The Role of Imidoselenium(II) Chlorides in the Formation of Cyclic Selenium Imides *via* Cyclocondensation

Aino J. Karhu, Olli J. Pakkanen, J. Mikko Rautiainen, Raija Oilunkaniemi, Tristram Chivers, and Risto S. Laitinen *

Electronic Supporting Information

1. QTAIM Analyses of ClSe[N(ᵗBu)Se]$_n$Cl (n = 1-3)

Computed gas phase QTAIM parameters charge density ρ, laplacian of charge density $\nabla^2\rho$, electronic energy density H, kinetic energy density per electron G/ρ and delocalization index DI are shown in Tables S1-S3.The numbering of the atoms in different chlorides is shown in Fig. 1S.

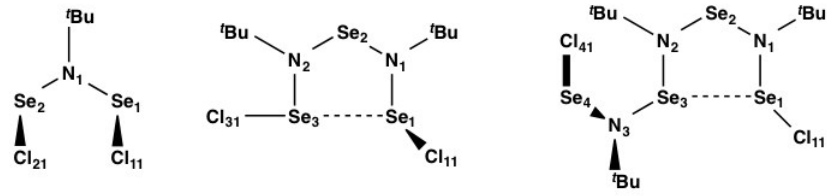


Fig. 1S. Numbering of atoms in ClSe[N(ᵗBu)Se]$_2$Cl (n = 1, 2, 3) for the QTAIM analysis.

Table S1. QTAIM parameters of ClSeN(ᵗBu)SeCl.

Bond	ρ	$\nabla^2\rho$	H	G	G/ρ	DI
Se1-Cl1	0.116	-0.008	-0.060	0.058	0.501	1.1
Se2-Cl2	0.118	-0.011	-0.062	0.059	0.501	1.2
Se1-N1	0.174	0.096	-0.122	0.146	0.840	1.1
Se2-N1	0.172	0.073	-0.120	0.139	0.804	1.1

Table S2. QTAIM parameters of ClSe[N(ᵗBu)Se]$_2$Cl.

Bond	ρ	$\nabla^2\rho$	H	G	G/ρ	DI
Se1-Cl11	0.110	0.008	-0.053	0.055	0.497	1.0
Se1-Cl31	0.109	0.007	-0.053	0.055	0.499	1.1
Se1-N1	0.187	0.152	-0.136	0.174	0.932	1.2
Se2-N1	0.144	-0.002	-0.089	0.088	0.615	0.9
Se2-N2	0.178	0.094	-0.127	0.150	0.846	1.1
Se3-N2	0.168	0.053	-0.117	0.130	0.770	1.1
Se1···Se3	0.027	0.044	-0.002	0.013	0.470	0.3

Table S3. Computed QTAIM parameters of ClSe[N(ᵗBu)Se]$_3$Cl.

Bond	ρ	$\nabla^2\rho$	H	G	G/ρ	DI
Se1-Cl11	0.109	0.008	-0.052	0.055	0.499	1.1
Se4-Cl41	0.110	0.004	-0.054	0.055	0.499	1.1
Se1-N1	0.185	0.149	-0.134	0.171	0.925	1.2
Se2-N1	0.145	-0.004	-0.090	0.089	0.615	0.9
Se2-N2	0.177	0.088	-0.126	0.148	0.836	1.1
Se3-N2	0.161	0.028	-0.108	0.115	0.716	1.0
Se3-N3	0.153	0.018	-0.100	0.104	0.679	1.0
Se4-N3	0.180	0.108	-0.129	0.156	0.866	1.2
Se1···Se3	0.019	0.037	0.000	0.010	0.504	0.2

In all bonds of ClSe[N(ᵗBu)Se]$_n$Cl (n = 1, 2, 3), the charge density is high (> 10^{-1}). Electronic energy density values are negative, which is typical for covalent bonds. In addition, G/ρ values are < 1 also indicating covalent bonding. $\nabla^2\rho$ values of the Se-N bonds decrease when bond lengths increase in ClSe[N(ᵗBu)Se]$_n$Cl (n = 1, 2, 3). This kind of behavior is typical for polar covalent bonds as observed by Love.[1] $\nabla^2\rho$ values of the Se-Cl bonds do not show similar behavior as the Se-N bonds and do not behave as systematically as those of the Se-N bonds, because Se-Cl bonds are less polar than the Se-N bonds. Delocalization indices are in a good agreement with bond lengths. ρ and $\nabla^2\rho$ values at the bond critical point of the Se···Se interactions in ClSe[N(ᵗBu)Se]$_n$Cl (n = 2, 3) indicate weak closed-shell interactions. H values are zero so they fall between shared-shell and closed-shell interactions. Delocalization indices of 0.3 and 0.2 also show that the bonding is weak.

