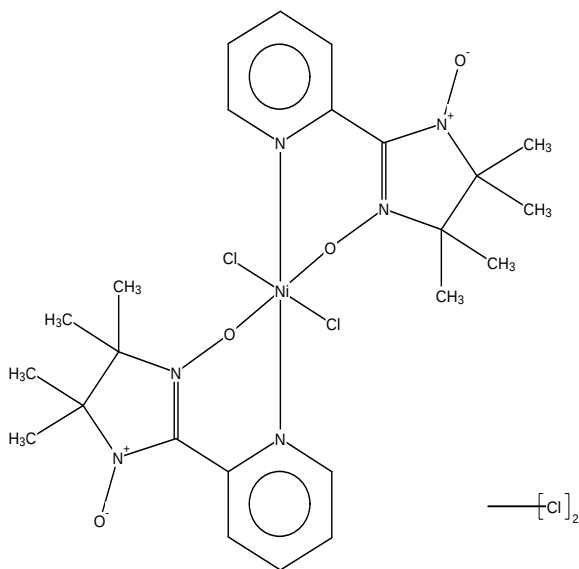
Reference: Y.Yamamoto, T.Yoshida, T.Suzuki, S.Kaizaki (2001)
Inorg.Chim.Acta ,325,187

Formula: C₂₄ H₃₂ Cl₂ N₆ Ni₁ O₄ C₁ H₂ Cl₂

Compound Name: Dichloro-bis(2-(2-pyridyl)-4,5,5-tetramethylimidazoline-1-oxyl-3-oxide)-nickel(ii) dichloromethane solvate

Space Group: P-1 **Cell:** a 10.854(3) b 12.434(4) c 13.489(4)
Space Group No.: 2 **Cell:** (Å,°) α 63.14(2) β 73.65(2) γ 71.16(2)

R-Factor (%): 4.23 **Temperature(K)**: 296 **Density(g/cm³)**: 1.495



MINJIC

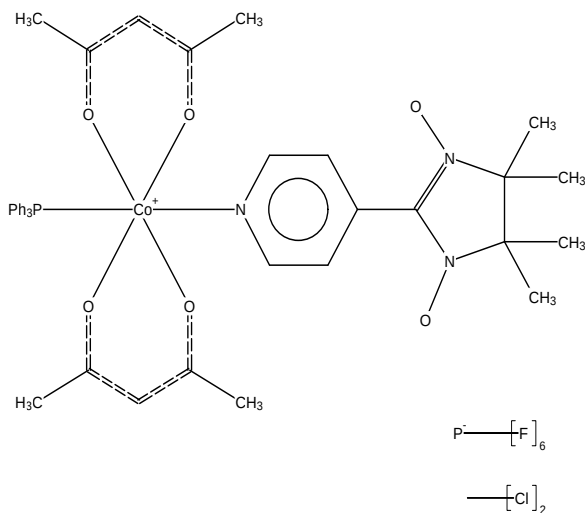
Reference: M.Ogita, Y.Yamamoto, T.Suzuki, S.Kaizaki (2002)
Eur.J.Inorg.Chem. ,886

Formula: C₄₀ H₄₅ Co₁ N₃ O₆ P₁¹⁺ F₆ P₁¹⁻ C₁ H₂ Cl₂

Compound Name: trans-(bis(Acetylacetonato)-(4,4,5,5-tetramethyl-2-(4-pyridyl)imidazolin-1-oxyl 3-oxide)-(triphenylphosphine)-cobalt(iii)) hexafluorophosphate dichloromethane solvate

Space Group: P-1 **Cell:** a 13.558(2) b 14.654(2) c 13.174(1)
Space Group No.: 2 **Cell:** (Å,°) α 103.35(1) β 94.46(1) γ 65.41(1)

R-Factor (%): 5.44 **Temperature(K)**: 296 **Density(g/cm³)**: 1.411



MINJOI

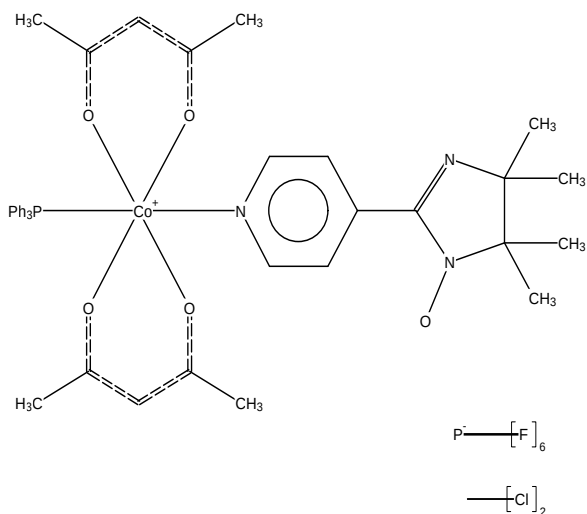
Reference: M.Ogita, Y.Yamamoto, T.Suzuki, S.Kaizaki (2002)
Eur.J.Inorg.Chem. ,886

Formula: C₄₀ H₄₅ Co₁ N₃ O₅ P₁¹⁺ F₆ P₁¹⁻ C₁ H₂ Cl₂

Compound Name: trans-(bis(Acetylacetonato)-(4,4,5,5-tetramethyl-2-(4-pyridyl)imidazolin-1-oxyl)-(triphenylphosphine)-cobalt(iii)) hexafluorophosphate dichloromethane solvate

Space Group: P-1 **Cell:** a 13.371(3) b 14.520(4) c 13.148(6)
Space Group No.: 2 **Cell:** (Å,°) α 101.76(4) β 93.41(4) γ 68.27(2)

R-Factor (%): 7.73 **Temperature(K)**: 296 **Density(g/cm³)**: 1.384



MUSDAP

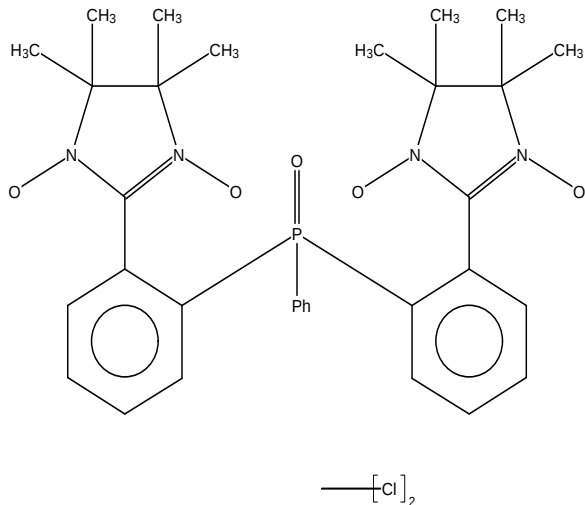
Reference: C.Rancurel, N.Daro, O.B.Borobia, E.Herdtwack,
J.-P.Sutter (2003) *Eur.J.Org.Chem.* ,167

Formula: C₃₂ H₃₇ N₄ O₅ P₁ C₁ H₂ Cl₂

Compound Name: bis(2-(4,4,5,5-Tetramethyl-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl) phenyl)(phenyl)phosphine oxide dichloromethane solvate

Space Group: Cc **Cell:** a 10.123(0) b 29.491(0) c 11.581(0)
Space Group No.: 9 **Cell:** (Å,°) α 90.00 β 104.24(0) γ 90.00

R-Factor (%): 2.58 **Temperature(K)**: 143 **Density(g/cm³)**: 1.335



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 33-36

NUDJAX

Reference: J.-P. Sutter, M.L.Kahn, S.Golhen, L.Ouahab, O.Kahn (1998) *Chem.-Eur.J.* ,4,571

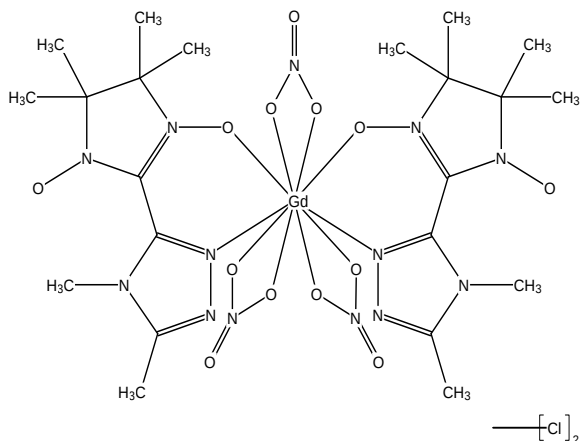
Formula: $C_{22}H_{36}Gd_1N_{13}O_{13} \cdot 3(C_1H_2Cl_2)$

Compound Name: bis(2-(4,5-Dimethyl-4H-1,2,4-triazol-3-yl)-4,4,5,5-tetramethyl-3-oxo-4,5-dihydro-1H-imidazol-1-oxyl)-tris(nitrato-O,O')-gadolinium(III) dichloromethane solvate

Space Group: P21/n **Cell:** a 11.135(3) b 15.156(7) c 26.490(7) α 90.00 β 100.50(1) γ 90.00

Space Group No.: 14

R-Factor (%): 9.54 **Temperature(K):** 263 **Density(g/cm³):** 1.666



OKUHEI

Reference: S.Suzuki, N.Itoh, K.Furuichi, M.Kozaki, D.Shiomi, K.Sato, T.Takui, H.Ohi, S.Itoh, K.Okada (2011) *Chem.Lett.* ,40,22

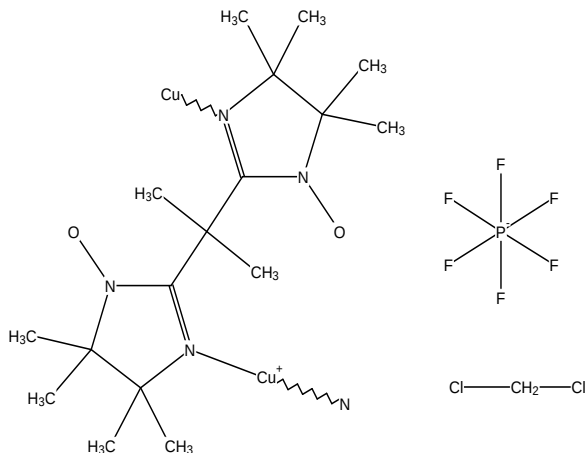
Formula: $(C_{17}H_{30}Cu_1N_4O_2)^{1+}n,n(F_6P_1)^{1-},2n(C_1H_2Cl_2)$

Compound Name: catena-((μ₂-2,2'-propane-2,2'-diylbis(4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole 1-oxide radical))-copper(I) hexafluorophosphate dichloromethane solvate)

Space Group: I-42d **Cell:** a 11.789(6) b 11.789(6) c 42.570(20) α 90.00 β 90.00 γ 90.00

Space Group No.: 122

R-Factor (%): 5.72 **Temperature(K):** 171 **Density(g/cm³):** 1.574



OKUWOG

Reference: E.V.Tretyakov, I.V.Eltsov, S.V.Fokin, Y.G.Shvedenkov, G.V.Romanenko, V.I.Ovcharenko (2003) *Polyhedron* ,22,2499

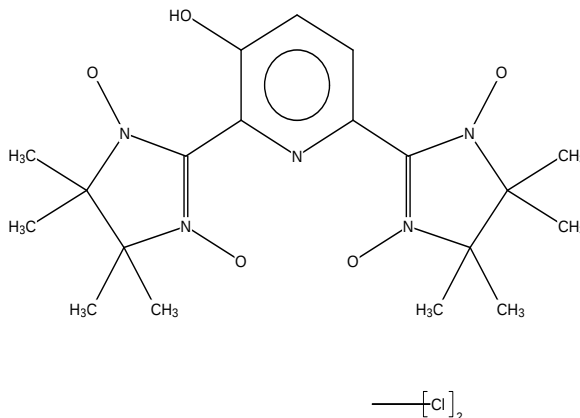
Formula: $C_{19}H_{27}N_5O_5 \cdot C_1H_2Cl_2$

Compound Name: 2,6-bis(4,4,5,5-tetramethyl-3-oxy-1-oxyl-4,5-dihydro-1H-imidazol-2-yl)-3-hydroxypyridine dichloromethane solvate

Space Group: P21/c **Cell:** a 12.338(5) b 16.533(5) c 11.786(5) α 90.00 β 92.38(0) γ 90.00

Space Group No.: 14

R-Factor (%): 6.57 **Temperature(K):** 293 **Density(g/cm³):** 1.356



OKUXIB

Reference: E.V.Tretyakov, I.V.Eltsov, S.V.Fokin, Y.G.Shvedenkov, G.V.Romanenko, V.I.Ovcharenko (2003) *Polyhedron* ,22,2499

