ESI index

Solid-state structures (CIF)

CIF filename	Compound	Compound number
16srv167	$Cp_2NbCl(NDipp)$	**3**
16srv289	$\{CpNb(\mu\text{-}Cl)(NDipp)\}_2$	**5**
18srv005	$Cp_2Nb(NDipp)(PCO) \cdot 5\{Cp_2NbCl(NDipp)\}$	**12** · 5{**3**}
18srv112	$Cp_2NbMe(NDipp)$	**11**
18srv116	$Cp_2Nb(ClGaCl_3)(NDipp) \cdot C_6D_6$	**9** · C_6D_6
18srv197	$Cp_2Nb(ClGaCl_3)(N\{Dipp{\cdot}Ga_2Cl_6\})$	**10**
18srv406	$[\{Cp_2NbCl\}_2(N\{2,6\text{-}^iPr_2C_6H_2\}_2N)][BAr^F{}_4]_2$	[**18**][$BAr^F{}_4$]$_2$
18srv467s	$TrBAr^F{}_4$	**15**
18srv502	$[Cp_2NbCl(NHDipp)]BAr^F{}_4$	[**13**]$BAr^F{}_4$
19srv036	$\{Cp_2NbCl\}_2(N\{2,6\text{-}^iPr_2C_6H_2\}_2N)$	**20**
19srv084	$[Cp_2NbCl(NHDipp)]OTf \cdot DCM$	[**13**]OTf · DCM
19srv177	$Cp_2NbCl(NDipp^{Tr})$	**17**

Computed structures (MOL2)

MOL2 filename	Compound	Compound reference	Calculation type
(CpTMS)2NbCl(NtBu)	$Cp^{TMS}{}_2NbCl(N^tBu)$		Gas-phase
(CpTMS)NbCl2(NtBu)	$Cp^{TMS}NbCl_2(N^tBu)$		Gas-phase
(eta5-Flu)Nb(NDipp)	(η^5-Flu)Nb(NDipp)		Gas-phase
(eta9-Flu)Nb(NDipp)	(η^9-Flu)Nb(NDipp)		Gas-phase
3	$Cp_2NbCl(NDipp)$	**3**	Gas-phase
3_RadicalCation	$[Cp_2NbCl(NDipp)]^{\bullet+}$	$\mathbf{3}^{\bullet+}$	Gas-phase
4	$\{CpNb(NDipp)\}_2(\mu,\eta^2,\eta^2\text{-}N_2)$	**4**	Gas-phase
5	$\{CpNb(\mu\text{-}Cl)(NDipp)\}_2$	**5**	Gas-phase
8_Cation	$[Cp_2Nb(NDipp)]^+$	$\mathbf{8}^+$	Gas-phase
9	$Cp_2Nb(ClGaCl_3)(NDipp)$	**9**	Gas-phase
10	$Cp_2Nb(ClGaCl_3)(N\{Dipp\cdot Ga_2Cl_6\})$	**10**	Gas-phase
12	$Cp_2Nb(NDipp)(PCO)$	**12**	Gas-phase
13_Cation	$[Cp_2NbCl(NHDipp)]^+$	$\mathbf{13}^+$	Gas-phase
14a_Cation	$[Cp_2NbCl(N\{Me\}Dipp)]^+$	$\mathbf{14a}^+$	Gas-phase
14b_Cation	$[Cp_2NbCl(N\{Dipp\text{-}4\text{-}Me\})]^+$	$\mathbf{14b}^+$	Gas-phase
16_Cation	$[Cp_2NbCl(N\{Dipp\text{-}4\text{-}Tr\})]^+$	$\mathbf{16}^+$	Gas-phase
18_Singlet_Dication_DCM	$[\{Cp_2NbCl\}_2(N\{2,6\text{-}^iPr_2C_6H_2\}_2N)]^{2+}$ (Singlet)	$\mathbf{18_S}^{2+}$	DCM solution (SMD)
18_Singlet_Dication_GasPhase	$[\{Cp_2NbCl\}_2(N\{2,6\text{-}^iPr_2C_6H_2\}_2N)]^{2+}$ (Singlet)	$\mathbf{18_S}^{2+}$	Gas-phase
18_Triplet_Dication_DCM	$[\{Cp_2NbCl\}_2(N\{2,6\text{-}^iPr_2C_6H_2\}_2N)]^{2+}$ (Triplet)	$\mathbf{18_T}^{2+}$	DCM solution (SMD)
18_Triplet_Dication_GasPhase	$[\{Cp_2NbCl\}_2(N\{2,6\text{-}^iPr_2C_6H_2\}_2N)]^{2+}$ (Triplet)	$\mathbf{18_T}^{2+}$	Gas-phase
19_Dication	$[\{Cp_2NbCl\}_2(N\{4,4'\text{-}Dipp_2\}N)]^{2+}$	$\mathbf{19}^{2+}$	Gas-phase
20	$\{Cp_2NbCl\}_2(N\{2,6\text{-}^iPr_2C_6H_2\}_2N)$	**20**	Gas-phase
AQ	$\{Cp^{\dagger}{}_2Zr\}_2(\mu,\eta^2,\eta^2\text{-}N_2)$	**AQ**	Gas-phase

Cp2NbCl(N(Dipp-4-H))_Cation	$[Cp_2NbCl(N\{Dipp\text{-}4\text{-}H\})]^+$,		Gas-phase
Ga2Cl6	Ga_2Cl_6		Gas-phase
KOHLID_GasPhase	$Cp^*AlI(N\{2,6\text{-}Mes_2C_6H_3\})\cdot AlI\{\kappa^2\text{-}N_3(Cp^*)(2,6\text{-}Mes_2C_6H_3)\}$	KOHLID	Gas-phase
MABHAB_GasPhase	$(TMS)N(Mes^*\text{-}4\text{-}\{CH_2CMe_2[C_6H_2\text{-}3,5\text{-}^tBu_2\text{-}2\text{-}\{NH(TMS)\}]\})$	MABHAB	Gas-phase
MeOTf_Et2O	MeOTf		Et_2O solution (SMD)
MeOTf_GasPhase	MeOTf		Gas-phase
Tr_Cation	Tr^+		Gas-phase