2. Thermochemical cycles

The Gibbs energy of sublimation of ᵗBuNH$_3$Cl was estimated as the difference between gas phase ion pair (ᵗBuNH$_3$)$^+$(Cl)$^-$ and formula unit energy in optimized crystal structure of orthorhombic ᵗBuNH$_3$Cl. Both the structure of (ᵗBuNH$_3$)$^+$(Cl)$^-$ ion pair and crystal structure were optimized utilizing a Crystal14 program [2] using the PBE0 functional [3] and the pob-TZVP basis sets.[4] Both the cell parameters and the atomic

1 I. Love, *J. Phys. Chem. A* 2009, **113**, 2649-2646.

2 (*a*) R. Dovesi, R. Orlando, A. Erba, C. M. Zicovich-Wilson, B. Civalleri, S. Casassa, L. Maschio, M. Ferrabone, M. De La Pierre, P. D'Arco, Y. Noel, M. Causa, M. Rerat and B. Kirtman, *Int. J. Quantum Chem.* 2014, **114**, 1287-1317; (*b*) R. Dovesi, V. R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N. M. Harrison, I. J. Bush, P. D'Arco, M. Llunell, M. Causà and Y. Noël CRYSTAL14, 2014, CRYSTAL14 User's Manual, University of Torino, Torino.

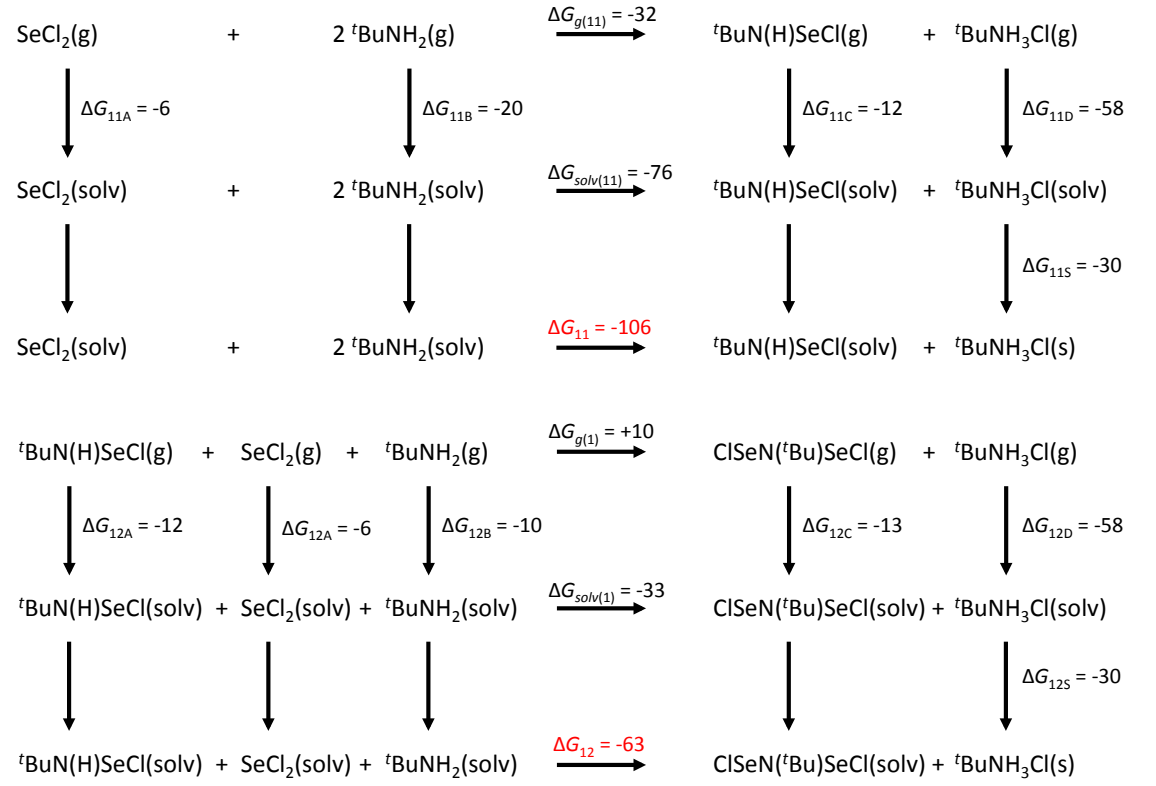
3 (*a*) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.,* 1996, **77**, 3865-3868; (*b*) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.,* 1997, **78**, 1396; (*c*) J. P. Perdew, M. Ernzerhof, and K. Burke, *J. Chem. Phys*., 1996, **105**, 9982-9985; (*d*) C. Adamo, and V. Barone, *J. Chem. Phys*., 1999, **110**, 6158-6170.

4 M. F. Peintinger, D. Vilela Oliveira, and T. Bredow, *J. Comput. Chem.*, 2013, **34**, 451-459.

coordinates were optimized. The optimization was started from experimental crystal structure with the orthorombic cell, *Pbca*, *a* = 17.770(8), *b* = 8.877(4), *c* = 8.647(3) Å, *V* = 1364.0 Å^3, *Z* = 8.[5] The corresponding optimized cell parameters were a = 17.758, b = 8.925, c = 8.593 Å, V = 1362 Å^3.
The calculated enthalpy and Gibbs energy differences for gaseous ion pair and ^{t}BuNH$_3$Cl in the crystal structure with vibrational and thermal energy corrections (298 K) were ΔH = –149 kJ mol^{-1} and ΔG = –88 kJ mol^{-1}.

The computed solvation energy was taken as the energy difference between the ion pair in the gaseous state and in THF. It has a ΔG value of –58 kJ mol^{-1}. The energy difference from the solvated ion pair to solid crystal structure (per formula unit) is -30 kJ mol^{-1}. These three values have been taken into account in the thermochemical cycles below.