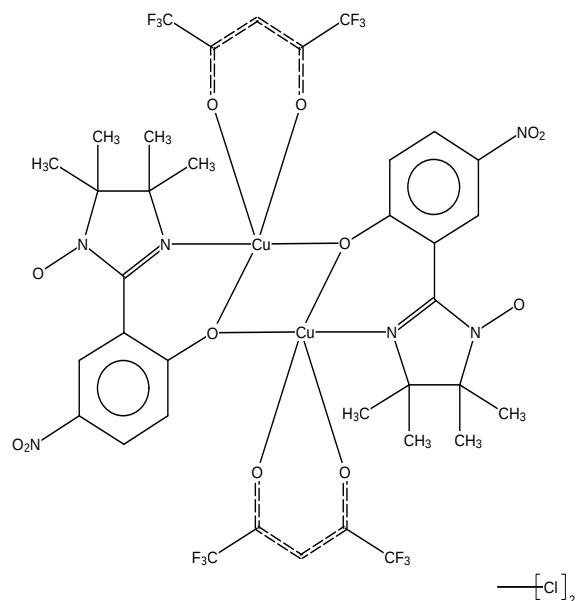
Formula: $C_{36}H_{32}Cu_2F_{12}N_6O_{12} \cdot C_1H_2Cl_2$

Compound Name: bis(μ₂-2-(2-Oxy-5-nitrophenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl)-bis(hexafluoroacetylacetonato)-di-copper dichloromethane solvate

Space Group: C2/c **Cell:** a 18.457(3) b 19.490(2) c 14.998(2) α 90.00 β 117.31(1) γ 90.00

Space Group No.: 15

R-Factor (%): 6.04 **Temperature(K):** 293 **Density(g/cm³):** 1.636



S18 Search: search3 (Sun Jan 12 22:45:21 2014): Hits 37-40

OKUXOH

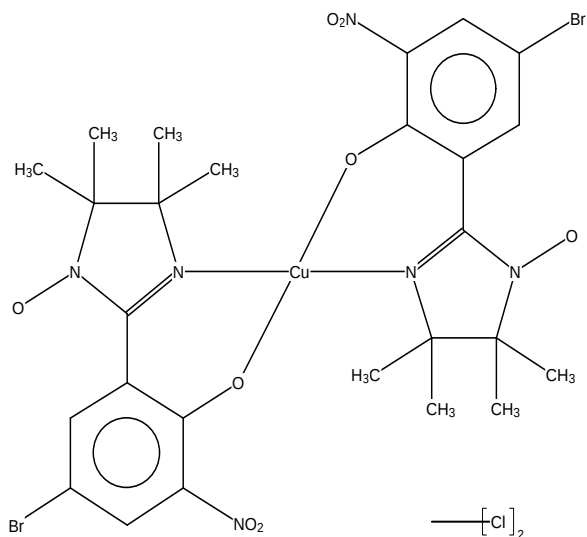
Reference: E.V.Tretyakov, I.V.Eltsov, S.V.Fokin, Y.G.Shvedenkov, G.V.Romanenko, V.I.Ovcharenko (2003) *Polyhedron*, **22**,2499

Formula: C₂₆ H₂₈ Br₂ Cu₁ N₆ O₉.0.5(C₁ H₂ Cl₂)

Compound Name: bis(2-(2-Oxy-5-bromo-3-nitrophenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl)-copper dichloromethane solvate

Space Group: P-1 **Cell:** **a** 11.063(5) **b** 11.930(5) **c** 12.656(5)
Space Group No.: 2 **(Å,°)** **α** 89.96(0) **β** 80.73(0) **γ** 82.69(0)

R-Factor (%): 6.92 **Temperature(K)**: 293 **Density(g/cm³)**: 1.662



OKUZUP

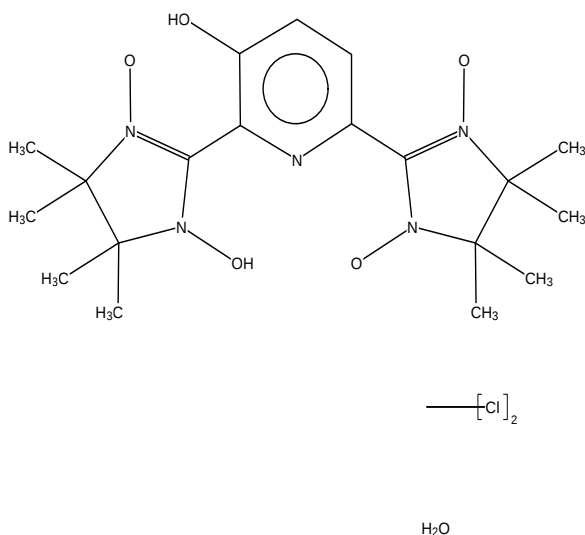
Reference: E.V.Tretyakov, I.V.Eltsov, S.V.Fokin, Y.G.Shvedenkov, G.V.Romanenko, V.I.Ovcharenko (2003) *Polyhedron*, **22**,2499

Formula: C₁₉ H₂₈ N₅ O₅.C₁ H₂ Cl₂.H₂ O₁

Compound Name: 2-(1-Hydroxy-4,4,5,5-tetramethyl-3-oxy-4,5-dihydro-1H-imidazol-2-yl)-6-(4,4,5,5-tetramethyl-3-oxy-1-oxyl-4,5-dihydro-1H-imidazol-2-yl)-3-hydroxypyridine dichloromethane solvate monohydrate

Space Group: P-1 **Cell:** **a** 11.810(2) **b** 11.934(2) **c** 11.945(2)
Space Group No.: 2 **(Å,°)** **α** 116.70(3) **β** 116.61(3) **γ** 92.68(3)

R-Factor (%): 10.29 **Temperature(K)**: 293 **Density(g/cm³)**: 1.324



ONIHUP

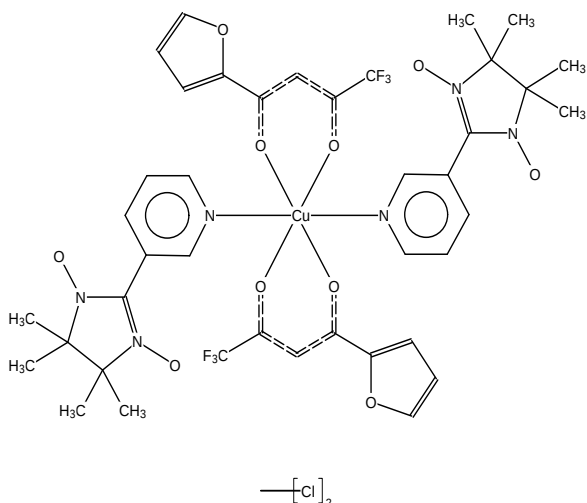
Reference: D.A.Souza, Y.Moreno, E.A.Ponzio, J.A.L.C.Resende, A.K.Jordao, A.C.Cunha, V.F.Ferreira, M.A.Novak, M.G.F.Vaz (2011) *Inorg.Chim.Acta*, **370**,469

Formula: C₄₀ H₄₀ Cu₁ F₆ N₆ O₁₀.C₁ H₂ Cl₂

Compound Name: bis(4,4,4-Trifluoro-1-furoylbutane-1,3-dionato)-bis(2-(3-pyridyl)-4,4,5-tetramethylimidazoline-1-oxyl-3-oxide)-copper(ii) dichloromethane solvate

Space Group: P-1 **Cell:** **a** 7.502(1) **b** 11.269(2) **c** 13.938(3)
Space Group No.: 2 **(Å,°)** **α** 75.28(3) **β** 80.27(3) **γ** 88.36(3)

R-Factor (%): 7.09 **Temperature(K)**: 298 **Density(g/cm³)**: 1.519



OYELAG

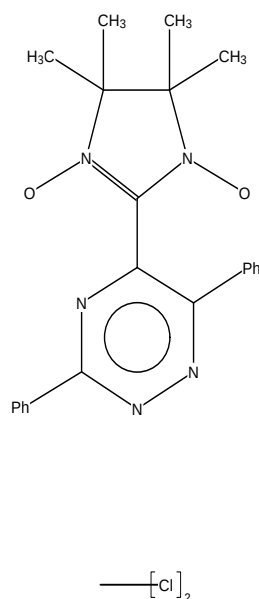
Reference: E.V.Tretyakov, I.A.Utepova, M.V.Varaksin, S.E.Tolstikov, G.V.Romanenko, A.S.Bogomyakov, D.V.Stass, V.I.Ovcharenko, O.N.Chupakhin (2011) *ARKIVOC*, **12**,76-8

Formula: C₂₂ H₂₂ N₅ O₂.0.5(C₁ H₂ Cl₂)

Compound Name: 4,4,5,5-Tetramethyl-2-(3,6-diphenyl-1,2,4-triazin-5-yl)-4,5-dihydro-1H-imidazol-3-oxide-1-oxyl dichloromethane solvate

Space Group: P21/n **Cell:** **a** 12.761(7) **b** 10.899(6) **c** 15.916(8)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 94.62(0) **γ** 90.00

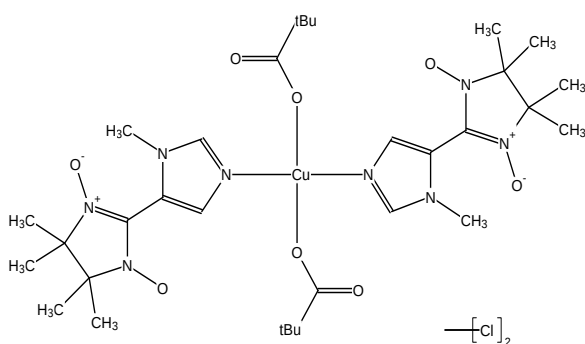
R-Factor (%): 5.29 **Temperature(K)**: 296 **Density(g/cm³)**: 1.297



S19 Search: search3 (Sun Jan 12 22:45:21 2014): Hits 41-44

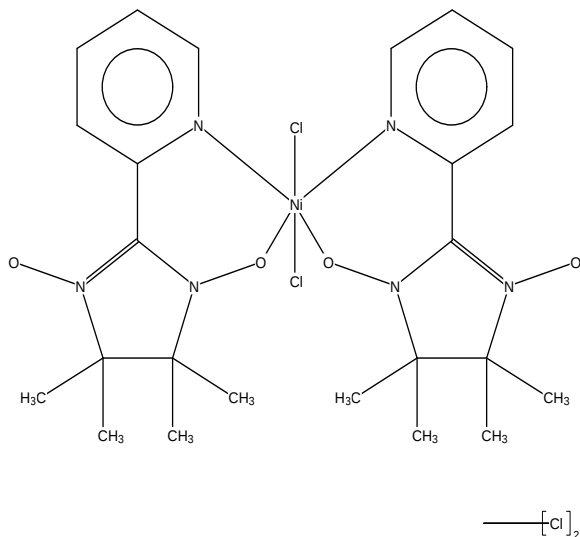
OZUVAH

Reference:	V.I.Ovcharenko, S.V.Fokin, E.Yu.Fursova, O.V.Kuznetsova, E.V.Tretyakov, G.V.Romanenko, A.S.Bogomyakov (2011) <i>Inorg.Chem.</i> , 50 ,4307					
Formula:	C ₃₂ H ₅₂ Cu ₁ N ₈ O ₈ ·2(C ₁ H ₂ Cl ₂)					
Compound Name:	bis(Pivalato-O)-bis(4,4,5,5-tetramethyl-2-(1-methyl-1H-imidazol-5-yl)-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl radical-N)-copper dichloromethane solvate					
Space Group:	P-1	Cell:	a	b	c	
Space Group No.:	2	(Å, °)	α	β	γ	
R-Factor (%) :	5.08	Temperature(K) :	298	Density(g/cm³) :	1.358	



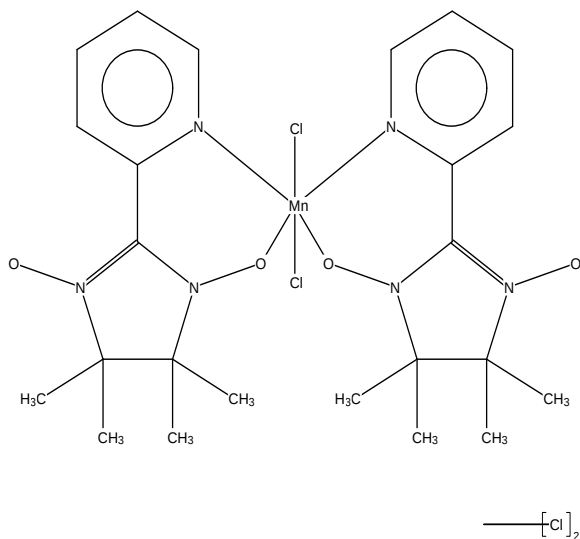
PIFROL

Reference:	D.Luneau, G.Risoan, P.Rey, A.Grand, A.Caneschi, D.Gatteschi, J.Laugier (1993) <i>Inorg.Chem.</i> , 32 ,5616					
Formula:	C ₂₄ H ₃₂ Cl ₂ Ni ₁ O ₄ ·2(C ₁ H ₂ Cl ₂)					
Compound Name:	Dichloro-bis(2-(2-pyridyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-oxy-3-oxide)-nickel(ii) dichloromethane solvate					
Space Group:	P21/c	Cell:	a	b	c	
Space Group No.:	14	(Å, °)	α	β	γ	
R-Factor (%) :	3.80	Temperature(K) :	295	Density(g/cm³) :	1.529	