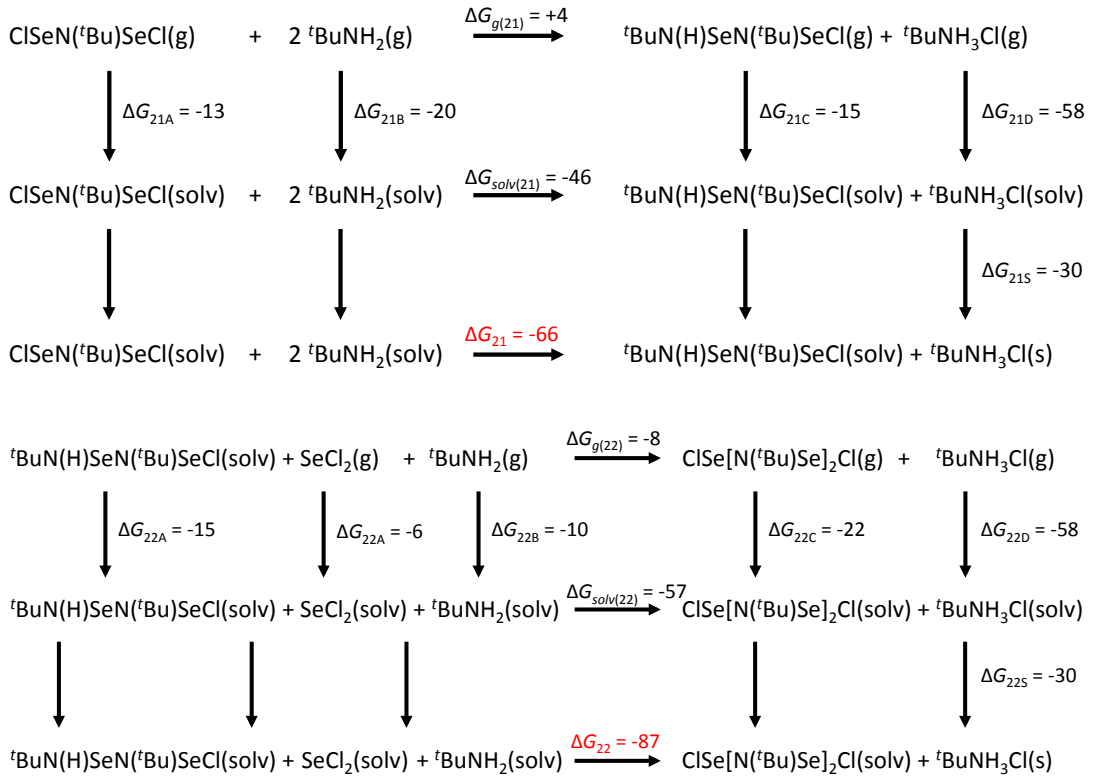
2.1 $SeCl_2$(solv) → ClSeN(^{t}Bu)SeCl(solv)



2 $SeCl_2$(solv) + 3 ^{t}BuNH$_2$(solv) ⟶ ClSeN(^{t}Bu)SeCl(solv) + 2 ^{t}BuNH$_3$Cl(s) ΔG_1 = (-106) + (-63) = -169

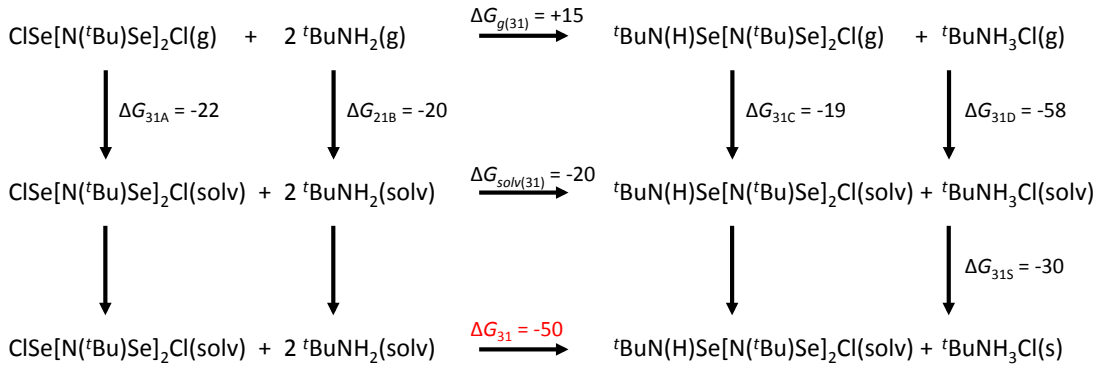
5 K. N. Trueblood, *Acta Crystallogr.* 1987, **C43**, 711-713.