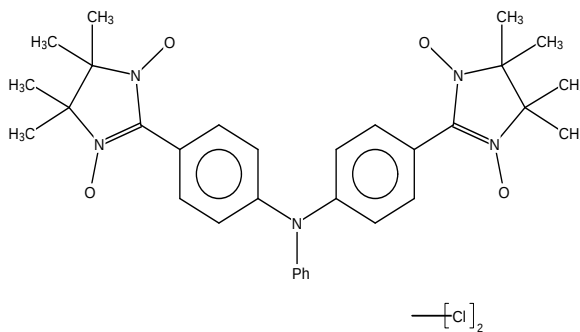
PIFRUR

Reference:	D.Luneau, G.Risoan, P.Rey, A.Grand, A.Caneschi, D.Gatteschi, J.Laugier (1993) <i>Inorg.Chem.</i> , 32 ,5616					
Formula:	C ₂₄ H ₃₂ Cl ₂ Mn ₁ N ₆ O ₄ ·2(C ₁ H ₂ Cl ₂)					
Compound Name:	Dichloro-bis(2-(2-pyridyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-oxy-3-oxide)-manganese(ii) dichloromethane solvate					
Space Group:	P21/c	Cell:	a	b	c	
Space Group No.:	14	(Å, °)	α	β	γ	
R-Factor (%) :	5.70	Temperature(K) :	295	Density(g/cm³) :	1.483	



QURNUM

Reference:	De-Qing Zhang, Zhe-Ming Wang, Liang Ding, Bin Zhang, Wei Xu, Dao-Ben Zhu, Chun-Hua Yan (2001) <i>Chin.J.Chem.</i> , 19 ,966					
Formula:	C ₃₂ H ₃₇ N ₅ O ₄ ·0.75(C ₁ H ₂ Cl ₂)					
Compound Name:	bis(4-(4,4,5,5-Tetramethyl-2-imidazoline-1,3-dioxy)phenyl)-phenylamine dichloromethane solvate					
Space Group:	Pbca	Cell:	a	b	c	
Space Group No.:	61	(Å, °)	α	β	γ	
R-Factor (%) :	6.46	Temperature(K) :	120	Density(g/cm³) :	1.302	



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 45-48

RATCOE

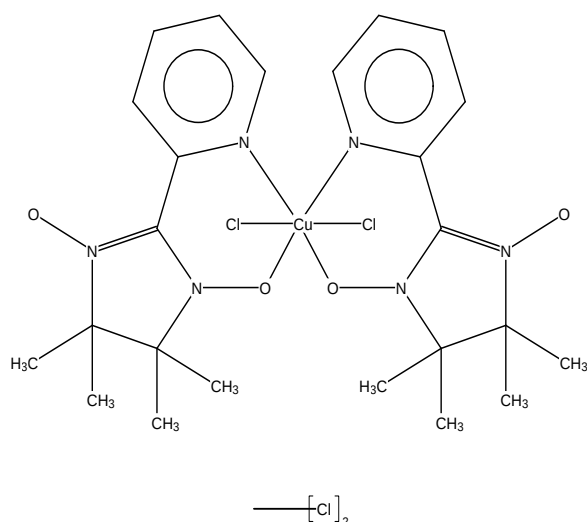
Reference: S.Ohba, T.Kato, N.Yoshioka, H.Inoue (1997) *Acta Crystallogr., Sect.C: Cryst. Struct. Commun.*, **53**,9700004

Formula: $C_{24}H_{32}Cl_2Cu_1N_6O_4 \cdot 2(C_1H_2Cl_2)$

Compound Name: bis(2-(2-Pyridyl)-4,4,5,5-tetramethyl-4,5-dihydro-(1H-imidazolyl-1-oxyl 3-oxide))-dichloro-copper(ii) dichloromethane solvate

Space Group: P21/c **Cell:** a 8.804(2) b 14.208(1) c 13.931(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 103.57(1) γ 90.00

R-Factor (%): 3.74 **Temperature(K):** 295 **Density(g/cm³):** 1.515



SUPFAL

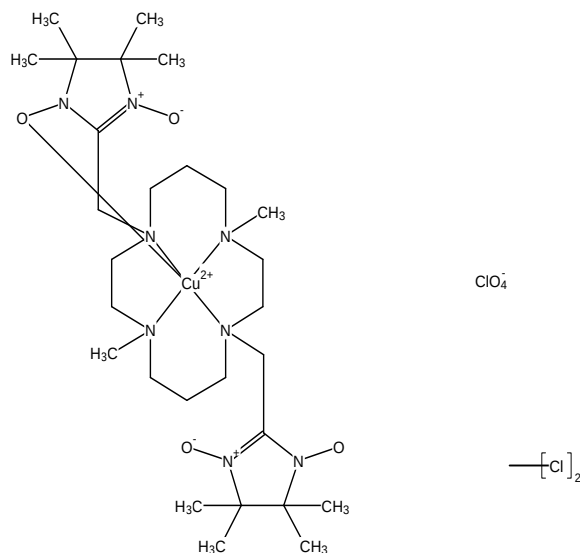
Reference: K.Igarashi, T.Nogami, T.Ishida (2009) *Polyhedron*, **28**,1672

Formula: $C_{28}H_{54}Cu_1N_8O_4 \cdot 2(Cl_1O_4^{1-}) \cdot 2(C_1H_2Cl_2)$

Compound Name: (1,8-Dimethyl-4,11-bis(4,4,5,5-tetramethylimidazolin-1-oxyl 3-oxide)-1,4,8,11-tetra-azacyclotetradecane-N,N',N'',N''',O)-copper(ii) diperchlorate dichloromethane solvate

Space Group: P-1 **Cell:** a 12.545(0) b 14.026(0) c 14.207(0)
Space Group No.: 2 **(Å,°)** α 74.17(0) β 64.30(0) γ 77.74(0)

R-Factor (%): 13.53 **Temperature(K):** 120 **Density(g/cm³):** 1.540



TIJREJ

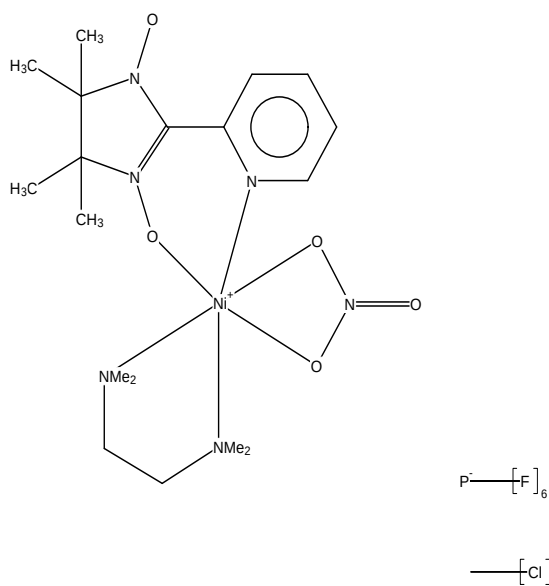
Reference: T.Yoshida, T.Suzuki, S.Kaizaki (2001) *Acta Crystallogr., Sect.C: Cryst. Struct. Commun.*, **57**,1274

Formula: $C_{18}H_{32}N_6Ni_1O_5^{1+}F_6P_1^{1-} \cdot C_1H_2Cl_2$

Compound Name: (4,5-Dihydro-4,4,5,5-tetramethyl-2-(2-pyridyl-κN)imidazol-1-oxyl 3-oxide)-κO³-(nitrate-κ²O,O')-(N,N,N',N'-tetramethyl-1,2-ethanediamine-κ²N,N')-nickel(ii) hexafluorophosphate dichloromethane solvate

Space Group: P21/c **Cell:** a 8.631(1) b 26.690(6) c 13.119(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 102.31(1) γ 90.00

R-Factor (%): 4.73 **Temperature(K):** 296 **Density(g/cm³):** 1.577



VENXOD

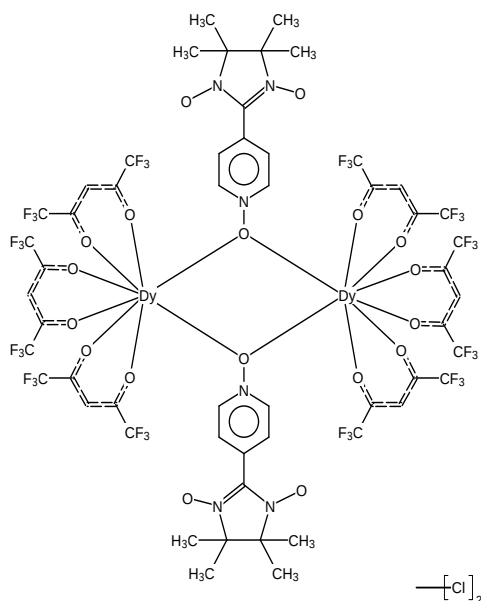
Reference: Tian Han, Wei Shi, Xiao-Ping Zhang, Lei-Lei Li, Peng Cheng (2012) *Inorg.Chem.*, **51**,13009

Formula: $C_{54}H_{38}Dy_2F_{36}N_6O_{18} \cdot C_1H_2Cl_2$

Compound Name: bis(μ₂-2-(4-Oxidopyridyl)-4,4,5,5-tetramethylimidazolin-1-oxyl 3-oxide)-hexakis(1,1,1,5,5,5-hexafluoroacetylacetonato)-di-dysprosium dichloromethane solvate

Space Group: P-1 **Cell:** a 12.216(0) b 12.779(0) c 25.832(1)
Space Group No.: 2 **(Å,°)** α 85.87(0) β 88.92(0) γ 68.76(0)

R-Factor (%): 5.52 **Temperature(K):** 120 **Density(g/cm³):** 1.907



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 49-52

VEQBEA

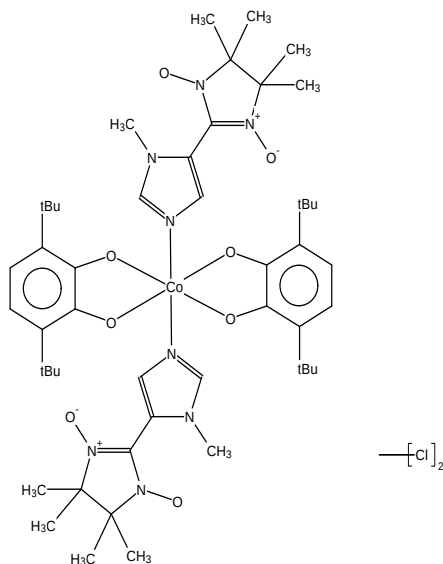
Reference: E.Yu.Fursova, O.V.Kuznetsova, E.V.Tret'yakov, G.V.Romanenko, A.S.Bogomyakov, V.I.Ovcharenko, R.Z.Sagdeev, V.K.Cherkasov, M.P.Bubnov, G.A.Abakumov (2011) *Izv.Akad.Nauk SSSR, Ser.Khim.(Russ.)(Russ.Chem.Bull.)*, 791

Formula: C₅₀ H₇₄ Co₁ N₈ O₈, 8(C₁ H₂ Cl₂)

Compound Name: bis(3,6-Di-*t*-butyl-*o*-semiquinolato)-bis(4,4,5,5-tetramethyl-2-(1-methyl-1H-imidazol-5-yl)-1-oxyl-4,5-dihydro-1H-imidazole-3-oxide-N)-cobalt(ii) dichloromethane solvate

Space Group: P-1 **Cell:** **a** 11.542(3) **b** 12.868(3) **c** 14.380(4)
Space Group No.: 2 **(Å, °)** **α** 97.25(0) **β** 104.41(0) **γ** 99.76(0)