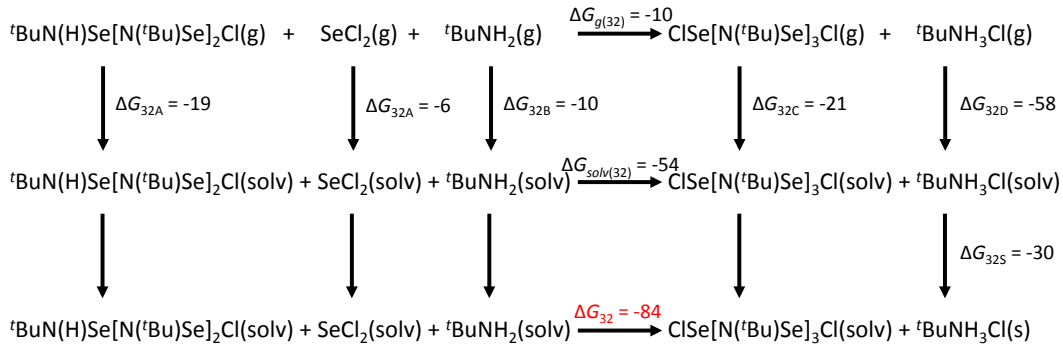
2.2 $ClSeN(^tBu)SeCl(solv) \rightarrow ClSe[N(^tBu)Se]_2Cl(solv)$



$ClSeN(^tBu)SeCl(solv) + 3\ ^tBuNH_2(solv) \longrightarrow ClSe[N(^tBu)Se]_2Cl(solv) + ^tBuNH_3Cl(s)$ $\Delta G_2 = (-66) + (-87) = -153$

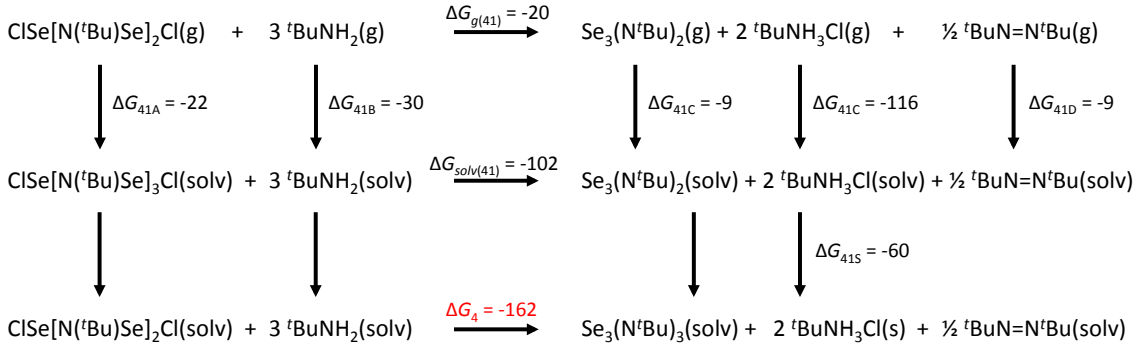
2.3 $ClSeN(^tBu)Se]_2Cl(solv) \rightarrow ClSe[N(^tBu)Se]_3Cl(solv)$



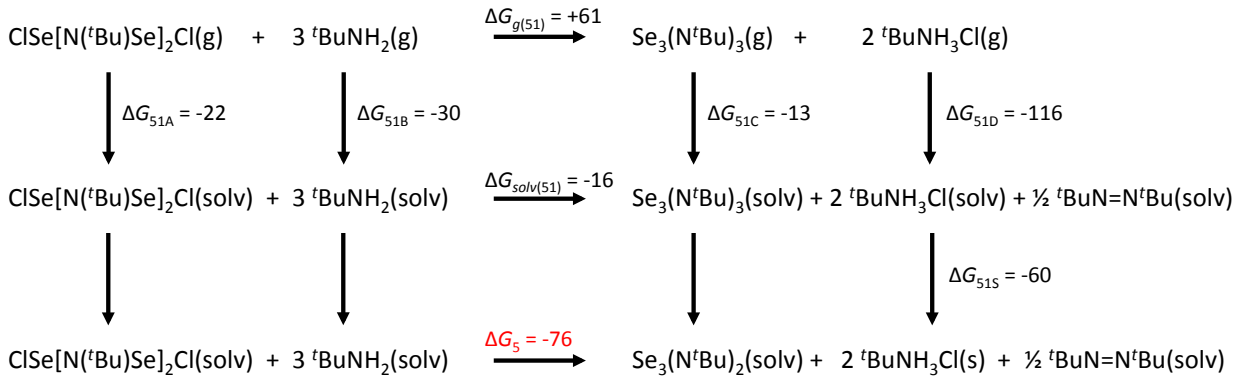


ClSeN[(ᵗBu)Se]$_2$Cl(solv) + 3 ᵗBuNH$_2$(solv) ⟶ ClSe[N(ᵗBu)Se]$_2$Cl(solv) + ᵗBuNH$_3$Cl(s) ΔG_3 = (-50) + (-84) = -134

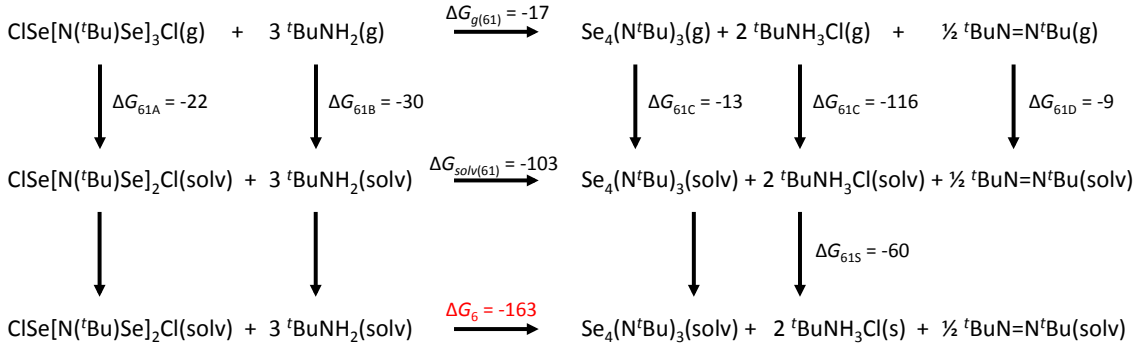
2.4 ClSe[N(ᵗBu)Se]$_2$Cl → 1,3-Se$_3$(NᵗBu)$_2$



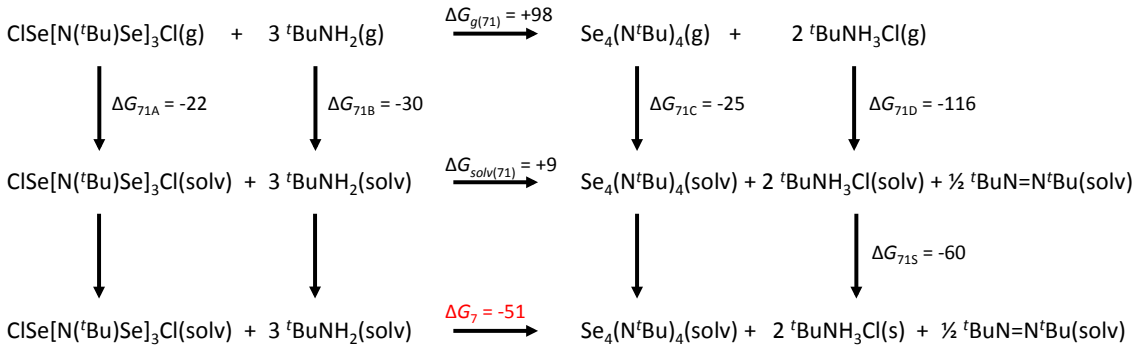
2.5 ClSe[N(ᵗBu)Se]$_2$Cl → 1,3,5-Se$_3$(NᵗBu)$_3$



2.6 ClSe[N(ᵗBu)Se]$_3$Cl → 1,3,5-Se$_4$(NᵗBu)$_3$



2.7 $ClSe[N(^tBu)Se]_3Cl \rightarrow 1,3,5,7\text{-}Se_4(N^tBu)_4$



3. Selected bond parameters of $[PdCl_2\{Se,Se'\text{-}(SeCl)_2N(^tBu)\}]\cdot[PdCl_2\{Se,Se'\text{-}Se_4(N^tBu)_3]\cdot MeCN$ and their comparison to the corresponding parameters in $[PdCl_2\{Se,Se'\text{-}Se_4(N^tBu)_3]$ and $ClSeN(^tBu)SeCl$

$[PdCl_2\{Se,Se'\text{-}Se_4(N^tBu)_3]$ in **10**·MeCN		$[PdCl_2\{Se,Se'\text{-}Se_4(N^tBu)_3]$ [a]		$[PdCl_2\{Se,Se'\text{-}(SeCl)_2N(^tBu)\}]$ in **10**·MeCN		$ClSe(N^tBu)SeCl$ [b]	
Pd1-Se1	2.3532(10)	Pd1-Se1	2.3439(8)	Pd2-Se5	2.3647(10)		
Pd1-Se2	2.3689(10)	Pd1-Se2	2.3830(10)	Pd2-Se6	2.3520(10)		
Pd1-Cl1	2.374(2)	Pd1-Cl1	2.3471(17)	Pd2-Cl3	2.3138(19)		
Pd1-Cl2	2.3550(18)	Pd1-Cl2	2.3417(16)	Pd2-Cl4	2.315(2)		
Se1-N1	1.799(6)	Se1-N1	1.879(5)	Se5-N4	1.811(6)	Se1-N1	1.804(6)
Se2-N1	1.883(7)	Se2-N1	1.825(5)	Se6-N4	1.825(6)	Se2-N1	1.816(7)
Se2-N2	1.808(6)	Se2-N2	1.902(6)	Se5-Cl5	2.233(2)	Se1-Cl1	2.223(2)
Se3-N2	1.873(6)	Se3-N2	1.853(6)	Se6-Cl6	2.250(2)	Se2-Cl2	2.215(2)
Se4-N3	1.870(7)	Se4-N3	1.863(5)				
Se1-N3	1.871(7)	Se1-N3	1.833(5)				
Se3-Se4	2.3293(12)	Se3-Se4	2.3307(11)				
Se1-Pd1-Se2	77.67(3)	Se1-Pd1-Se2	77.85(4)	Se5-Pd2-Se6	77.07(3)		
Cl1-Pd1-Se2	95.25(5)	Cl1-Pd1-Se1	90.10(5)	Cl3-Pd2-Se5	94.69(6)		
Cl2-Pd1-Se1	93.78(5)	Cl2-Pd1-Se2	97.91(5)	Cl4-Pd2-Se6	93.70(5)		
Cl1-Pd1-Cl2	93.28(7)	Cl1-Pd1-Cl2	94.06(6)	Cl13-Pd2-Cl4	94.45(7)		
Cl2-Pd1-Se2	169.55(6)	Cl2-Pd1-Se1	175.48(5)	Cl4-Pd2-Se5	170.66(5)		
N1-Se1-N2	109.6(3)	N1-Se1-N2	99.5(2)	N4-Se5-Cl5	100.8(2)	N1-Se1-Cl1	103.9(2)
N1-Se2-N3	101.1(3)	N1-Se1-N3	107.4(2)	N4-Se6-Cl6	101.0(2)	N1-Se2-Cl2	103.8(2)
N2-Se3-Se4	101.2(2)	N2-Se3-Se4	104.57(17)	C4-N4-Se5	127.9(5)	C1-N1-Se1	119.9(5)
N3-Se4-Se3	108.5(2)	N3-Se4-Se3	103.93(17)	C4-N4-Se6	124.0(5)	C1-N1-Se2	123.1(5)
Se1-N1-Se2	107.0(3)	Se1-N1-Se2	106.6(3)	Se5-N4-Se6	107.8(3)	Se1-N1-Se2	116.7(4)
Se2-N2-Se3	116.6(3)	Se2-N2-Se3	117.6(3)				
Se1-N3-Se4	118.1(3)	Se1-N3-Se4	116.0(3)				
C1-N1-Se1	122.8(5)	C1-N1-Se1	125.9(4)				
C1-N1-Se2	127.3(5)	C1-N1-Se2	122.1(4)				
C2-N2-Se2	121.6(5)	C2-N2-Se2	114.5(4)				
C2-N2-Se3	118.7(5)	C2-N2-Se3	116.8(4)				
C3-N3-Se1	116.6(5)	C3-N3-Se1	121.8(4)				
C3-N3-Se4	117.1(5)	C3-N3-Se4	118.4(4)				