R-Factor (%): 9.26 **Temperature(K):** 295 **Density(g/cm³):** 1.368



VEQCAX

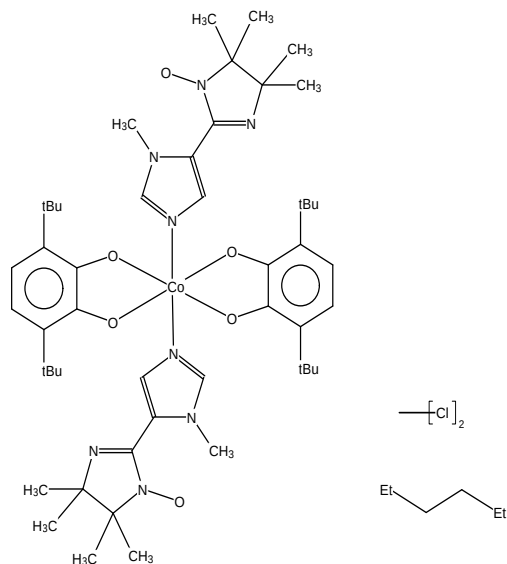
Reference: E.Yu.Fursova, O.V.Kuznetsova, E.V.Tret'yakov, G.V.Romanenko, A.S.Bogomyakov, V.I.Ovcharenko, R.Z.Sagdeev, V.K.Cherkasov, M.P.Bubnov, G.A.Abakumov (2011) *Izv.Akad.Nauk SSSR, Ser.Khim.(Russ.)(Russ.Chem.Bull.)*, 791

Formula: C₅₀ H₇₄ Co₁ N₈ O₆, 2(C₁ H₂ Cl₂), C₆ H₁₄

Compound Name: bis(3,6-Di-*t*-butyl-*o*-semiquinolato)-bis(4,4,5,5-tetramethyl-2-(1-methyl-1H-imidazol-5-yl)-1-oxyl-4,5-dihydro-1H-imidazole-N)-cobalt(ii) dichloromethane hexane solvate

Space Group: P-1 **Cell:** **a** 10.442(9) **b** 11.857(9) **c** 14.408(12)
Space Group No.: 2 **(Å, °)** **α** 71.59(1) **β** 84.66(1) **γ** 72.49(1)

R-Factor (%): 16.14 **Temperature(K):** 295 **Density(g/cm³):** 1.233



WODHOM

Reference: K.Matsuda, M.Irie (2000) *J.Am.Chem.Soc.*, **122**, 7195

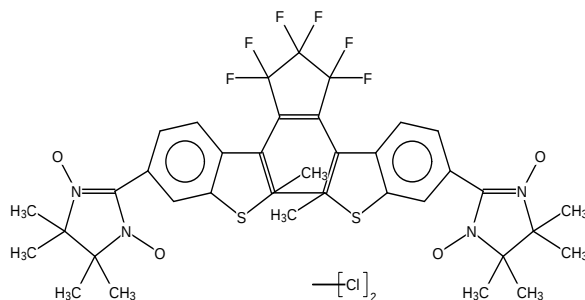
Formula: C₃₇ H₃₆ F₆ N₄ O₄ S₂, C₁ H₂ Cl₂

Compound Name: 3,3,4,4,5,5-Hexafluoro-11,20-bis(1-oxyl-3-oxide-4,4,5,5-tetramethylimidazolin-2-yl)-15,16-dimethyl-14,17-dithiahexacyclo[14.7.0.0^{2,6}.0^{7,15}.0^{8,13}.0^{18,23}]tricoso-1(16),2(6),7(15),8(10),12,18,20,22-octaene dichloromethane solvate

Synonym: 2b

Space Group: P21/c **Cell:** **a** 12.277(1) **b** 23.850(4) **c** 26.549(4)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 90.51(0) **γ** 90.00

R-Factor (%): 11.53 **Temperature(K):** 111 **Density(g/cm³):** 1.476



WOTYOT

Reference: Y.Sayama, M.Handa, M.Mikuriya, I.Hiromitsu, K.Kasuga (2000) *Bull.Chem.Soc.Jpn.*, **73**, 2499

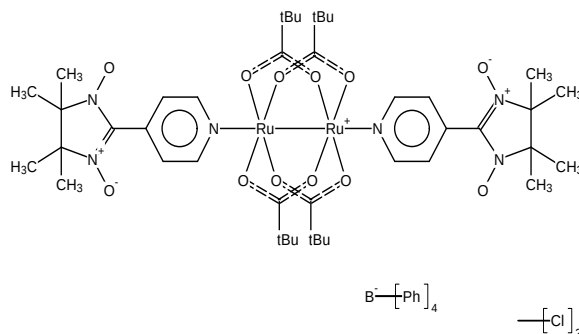
Formula: C₄₄ H₆₈ N₆ O₁₂ Ru₂ ¹⁺, C₂₄ H₂₀ B₁ ¹⁻, 0.5(C₁ H₂ Cl₂)

Compound Name: tetrakis(μ₂-Pivalato-O,O')-bis(4-(4,4,5,5-tetramethyl-1-oxyl-3-oxyl-4,5-dihydro-1H-imidazol-2-yl)pyridine-N)-di-ruthenium(ii,iii) tetraphenylborate dichloromethane solvate

Synonym: tetrakis(μ₂-Pivalato-O,O')-bis(4-(nitronyl nitroxide)pyridine-N)-di-ruthenium(ii,iii) tetraphenylborate dichloromethane solvate

Space Group: P21/n **Cell:** **a** 16.705(3) **b** 13.902(2) **c** 17.707(3)
Space Group No.: 13 **(Å, °)** **α** 90.00 **β** 110.40(1) **γ** 90.00

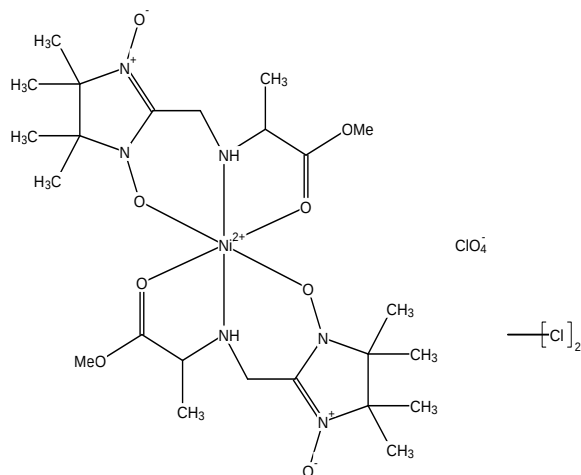
R-Factor (%): 5.20 **Temperature(K):** 295 **Density(g/cm³):** 1.238



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 53-56

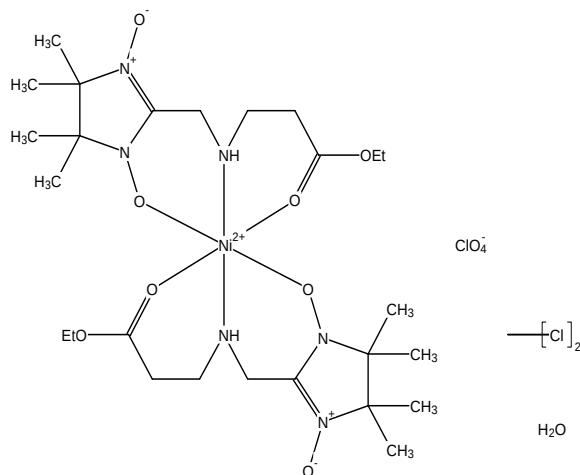
WUSCIX

Reference:	S.Osada, K.Igarashi, T.Nogami, T.Ishida (2010) <i>Chem.Lett.</i> , 39 ,576				
Formula:	$C_{24}H_{44}N_6Ni_1O_8^{2+} \cdot 2(Cl_1O_4^{1-}) \cdot 2(C_1H_2Cl_2)$				
Compound Name:	bis(Methyl N-((4,4,5,5-tetramethylimidazolin-1-oxyl-2-yl 3-oxide)methyl)-L-alaninato radical-N,O,O')-nickel(ii) diperchlorate dichloromethane solvate				
Synonym:	bis((S)-Methyl 2-(((4,4,5,5-tetramethylimidazolin-1-oxyl-2-yl 3-oxide)methyl)amino)propanoato radical-N,O,O')-nickel(ii) diperchlorate dichloromethane solvate				
Space Group:	P21	Cell:	a 13.209(0)	b 16.405(0)	c 13.204(0)
Space Group No.:	4	(Å, °)	α 90.00	β 134.66(0)	γ 90.00
R-Factor (%) :	9.88	Temperature(K) :	100	Density(g/cm³) :	1.586



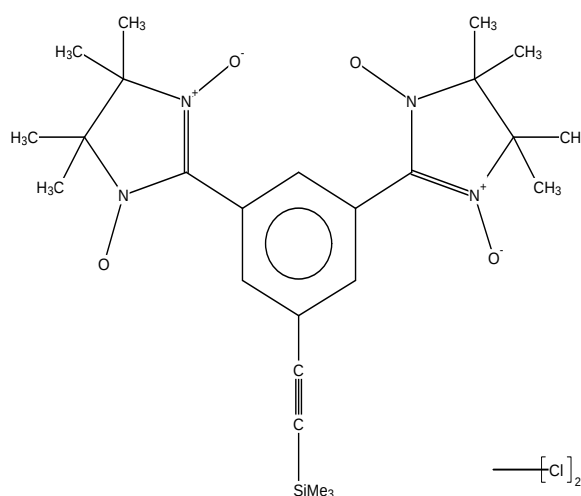
WUSCOD

Reference:	S.Osada, K.Igarashi, T.Nogami, T.Ishida (2010) <i>Chem.Lett.</i> , 39 ,576				
Formula:	$C_{26}H_{48}N_6Ni_1O_8^{2+} \cdot 2(Cl_1O_4^{1-}) \cdot C_1H_2Cl_2 \cdot 1.83(H_2O_1)$				
Compound Name:	bis(Ethyl N-((4,4,5,5-tetramethylimidazolin-1-oxyl-2-yl 3-oxide)methyl)-β-alaninato radical-N,O,O')-nickel(ii) diperchlorate dichloromethane solvate hydrate				
Synonym:	bis(Ethyl 3-(((4,4,5,5-tetramethylimidazolin-1-oxyl-2-yl 3-oxide)methyl)amino)propanoato radical-N,O,O')-nickel(ii) diperchlorate dichloromethane solvate hydrate				
Space Group:	P-1	Cell:	a 11.248(0)	b 12.429(0)	c 15.668(1)
Space Group No.:	2	(Å, °)	α 72.42(0)	β 78.82(0)	γ 86.92(0)
R-Factor (%) :	11.44	Temperature(K) :	106	Density(g/cm³) :	1.537



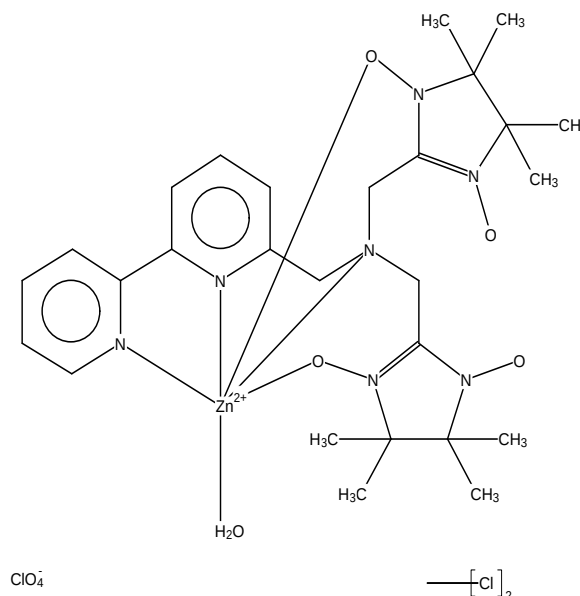
XEZXIJ

Reference:	L.Catala, J.Le Moigne, N.Kyritsakas, P.Rey, J.J.Novoa, P.Turek (2001) <i>Chem.-Eur.J.</i> , 7 ,2466				
Formula:	$C_{25}H_{36}N_4O_4Si_1C_1H_2Cl_2$				
Compound Name:	1,3-bis(1-Oxyl-3-oxo-4,4,5,5-tetramethylimidazolin-2-yl)-5-trimethylsilylacetylenebenzene dichloromethane solvate				
Space Group:	Pbca	Cell:	a 15.269(0)	b 13.288(0)	c 30.189(0)
Space Group No.:	61	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%) :	7.60	Temperature(K) :	174	Density(g/cm³) :	1.235



XOTLEX

Reference:	C.Stroh, R.Ziessel (2002) <i>Chem. Commun.</i> ,1916				
Formula:	$C_{27}H_{39}N_7O_5Zn_1^{2+} \cdot 2(Cl_1O_4^{1-}) \cdot C_1H_2Cl_2$				
Compound Name:	mer-Aqua-(6-(N,N-bis((4,5-dihydro-4,4,5,5-tetramethylimidazolinyl-3-oxide-1-oxyl-2-yl)methyl)aminomethyl)-2,2'-bipyridine-N,N',N'',O,O')-zinc diperchlorate dichloromethane solvate				
Space Group:	P32	Cell:	a 15.455(0)	b 15.455(0)	c 13.559(0)
Space Group No.:	145	(Å, °)	α 90.00	β 90.00	γ 120.00
R-Factor (%) :	7.50	Temperature(K) :	173	Density(g/cm³) :	1.582



Search: search3 (Sun Jan 12 22:45:21 2014): Hits 57-58

XOTLEX01

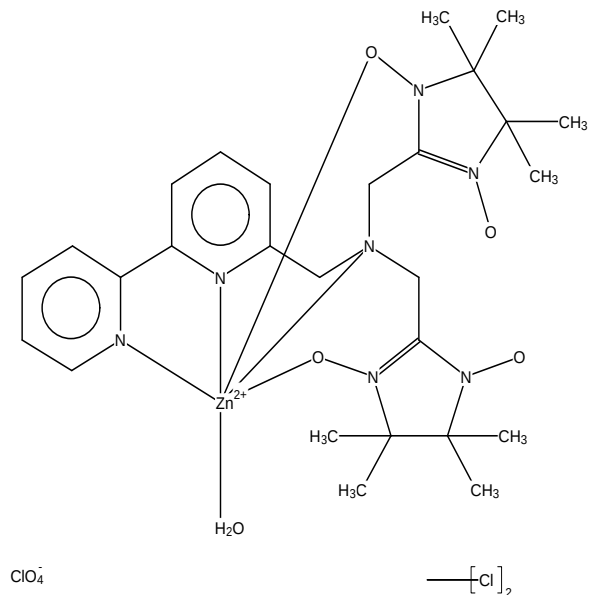
Reference: C.Stroh, E.Belorizky, P.Turek, H.Bolvin, R.Ziessel (2003)
Inorg.Chem. ,**42**,2938

Formula: $C_{27}H_{39}N_7O_5Zn^{2+} \cdot 2(Cl_1O_4^{1-}) \cdot C_1H_2Cl_2$

Compound Name: mer-Aqua-(6-(N,N-bis((4,5-dihydro-4,4,5,5-tetramethylimidazolyl-3-oxide-1-oxyl-2-yl)methyl)aminomethyl)-2,2'-bipyridine-N,N'',N'',O,O')-zinc diperchlorate dichloromethane solvate

Space Group: P32 **Cell:** **a** 15.455(0) **b** 15.455(0) **c** 13.559(0)
Space Group No.: 145 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 120.00

R-Factor (%): 7.50 **Temperature(K):** 173 **Density(g/cm³):** 1.582



XUDSIZ

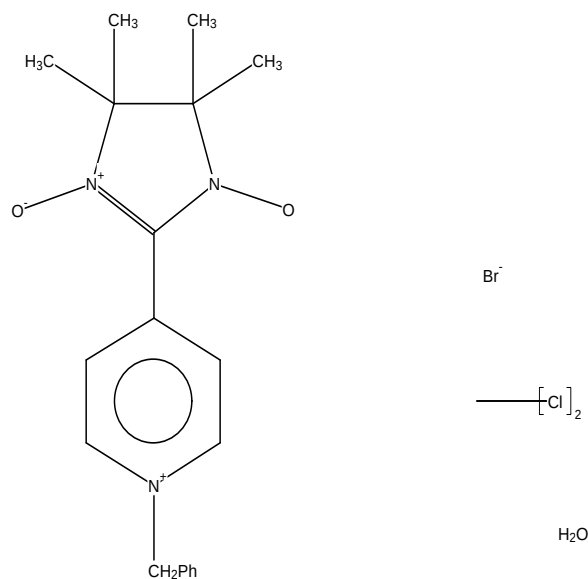
Reference: Hai-Rong Zhao, Jia-Sen Sun, Yun-Xia Sui,
Xiao-Ming Ren, Bin-Qian Yao, Lin-Jiang Shen, Qing-Jin Meng (2009)
J.Mol.Struct. ,**930**,167

Formula: $C_{19}H_{23}N_3O_2^{1+} \cdot Br_1^{1-} \cdot 0.33(C_1H_2Cl_2) \cdot 0.67(H_2O_1)$

Compound Name: (2-(N-Benzylpyridinium-4-yl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide radical) bromide dichloromethane solvate hydrate

Space Group: P-1 **Cell:** **a** 15.889(4) **b** 16.133(2) **c** 16.459(2)
Space Group No.: 2 **(Å,°)** **α** 118.88(0) **β** 95.95(0) **γ** 109.44(0)

R-Factor (%): 6.97 **Temperature(K):** 296 **Density(g/cm³):** 1.345



Search Overview

S24

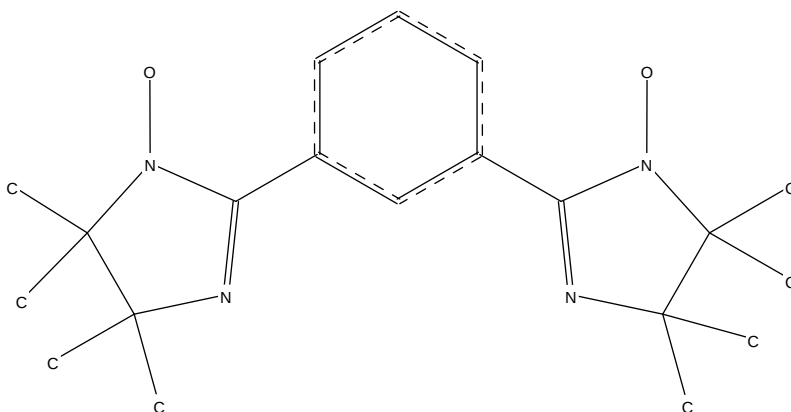
Search: search1
Date/Time done: Thu Jan 16 10:36:36 2014
Database(s): CSD version 5.35 updates (Nov 2013)
CSD version 5.35 (November 2013)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 27

Single query used. Search found structures that:

match

Query 1

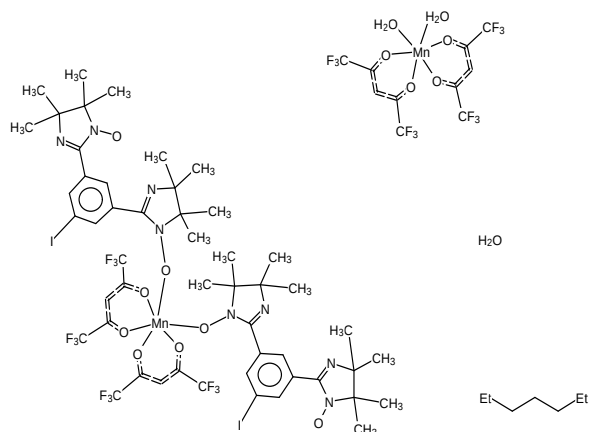
Query 1



Search: search1 (Thu Jan 16 10:36:36 2014): Hits 1-4

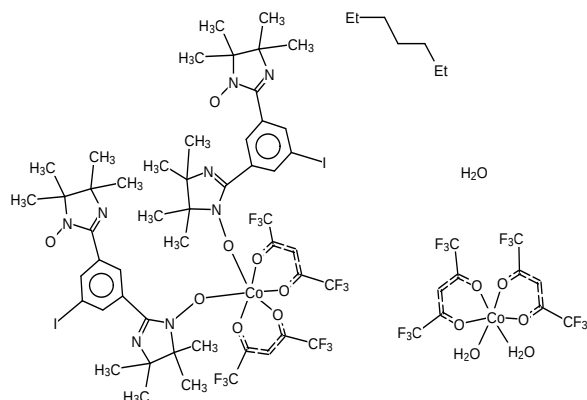
VIBRIJ

Reference:	M.G.F.Vaz, H.Akpınar, G.P.Guedes, S.Santos, M.A.Novak, P.M.Lahti (2013) <i>New J.Chem.</i> , 37 ,1927				
Formula:	C ₅₀ H ₅₆ F ₁₂ I ₂ Mn ₁ N ₈ O ₈ C ₁₀ H ₆ F ₁₂ Mn ₁ O ₆ .0.5(H ₂ O ₁).0.5(C ₇ H ₁₆)				
Compound Name:	bis(2,2'-(5-Iodo-1,3-phenylene)bis(4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-olato))-bis(1,1,1,3,3,3-hexafluoroacetylacetonato)-manganese bis(1,1,1,3,3,3-hexafluoroacetylacetonato)-diaqua-manganese n-heptane solvate hemihydrate				
Space Group:	C2/c	Cell:	a 49.475(0)	b 16.483(0)	c 22.224(0)
Space Group No.:	15	(Å, °)	α 90.00	β 115.25(0)	γ 90.00
R-Factor (%) :	5.64	Temperature(K) :	100	Density(g/cm³) :	1.619



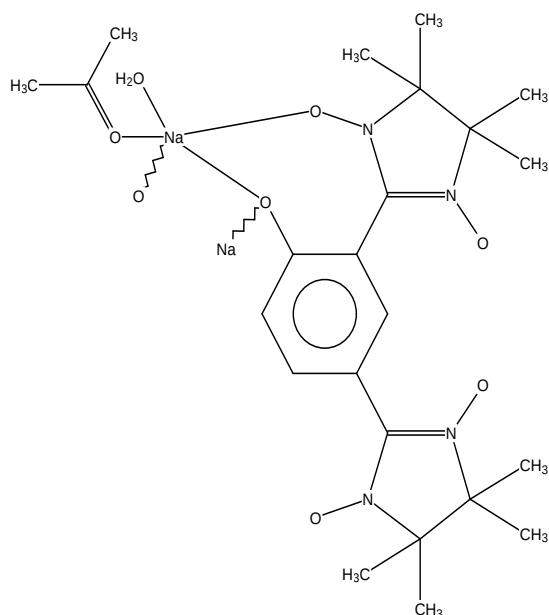
VIBROP

Reference:	M.G.F.Vaz, H.Akpınar, G.P.Guedes, S.Santos, M.A.Novak, P.M.Lahti (2013) <i>New J.Chem.</i> , 37 ,1927				
Formula:	C ₅₀ H ₅₆ Co ₁ F ₁₂ I ₂ N ₈ O ₈ C ₁₀ H ₆ Co ₁ F ₁₂ O ₆ .0.5(C ₇ H ₁₆).0.5(H ₂ O ₁)				
Compound Name:	bis(2,2'-(5-Iodo-1,3-phenylene)bis(4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-olato))-bis(1,1,1,3,3,3-hexafluoroacetylacetonato)-cobalt bis(1,1,1,3,3,3-hexafluoroacetylacetonato)-diaqua-cobalt n-heptane solvate hemihydrate				
Space Group:	C2/c	Cell:	a 49.363(0)	b 16.337(0)	c 22.309(0)
Space Group No.:	15	(Å, °)	α 90.00	β 115.93(0)	γ 90.00
R-Factor (%) :	5.75	Temperature(K) :	100	Density(g/cm³) :	1.647



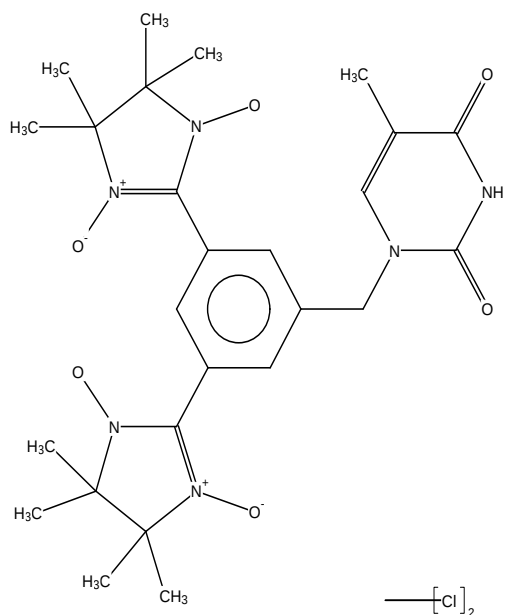
AJISER

Reference:	Y.Kanzaki, D.Shiomi, K.Sato, T.Takui (2003) <i>Polyhedron</i> , 22 ,1817				
Formula:	(C ₂₃ H ₃₅ N ₄ Na ₁ O ₇) _n				
Compound Name:	catena-((μ ₂ -2,4-bis(1-Oxyl-3-oxido-dioxy-4,4,5,5-tetramethyl-imidazolin-2-yl))phenolato-O,O')-aqua-acetone-sodium)				
Space Group:	P212121	Cell:	a 7.540(4)	b 10.817(6)	c 32.080(20)
Space Group No.:	19	(Å, °)	α 90.00	β 90.00	γ 90.00
R-Factor (%) :	11.33	Temperature(K) :	173	Density(g/cm³) :	1.276