[a] Ref. 6. [b] Ref. 7.

6 M. Risto, A. Eironen, E. Männistö, R. Oilunkaniemi, R. S. Laitinen and T. Chivers, *Dalton Trans.,* 2009, 8473-8475.

7 T. Maaninen, T. Chivers, R. Laitinen and E. Wegelius, *Chem. Commun.,* 2000, 759-760.

4. PBE0/def2-TZVPP optimized Cartesian coordinates of ClSe[N(^{t}Bu)Se]$_n$Cl (n = 1-3) and Se$_m$(N^{t}Bu)$_m$ and Se$_m$(N^{t}Bu)$_{m-1}$ (m = 3, 4) in the gas phase

4.1 ClSe(N^{t}Bu)SeCl

Se	-1.48876	-0.39349	-0.84591
Se	1.59545	-0.26608	-0.72335
Cl	-2.00556	-1.46667	0.99294
Cl	1.89574	-1.61173	0.97106
N	-0.00305	0.53329	-0.40355
C	-0.04303	1.77666	0.44660
C	0.46001	1.45499	1.84813
H	1.49688	1.11887	1.82866
H	0.40604	2.35166	2.46810
H	-0.14630	0.67489	2.30860
C	-1.46478	2.30974	0.52523
H	-1.44359	3.23841	1.09776
H	-1.87106	2.52723	-0.46299
H	-2.13490	1.61533	1.03175
C	0.84265	2.82684	-0.21364
H	1.87637	2.48772	-0.28161
H	0.48138	3.05995	-1.21678
H	0.82692	3.74197	0.38035

4.2 ClSe[N(^{t}Bu)Se]$_2$Cl

C	2.84288	0.93888	-0.21535
C	-1.73652	1.73681	0.75299
C	3.85508	0.38734	0.77570
H	4.81870	0.86206	0.58345
H	3.97985	-0.69072	0.67000
H	3.56528	0.60454	1.80447
C	2.76443	2.45445	-0.05437
H	2.04222	2.89278	-0.74316
H	3.74121	2.89613	-0.25803
H	2.47317	2.71437	0.96447
C	3.26920	0.56614	-1.63356
H	4.27209	0.94626	-1.83572
H	2.60080	1.00146	-2.38132
H	3.27156	-0.51669	-1.76173
C	-1.46281	3.09561	0.12452
H	-1.89458	3.86838	0.76229
H	-1.92327	3.16885	-0.86214
H	-0.39620	3.29326	0.02553
C	-1.00031	1.61960	2.08248
H	-1.35990	2.38151	2.77661
H	0.07268	1.75700	1.94706
H	-1.17874	0.64139	2.53355
C	-3.23638	1.59658	0.97547
H	-3.56881	2.38843	1.64873
H	-3.48666	0.63858	1.43074
H	-3.78123	1.68031	0.03568
N	1.48736	0.38268	0.05684
N	-1.29439	0.66035	-0.19446
Cl	1.74635	-2.82040	-0.21315
Cl	-3.68258	-1.16726	-0.96465
Se	1.19511	-1.05986	1.02874