EDEDIB

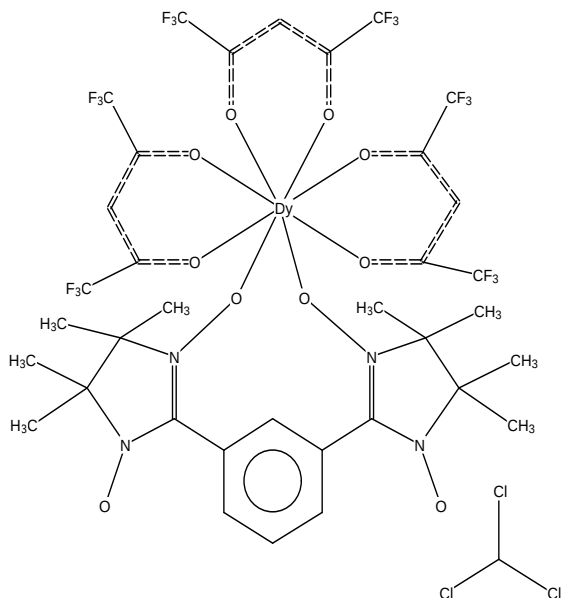
Reference:	H.Tanaka, D.Shiomi, T.Ise, K.Sato, T.Takui (2007) <i>Polyhedron</i> , 26 ,2230				
Formula:	C ₂₆ H ₃₄ N ₆ O ₆ C ₁ H ₂ Cl ₂				
Compound Name:	1-(3,5-bis(1-Oxyl-3-oxido-4,4,5,5-tetramethylimidazolidin-2-yl)benzyl)-5-methyl-1H-pyrimidin-2,4-dione dichloromethane solvate				
Space Group:	P-1	Cell:	a 10.786(1)	b 12.118(3)	c 12.522(2)
Space Group No.:	2	(Å, °)	α 78.15(1)	β 69.17(1)	γ 75.16(1)
R-Factor (%) :	6.79	Temperature(K) :	293	Density(g/cm³) :	1.385



Search: search1 (Thu Jan 16^{S26} 10:36:36 2014): Hits 5-8

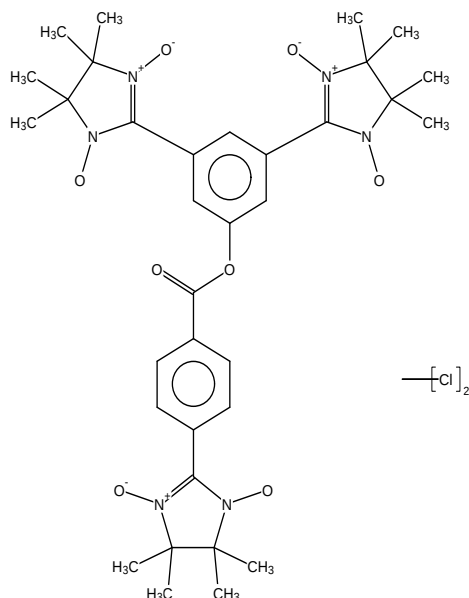
FUYDUZ

Reference:	K.Bernot, F.Pointillart, P.Rosa, M.Etienne, R.Sessoli, D.Gatteschi (2010) <i>Chem. Commun.</i> , 46 ,6458					
Formula:	C ₃₅ H ₃₁ Dy ₁ F ₁₈ N ₄ O ₁₀ ·C ₁ H ₁ Cl ₃					
Compound Name:	(1,3-bis-(1'-oxyl-3'-oxido-4',4',5',5'-tetramethyl-4,5-hydro-1H-imidazol-2-yl)benzene)-tris(hexafluoroacetylacetonato)-dysprosium chloroform solvate					
Space Group:	P-1	Cell:	a 12.187(0)	b 13.163(0)	c 31.581(1)	
Space Group No.:	2	Cell:	α 90.00(0)	β 79.83(0)	γ 76.74(0)	
R-Factor (%) :	5.12	Temperature(K) :	150	Density(g/cm³) :	1.769	



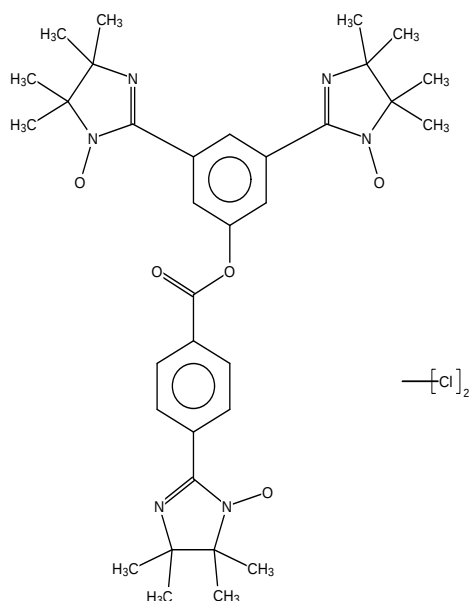
KEHPET

Reference:	Y.Kanzaki, D.Shiomi, C.Kaneda, T.Ise, K.Sato, T.Takui (2006) <i>J.Mater.Chem.</i> , 16 ,2064					
Formula:	C ₃₄ H ₄₃ N ₆ O ₈ ·0.5(C ₁ H ₂ Cl ₂)					
Compound Name:	4-(1',3'-Oxyl-4',4',5',5'-tetramethylimidazolin-2'-yl)-benzoic acid 3,5-bis-(1'',3''-oxyl-4'',4'',5'',5''-tetramethylimidazolin-2''-yl)phenyl ester dichloromethane solvate					
Space Group:	P-1	Cell:	a 11.390(1)	b 12.091(2)	c 14.386(3)	
Space Group No.:	2	Cell:	α 74.85(2)	β 78.45(2)	γ 68.70(2)	
R-Factor (%) :	7.20	Temperature(K) :	173	Density(g/cm³) :	1.325	



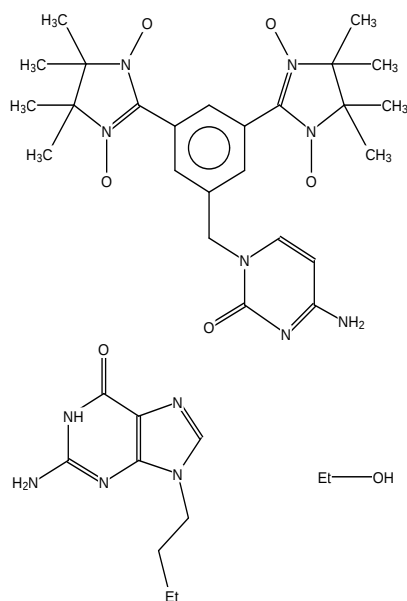
KEHPIX

Reference:	Y.Kanzaki, D.Shiomi, C.Kaneda, T.Ise, K.Sato, T.Takui (2006) <i>J.Mater.Chem.</i> , 16 ,2064					
Formula:	C ₃₄ H ₄₃ N ₆ O ₅ ·0.5(C ₁ H ₂ Cl ₂)					
Compound Name:	4-(1'-Oxyl-4',4',5',5'-tetramethylimidazolin-2'-yl)-benzoic acid 3,5-bis-(1''-oxyl-4'',4'',5'',5''-tetramethylimidazolin-2''-yl)-phenyl ester dichloromethane solvate					
Space Group:	P-1	Cell:	a 11.280(7)	b 11.995(7)	c 14.345(9)	
Space Group No.:	2	Cell:	α 74.99(2)	β 78.72(3)	γ 69.63(2)	
R-Factor (%) :	9.90	Temperature(K) :	293	Density(g/cm³) :	1.252	



MILFAP

Reference:	H.Tanaka, D.Shiomi, T.Ise, K.Sato, T.Takui (2007) <i>CrystEngComm</i> , 9 ,767					
Formula:	C ₂₅ H ₃₃ N ₇ O ₅ ·C ₉ H ₁₃ N ₅ O ₁ ·C ₂ H ₆ O ₁					
Compound Name:	4-Amino-1-(3,5-bis-(1-oxyl-3-oxido-4,4,5,5-tetramethyl-imidazolidin-2-yl)-benzyl)-1H-pyrimidin-2-one biradical 2-amino-9-butyl-1,9-dihydro-purin-6-one ethanol solvate					
Space Group:	P-1	Cell:	a 7.596(6)	b 12.988(11)	c 20.897(17)	
Space Group No.:	2	Cell:	α 100.89(1)	β 95.41(1)	γ 95.52(1)	
R-Factor (%) :	9.99	Temperature(K) :	143	Density(g/cm³) :	1.269	



Search: search1 (Thu Jan 16^{S27} 10:36:36 2014): Hits 9-12

OLABEI

Reference: T.Ichimura, K.Doi, C.Mitsuhashi, T.Ishida, T.Nogami (2003) *Polyhedron* ,**22**,2557

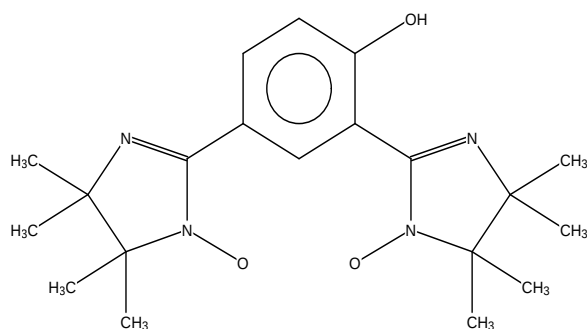
Formula: C₂₀ H₂₈ N₄ O₃

Compound Name: 4-Hydroxy-1,3-phenylene-bis(4,4,5,5-tetramethylimidazolin-2-oxyl-3-yl)

Synonym: 4-Hydroxy-1,3-phenylene-bis(imino nitroxide)

Space Group: Pbc_a **Cell:** **a** 13.006(0) **b** 12.168(0) **c** 24.954(1)
Space Group No.: 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 9.89 **Temperature(K):** 100 **Density(g/cm³):** 1.253



QUFFIG

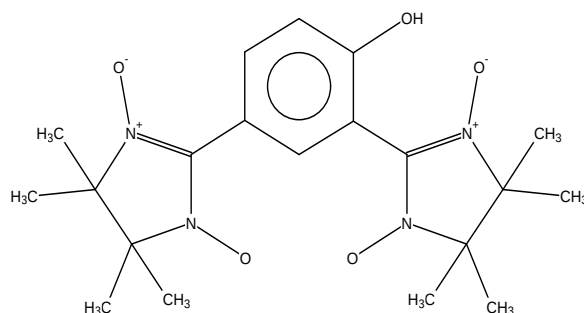
Reference: S.Hase, D.Shiomi, K.Sato, T.Takui (2001) *J.Mater.Chem.* ,**11**,756

Formula: C₂₀ H₂₈ N₄ O₅

Compound Name: 2,4-bis(1-Oxyl-3-oxide-4,4,5,5-tetramethyl-2-imidazolin-2-yl)phenol

Space Group: P2₁/n **Cell:** **a** 11.806(4) **b** 25.330(5) **c** 7.337(7)
Space Group No.: 14 **(Å,°)** α 90.00 β 104.65(4) γ 90.00

R-Factor (%): 6.17 **Temperature(K):** 296 **Density(g/cm³):** 1.266



QUFFOM

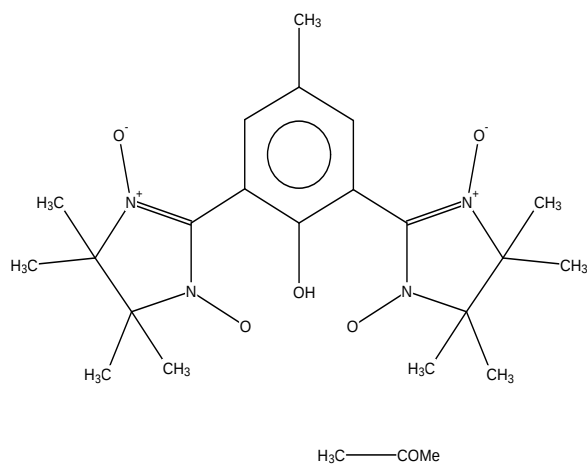
Reference: S.Hase, D.Shiomi, K.Sato, T.Takui (2001) *J.Mater.Chem.* ,**11**,756

Formula: C₂₁ H₃₀ N₄ O₅.0.5(C₃ H₆ O₁)

Compound Name: 4-Methyl-2,6-bis(1-oxyl-3-oxide-4,4,5,5-tetramethyl-2-imidazolin-2-yl)phenol acetone solvate

Space Group: Pbc_a **Cell:** **a** 20.206(4) **b** 40.405(4) **c** 11.888(3)
Space Group No.: 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.87 **Temperature(K):** 296 **Density(g/cm³):** 1.225



QUSCOW

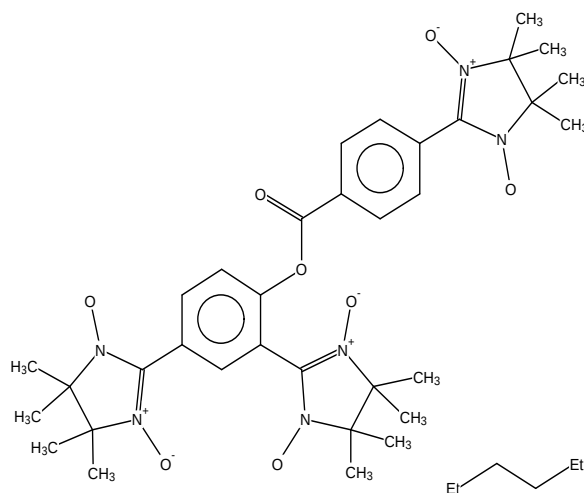
Reference: D.Shiomi, T.Kanaya, K.Sato, M.Mito, K.Takeda, T.Takui (2001) *J.Am.Chem.Soc.* ,**123**,11823

Formula: C₃₄ H₄₃ N₆ O₈.C₆ H₁₄

Compound Name: 4-(1-Oxyl-3-oxido-4,4,5,5-tetramethyl-2-imidazolin-2-yl)-benzoic acid 2,4-bis(1-oxyl-3-oxido-4,4,5,5-tetramethyl-2-imidazolin-2-yl)-phenyl ester hexane solvate

Space Group: C2/c **Cell:** **a** 34.160(20) **b** 12.551(9) **c** 17.770(30)
Space Group No.: 15 **(Å,°)** α 90.00 β 100.68(8) γ 90.00

R-Factor (%): 6.75 **Temperature(K):** 293 **Density(g/cm³):** 1.331



Search: search1 (Thu Jan 16^{S28} 10:36:36 2014): Hits 13-16

SUGCAY

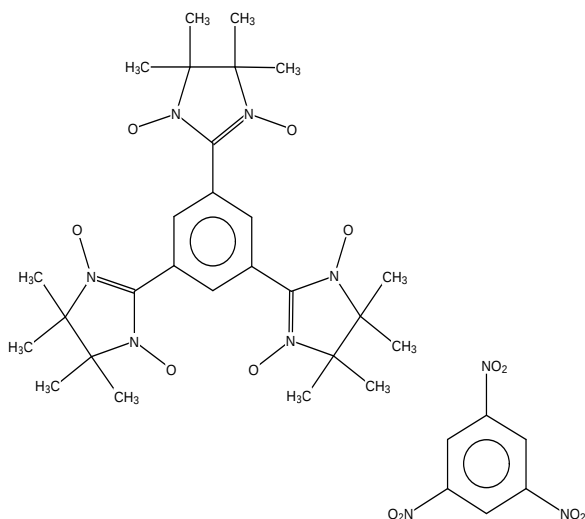
Reference: A.Izuoka, M.Fukada, T.Sagawara, M.Sakai, S.Bandow (1992) *Chem.Lett.* ,1627

Formula: $C_{27}H_{39}N_6O_6$

Compound Name: 1,3,5-tris(4',4',5',5'-Tetramethylimidazolin-2'-yl)benzene 3',3'',3'''-trioxide

Space Group: C2 **Cell:** a 21.158(3) b 12.374(2) c 7.285(1) **Space Group No.:** 5 **Cell:** $(\text{\AA},^\circ)$ α 90.00 β 104.79(1) γ 90.00

R-Factor (%): 6.00 **Temperature(K):** 295 **Density(g/cm³):** 1.362



SUKBOP

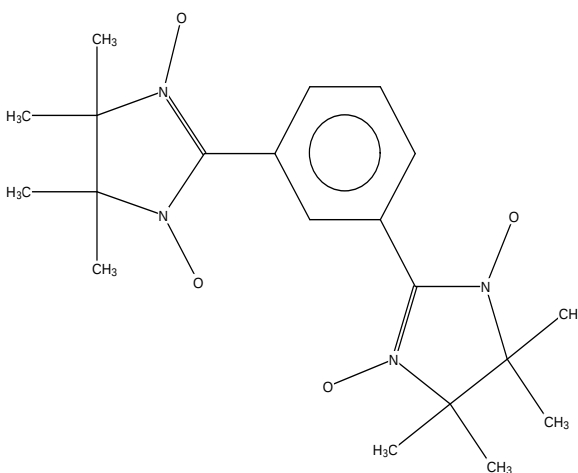
Reference: A.Caneschi, P.Chiesi, L.David, F.Ferraro, D.Gatteschi, R.Sessoli (1993) *Inorg.Chem.* ,32,1445

Formula: $C_{20}H_{28}N_4O_4$

Compound Name: 1,3-bis(1'-Oxyl-3'-oxido-4',4',5',5'-tetramethyl-4,5'-dihydro-1H-imidazol-2'-yl)benzene

Space Group: P21/n **Cell:** a 7.318(2) b 25.368(3) c 11.669(2) **Space Group No.:** 14 **Cell:** $(\text{\AA},^\circ)$ α 90.00 β 104.72(2) γ 90.00

R-Factor (%): 9.10 **Temperature(K):** 295 **Density(g/cm³):** 1.232



SUKCAC

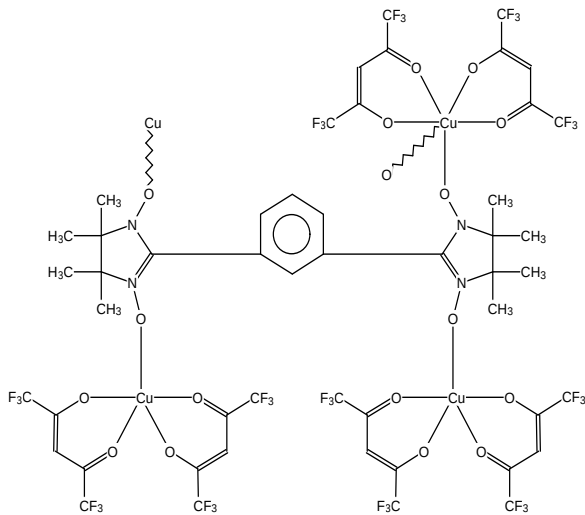
Reference: A.Caneschi, P.Chiesi, L.David, F.Ferraro, D.Gatteschi, R.Sessoli (1993) *Inorg.Chem.* ,32,1445

Formula: $(C_{50}H_{34}Cu_3F_{36}N_4O_{16})_n$

Compound Name: catena-((μ₄-1,3-bis(1'-Oxyl-3'-oxido-4',4',5',5'-tetramethyl-4,5'-dihydro-1H-imidazol-2'-yl)benzene)-tris(bis(hexafluoroacetylacetonato)-copper(ii))

Space Group: P21/n **Cell:** a 13.942(3) b 16.422(4) c 16.473(3) **Space Group No.:** 13 **Cell:** $(\text{\AA},^\circ)$ α 90.00 β 97.93(2) γ 90.00

R-Factor (%): 8.09 **Temperature(K):** 295 **Density(g/cm³):** 1.619



TICVUX

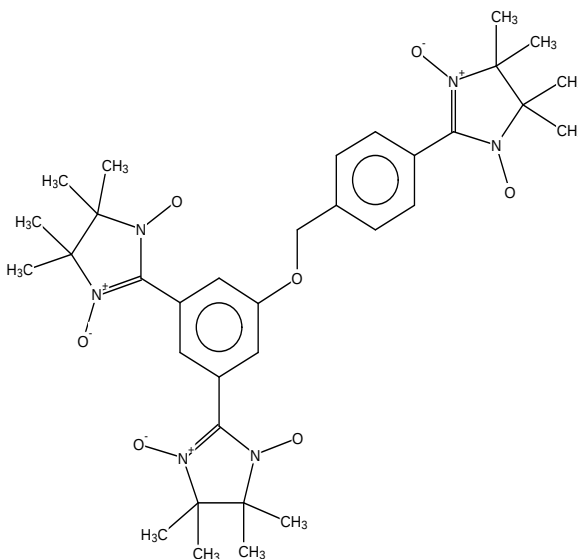
Reference: Y.Kanzaki, D.Shiomi, T.Ise, K.Sato, T.Takui (2007) *Polyhedron* ,26,1901

Formula: $C_{34}H_{45}N_6O_7$

Compound Name: 4-(1-Oxyl-4,4,5,5-tetramethyl-imidazolin-2-yl)benzyl 3,5-bis-(1-oxyl-4,4,5,5-tetramethyl-imidazolin-2-yl)phenyl ether

Space Group: P21/a **Cell:** a 12.874(10) b 27.517(20) c 10.723(8) **Space Group No.:** 14 **Cell:** $(\text{\AA},^\circ)$ α 90.00 β 117.57(0) γ 90.00

R-Factor (%): 9.88 **Temperature(K):** 143 **Density(g/cm³):** 1.282



Search: search1 (Thu Jan 16^{S29} 10:36:36 2014): Hits 17-20

TICWAE

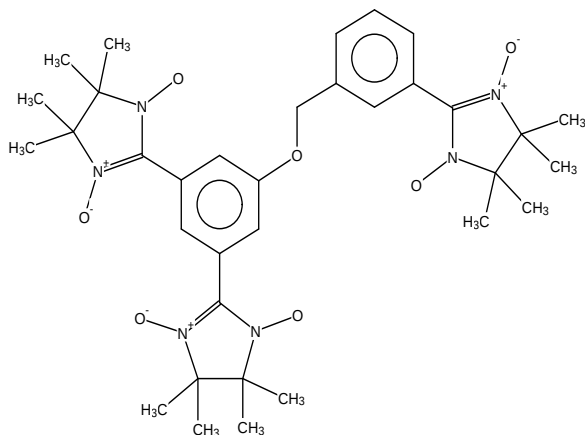
Reference: Y.Kanzaki, D.Shiomi, T.Ise, K.Sato, T.Takui (2007) *Polyhedron* ,**26**,1901

Formula: C₃₄ H₄₅ N₆ O₇

Compound Name: 3-(1-Oxyl-4,4,5,5-tetramethyl-imidazolin-2-yl)benzyl 3,5-bis-(1-oxyl-4,4,5,5-tetramethyl-imidazolin-2-yl)phenyl ether

Space Group: P21/n **Cell:** **a** 12.463(7) **b** 11.835(6) **c** 22.583(13)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 95.63(0) **γ** 90.00

R-Factor (%): 8.80 **Temperature(K)**: 193 **Density(g/cm³)**: 1.302



TICYAG

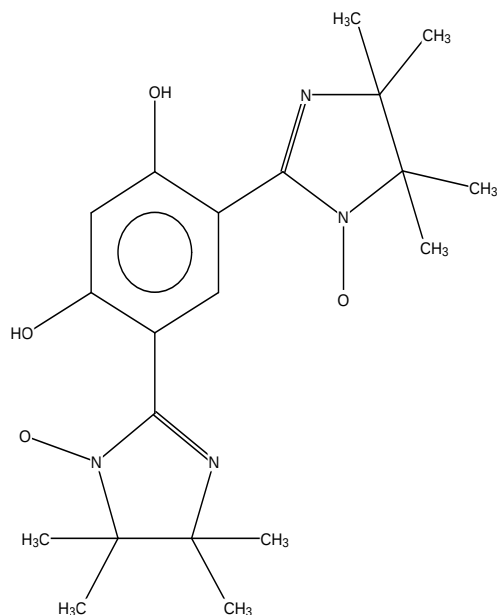
Reference: K.Tanaka, K.Furuichi, M.Kozaki, S.Suzuki, D.Shiomi, K.Sato, T.Takui, K.Okada (2007) *Polyhedron* ,**26**,2021

Formula: C₂₀ H₂₈ N₄ O₄

Compound Name: 1,3-Dihydroxy-4,6-bis(4,4,5,5-tetramethylimidazoline-1-oxyl-2-yl) benzene

Space Group: P21/c **Cell:** **a** 10.620(1) **b** 11.021(0) **c** 18.422(1)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 105.96(0) **γ** 90.00