Se	-1.74359	-1.08458	0.12289
Se	0.15270	0.83822	-1.24580

4.3 ClSe[N(^{t}Bu)Se]$_3$Cl

Se	-3.86182	0.33176	-0.69139
Se	-0.86644	-0.28291	-0.31709
Se	1.60030	0.84322	1.12132
Se	2.13929	-1.32086	-1.08724
Cl	-4.27636	-1.75342	-1.32486
Cl	2.04831	-3.09048	0.25719
N	-2.50281	0.22367	0.46733
N	0.19443	1.19432	0.05563
N	2.79396	0.00984	-0.12452
C	-2.74365	-0.16223	1.89540
C	-4.03084	0.48526	2.38737
H	-4.90970	0.07536	1.89211
H	-4.01258	1.56466	2.22337
H	-4.12642	0.30293	3.45903
C	-1.58380	0.37021	2.72576
H	-1.77136	0.15669	3.77931
H	-1.47696	1.44877	2.60105
H	-0.64429	-0.11055	2.45075
C	-2.83152	-1.67743	2.03691
H	-3.66501	-2.07522	1.45800
H	-2.97830	-1.94564	3.08506
H	-1.91014	-2.15041	1.69222
C	0.20770	2.34443	-0.90390
C	-1.23155	2.76563	-1.16509
H	-1.79532	1.97274	-1.65771
H	-1.23622	3.63726	-1.82174
H	-1.73599	3.02482	-0.23362
C	0.94787	3.51696	-0.27563
H	0.52665	3.76755	0.69959
H	0.84448	4.38547	-0.92812
H	2.00982	3.31103	-0.15033
C	0.87414	1.95117	-2.21750
H	1.92158	1.69464	-2.05900
H	0.82515	2.78015	-2.92634
H	0.36356	1.09506	-2.66287
C	4.23745	0.14488	0.22315
C	4.61614	1.61642	0.08080
H	4.45768	1.95252	-0.94508
H	5.67029	1.74977	0.32931
H	4.02755	2.24697	0.74714
C	5.09241	-0.67797	-0.72693
H	4.92249	-0.39139	-1.76548
H	4.89680	-1.74570	-0.62711
H	6.14197	-0.49860	-0.48746
C	4.46972	-0.33636	1.65435
H	5.52967	-0.26837	1.90595
H	4.14798	-1.37206	1.76717
H	3.92460	0.27631	2.37733

4.4 1,3-Se$_3$(N^{t}Bu)$_2$

Se	0.71363	-1.30917	-0.95629

Se	-0.71363	-1.30917	0.95629
N	-1.37646	0.35077	0.56399
C	-2.55381	-0.06092	-1.63721
H	-1.78937	0.48249	-2.19373
H	-3.51179	0.07143	-2.14449
H	-2.30245	-1.12157	-1.65290
C	-2.65609	0.45408	-0.20963
C	-3.70574	-0.33660	0.56194
H	-3.47884	-1.40281	0.56217
H	-4.68050	-0.19648	0.09154
H	-3.76526	0.00911	1.59521
C	-3.06548	1.92362	-0.20745
H	-3.10326	2.31145	0.81201
H	-4.05636	2.02506	-0.65341
H	-2.37566	2.53232	-0.79399
Se	-0.00000	1.49790	-0.00000
N	1.37646	0.35077	-0.56399
C	3.70574	-0.33660	-0.56194
H	3.47884	-1.40281	-0.56219
H	4.68050	-0.19648	-0.09153
H	3.76527	0.00913	-1.59521
C	2.65610	0.45408	0.20963
C	3.06547	1.92363	0.20745
H	3.10325	2.31146	-0.81200
H	4.05636	2.02506	0.65341
H	2.37566	2.53232	0.79400
C	2.55381	-0.06092	1.63721
H	1.78936	0.48248	2.19373
H	3.51179	0.07143	2.14450
H	2.30245	-1.12158	1.65290

4.5 1,3,5-$Se_3(N^tBu)_3$

Se	-1.75631	0.17078	-0.96882
N	-0.69433	1.53717	-0.34032
C	-0.17027	3.56778	0.94749
H	0.79213	3.21679	1.31708
H	-0.58051	4.27232	1.67330
H	0.00000	4.10316	0.01147
C	-1.16133	2.42895	0.75493
C	-2.49656	3.02597	0.31444
H	-2.37637	3.58305	-0.61600
H	-2.87705	3.70297	1.08198
H	-3.24103	2.24349	0.15777
C	-1.35146	1.68157	2.06683
H	-2.08187	0.88148	1.94366
H	-1.72184	2.35888	2.83927
H	-0.41348	1.25023	2.41134
Se	1.02605	1.43562	-0.96882
N	1.67839	-0.16728	-0.34032
C	3.17492	-1.63643	0.94749
H	2.38976	-2.29440	1.31708
H	3.99019	-1.63343	1.67330
H	3.55344	-2.05158	0.01147
C	2.68420	-0.20873	0.75493
C	3.86884	0.64911	0.31444
H	4.29120	0.26647	-0.61600
H	4.64539	0.64011	1.08198

H	3.56344	1.68507	0.15777
C	2.13202	0.32962	2.06683
H	1.80432	1.36221	1.94366
H	2.90377	0.31172	2.83927
H	1.28947	-0.26703	2.41134
Se	0.73025	-1.60640	-0.96882
N	-0.98406	-1.36989	-0.34032
C	-3.00465	-1.93135	0.94749
H	-3.18188	-0.92239	1.31708
H	-3.40968	-2.63889	1.67330
H	-3.55344	-2.05158	0.01147
C	-1.52287	-2.22022	0.75493
C	-1.37228	-3.67507	0.31444
H	-1.91483	-3.84952	-0.61600
H	-1.76834	-4.34309	1.08198
H	-0.32240	-3.92856	0.15777
C	-0.78055	-2.01119	2.06683
H	0.27755	-2.24369	1.94366
H	-1.18193	-2.67060	2.83927
H	-0.87599	-0.98320	2.41134

4.6 1,3,5-$Se_4(N^tBu)_3$

Se	1.49366	0.85162	-1.28844
Se	-1.52524	1.28430	-0.71664
Se	-0.80060	-1.16335	1.20919
Se	0.55680	-1.98855	-0.51549
N	0.17763	1.58234	-0.20037
N	-2.10535	-0.13463	0.46150
N	1.94198	-0.77242	-0.57795
C	0.41435	2.68191	0.79380
C	-3.30642	-0.82389	-0.09191
C	3.11675	-1.00829	0.31185
C	1.89260	2.80112	1.12239
H	2.28401	1.87663	1.54232
H	2.01668	3.58746	1.86882
H	2.48567	3.06377	0.24669
C	-0.35117	2.36946	2.07389
H	-1.41625	2.24610	1.87376
H	-0.22894	3.18802	2.78597
H	0.01879	1.44999	2.52789
C	-0.05954	4.00752	0.20386
H	0.48421	4.23068	-0.71645
H	0.11338	4.82071	0.91183
H	-1.12643	3.97309	-0.02052
C	-3.95272	-1.62519	1.03242
H	-3.29625	-2.42268	1.37875
H	-4.87797	-2.07753	0.66944
H	-4.18801	-0.97650	1.87763
C	-4.29986	0.25240	-0.53112
H	-4.46901	0.97408	0.26894
H	-5.25112	-0.22000	-0.78126
H	-3.96759	0.78726	-1.42400
C	-2.98329	-1.74046	-1.26721
H	-2.43359	-1.20674	-2.04365
H	-3.90552	-2.13395	-1.69986
H	-2.37844	-2.58767	-0.94054
C	3.69413	-2.37564	-0.04850

H	2.97109	-3.17111	0.13276
H	4.57628	-2.57485	0.56304
H	3.98480	-2.40119	-1.09985
C	4.18607	0.03848	0.02965
H	4.44374	0.05402	-1.03085
H	5.08329	-0.21857	0.59531
H	3.87461	1.03949	0.31864
C	2.73751	-0.99325	1.78865
H	2.23399	-0.06775	2.06417
H	3.63259	-1.09888	2.40514
H	2.06858	-1.82229	2.02385

4.7. 1,3,5,7-$Se_4(N^tBu)_4$

Se	1.55852	1.52699	-0.84335
Se	-1.55852	1.52699	-0.84335
Se	-1.55852	-1.52699	-0.84335
Se	1.55852	-1.52699	-0.84335
N	0.00000	2.26671	-0.09846
N	-1.73967	0.00000	0.15442
N	0.00000	-2.26671	-0.09846
N	1.73967	0.00000	0.15442
C	0.00000	3.76327	-0.03783
C	-2.62654	0.00000	1.35571
C	2.62654	0.00000	1.35571
C	0.00000	-3.76327	-0.03783
C	-1.22422	4.25816	0.72645
H	-2.15753	3.97460	0.24283
H	-1.18515	5.34781	0.77823
H	-1.22384	3.86760	1.74338
C	1.22422	4.25816	0.72645
H	1.22384	3.86760	1.74338
H	1.18515	5.34781	0.77823
H	2.15753	3.97460	0.24283
C	0.00000	4.36718	-1.44350
H	0.88407	4.05345	-2.00424
H	0.00000	5.45842	-1.39941
H	-0.88407	4.05345	-2.00424
C	-4.09045	0.00000	0.93298
H	-4.31309	0.88778	0.33680
H	-4.74810	0.00000	1.80498
H	-4.31309	-0.88778	0.33680
C	-2.32522	-1.23270	2.19467
H	-2.62410	-2.14245	1.67943
H	-2.88153	-1.17396	3.13188
H	-1.25977	-1.29579	2.41803
C	-2.32522	1.23270	2.19467
H	-1.25977	1.29579	2.41803
H	-2.88153	1.17396	3.13188
H	-2.62410	2.14245	1.67943
C	-1.22422	-4.25816	0.72645
H	-1.18515	-5.34781	0.77823
H	-2.15753	-3.97460	0.24283
H	-1.22384	-3.86760	1.74338
C	1.22422	-4.25816	0.72645
H	1.18515	-5.34781	0.77823
H	1.22384	-3.86760	1.74338
H	2.15753	-3.97460	0.24283

C	0.00000	-4.36718	-1.44350
H	0.88407	-4.05345	-2.00424
H	-0.88407	-4.05345	-2.00424
H	0.00000	-5.45842	-1.39941
C	2.32522	-1.23270	2.19467
H	1.25977	-1.29579	2.41803
H	2.88153	-1.17396	3.13188
H	2.62410	-2.14245	1.67943
C	2.32522	1.23270	2.19467
H	2.62410	2.14245	1.67943
H	2.88153	1.17396	3.13188
H	1.25977	1.29579	2.41803
C	4.09045	0.00000	0.93298
H	4.31309	-0.88778	0.33680
H	4.74810	0.00000	1.80498
H	4.31309	0.88778	0.33680