R-Factor (%): 4.40 **Temperature(K)**: 173 **Density(g/cm³)**: 1.245



XEQSOB

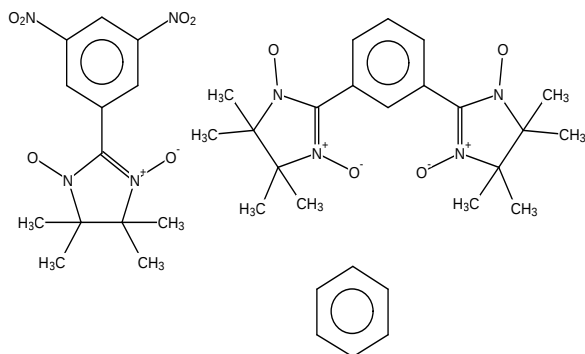
Reference: A.Izuoka, M.Fukada, R.Kumai, M.Itakura, S.Hikami, T.Sugawara (1994) *J.Am.Chem.Soc.* ,**116**,2609

Formula: C₁₃ H₁₅ N₄ O₆.C₂₀ H₂₈ N₄ O₄.C₆ H₆

Compound Name: 1-(Nitronyl nitroxide)-3,4-dinitrobenzene radical 1,3-bis(nitronyl nitroxide) benzene radical benzene solvate

Space Group: P1 **Cell:** **a** 11.526(3) **b** 13.260(2) **c** 7.288(2)
Space Group No.: 1 **(Å,°)** **α** 106.57(2) **β** 106.34(3) **γ** 90.38(2)

R-Factor (%): 5.90 **Temperature(K)**: 295 **Density(g/cm³)**: 1.286



XEQSOB01

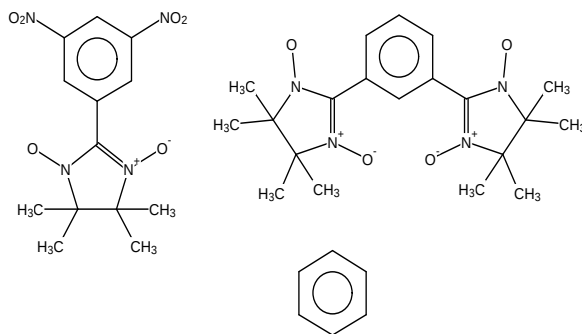
Reference: M.Nishizawa, D.Shiomi, K.Sato, T.Takui, K.Itoh, H.Sawa, R.Kato, H.Sakurai, A.Izuoka, T.Sugawara (2000) *J.Phys.Chem.B* ,**104**, 503

Formula: C₁₃ H₁₅ N₄ O₆.C₂₀ H₂₈ N₄ O₄.C₆ H₆

Compound Name: 1-(Nitronyl nitroxide)-3,4-dinitrobenzene radical 1,3-bis(nitronyl nitroxide) benzene radical benzene solvate

Space Group: P1 **Cell:** **a** 11.150(10) **b** 12.820(10) **c** 7.134(7)
Space Group No.: 1 **(Å,°)** **α** 105.90(10) **β** 101.90(10) **γ** 70.09(7)

R-Factor (%): 3.40 **Temperature(K)**: 30 **Density(g/cm³)**: 1.434



Search: search1 (Thu Jan 16 10:36:36 2014): Hits 21-24

XEQSOB02

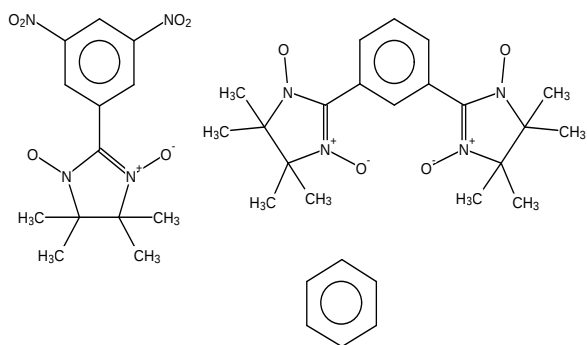
Reference: M.Nishizawa, D.Shiomi, K.Sato, T.Takui, K.Itoh, H.Sawa, R.Kato, H.Sakurai, A.Izuoka, T.Sugawara (2000) *J.Phys.Chem.B* ,**104**, 503

Formula: C₁₃ H₁₅ N₄ O₆, C₂₀ H₂₈ N₄ O₄, C₆ H₆

Compound Name: 1-(Nitronyl nitroxide)-3,4-dinitrobenzene radical 1,3-bis(nitronyl nitroxide) benzene radical benzene solvate

Space Group: P1 **Cell:** **a** 11.150(10) **b** 12.820(10) **c** 7.133(7)
Space Group No.: 1 **(Å, °)** α 105.90(10) β 101.80(10) γ 70.08(7)

R-Factor (%): 3.40 **Temperature(K):** 10 **Density(g/cm³):** 1.434



XEZWUU

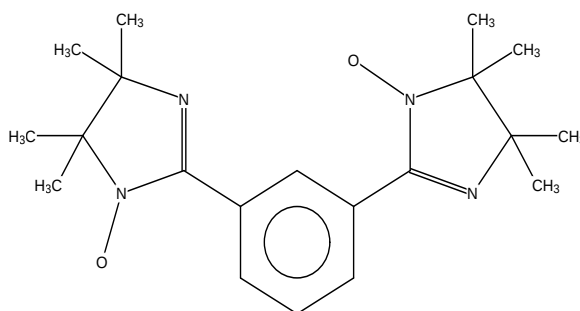
Reference: L.Catala, J.Le Moigne, N.Kyritsakas, P.Rey, J.J.Novoa, P.Turek (2001) *Chem.-Eur.J.* ,**7**,2466

Formula: C₂₀ H₂₈ N₄ O₂

Compound Name: 1,3-bis(1-Oxy-4,4,5,5-tetramethylimidazolin-2-yl)benzene

Space Group: P21/n **Cell:** **a** 7.158(0) **b** 25.553(2) **c** 11.503(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 102.43(0) γ 90.00

R-Factor (%): 13.60 **Temperature(K):** 295 **Density(g/cm³):** 1.152



XEXXAB

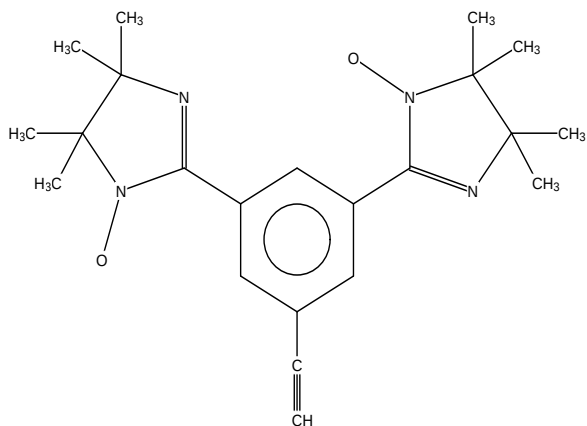
Reference: L.Catala, J.Le Moigne, N.Kyritsakas, P.Rey, J.J.Novoa, P.Turek (2001) *Chem.-Eur.J.* ,**7**,2466

Formula: C₂₂ H₂₈ N₄ O₂

Compound Name: 1,3-bis(1-Oxy-4,4,5,5-tetramethylimidazolin-2-yl)-5-ethynylbenzene

Space Group: P21/n **Cell:** **a** 12.150(0) **b** 10.776(0) **c** 16.693(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.78(0) γ 90.00

R-Factor (%): 11.30 **Temperature(K):** 295 **Density(g/cm³):** 1.164



XEXXEF

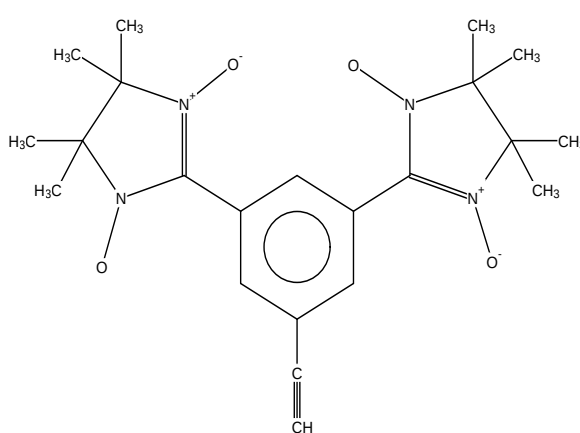
Reference: L.Catala, J.Le Moigne, N.Kyritsakas, P.Rey, J.J.Novoa, P.Turek (2001) *Chem.-Eur.J.* ,**7**,2466

Formula: C₂₂ H₂₈ N₄ O₄

Compound Name: 1,3-bis(1-Oxyl-3-oxo-4,4,5,5-tetramethylimidazolin-2-yl)-5-ethynylbenzene

Space Group: P21/n **Cell:** **a** 12.611(0) **b** 11.130(0) **c** 16.153(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 97.60(0) γ 90.00

R-Factor (%): 6.10 **Temperature(K):** 295 **Density(g/cm³):** 1.219



Search: search1 (Thu Jan 16 10:36:36 2014): Hits 25-27

XEZXIJ

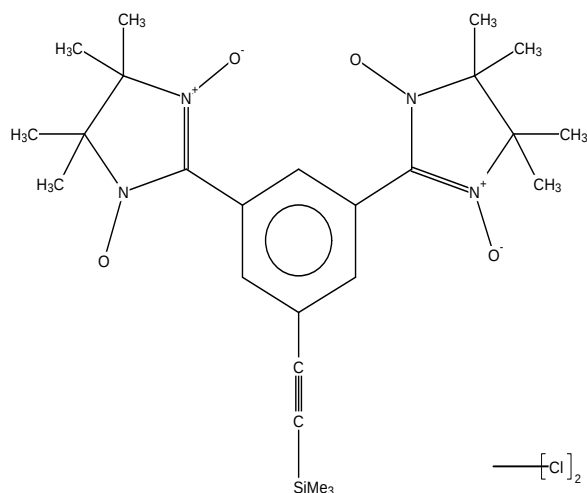
Reference: L.Catala, J.Le Moigne, N.Kyritsakas, P.Rey, J.J.Novoa, P.Turek (2001) *Chem.-Eur.J.* ,7,2466

Formula: C₂₅ H₃₆ N₄ O₄ Si₁.C₁ H₂ Cl₂

Compound Name: 1,3-bis(1-Oxyl-3-oxo-4,4,5,5-tetramethylimidazolin-2-yl)-5-trimethylsilylacetylenebenzene dichloromethane solvate

Space Group: Pbc_a **Cell:** **a** 15.269(0) **b** 13.288(0) **c** 30.189(0)
Space Group No.: 61 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 7.60 **Temperature(K)**: 174 **Density(g/cm³)**: 1.235



XEZXP

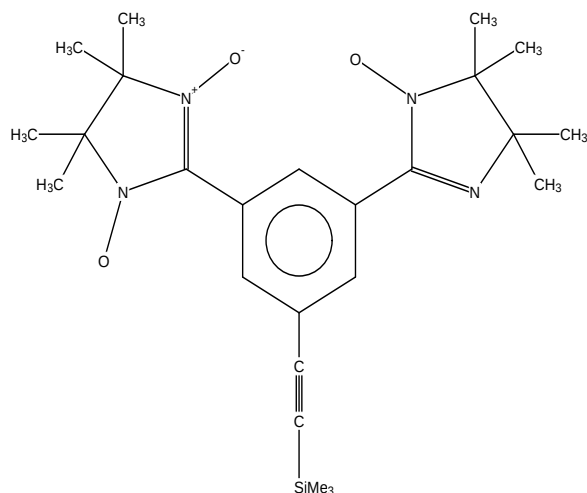
Reference: L.Catala, J.Le Moigne, N.Kyritsakas, P.Rey, J.J.Novoa, P.Turek (2001) *Chem.-Eur.J.* ,7,2466

Formula: C₂₅ H₃₆ N₄ O₃ Si₁

Compound Name: 1-(1-Oxyl-4,4,5,5-tetramethylimidazolin-2-yl)-3-(1-oxyl-3-oxo-4,4,5,5-tetramethylimidazolin-2-yl)-5-trimethylsilylacetylenebenzene

Space Group: P21/c **Cell:** **a** 11.866(0) **b** 21.524(0) **c** 10.960(0)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 109.72(0) **γ** 90.00

R-Factor (%): 5.00 **Temperature(K)**: 173 **Density(g/cm³)**: 1.181



XEZXUV

Reference: L.Catala, J.Le Moigne, N.Kyritsakas, P.Rey, J.J.Novoa, P.Turek (2001) *Chem.-Eur.J.* ,7,2466

Formula: C₂₀ H₂₈ N₄ O₃

Compound Name: 1-(1-Oxyl-4,4,5,5-tetramethylimidazolin-2-yl)-3-(1-oxyl-3-oxo-4,4,5,5-tetramethylimidazolin-2-yl)benzene

Space Group: P21/n **Cell:** **a** 7.229(0) **b** 25.462(4) **c** 11.596(1)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 103.79(0) **γ** 90.00

R-Factor (%): 10.30 **Temperature(K)**: 295 **Density(g/cm³)**: 1.194

