Supporting information for

Synthesis and Structural Characterization of Monomeric Mercury(II) Selenolate Complexes Derived from 2-Phenylbenzamide Ligands

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General Experimental Details

All reactions were carried out under nitrogen atmosphere using standard vacuum-line techniques. Spectroscopic grade methanol and toluene, DMF and DMSO with sealed septa and 1,10-phenanthroline were used as received. All other solvents were purified by standard procedure and freshly distilled prior to use. Elemental selenium, copper iodide, succinimide, $CdCl_2$, $ZnCl_2$ and Hg were purchased from commercial sources (Aldrich/ Fluka) and used as received. 2-iodobenzoic acid, thionyl chloride and amines were purchased from Spectrochem Pvt. Ltd. Dichloromethane used from MBRAUN solvent drying system. Silica gel (100-200 mesh size) was used for column chromatography purchased from RANKEM Pvt. Ltd. India. TLC analysis of reaction mixtures was performed using Merck silica gel (60 F_{254}) plates. Potassium carbonate and $ZnCl_2$ were stored in desiccator and used under anhydrous conditions. Diselenides (1a, 1b, 1c) are known and mercury selenolates are unknown.

TLC analysis of reaction mixtures was performed using silica gel coated aluminum plates. NMR spectra were recorded on a Bruker Bio Spin GmbH-400 MHz spectrometer operating at 400.13 (^{1}H), 100.61 (^{13}C) and 76.31 (^{77}SeMHz) .^{1}H and ^{13}C NMR chemical shifts were relative to internal chloroform peak ($\delta = 7.24$ ppm for ^{1}H and $\delta = 77.0$ for ^{13}C NMR). The ^{77}Se NMR chemical shifts were relative to external diphenyl diselenide (Ph_2Se_2) in $CDCl_3$ ($\delta= 463.0$ ppm relative to Me_2Se ($\delta = 0$ ppm)). High resolution mass spectral (HRMS) analysis was performed for ion of ^{80}Se on a quadrupole-time of flight (Q-TOF) mass spectrometer equipped with both, an ESI and APCI source. Silica gel (100-200mesh size) was used for column chromatography. The single-crystal diffraction studies were carried out on a Bruker APEX II diffractometer (Mo-Kα, λ = 0.71069 Å). All crystal structures were solved by direct methods. The program SAINT (version 6.22) was used for integration of the intensity of reflections and scaling. The program SADABS was used for absorption correction. The crystal structures were solved and refined using the SHELXTL package. All hydrogen atoms were included in idealized positions, and a riding model was used. Non-hydrogen atoms were refined with anisotropic displacement parameters.

VT NMR study and thermal studies. For better understanding of non-bonding interactions in the complex variable temperature ^{1}H NMR study has been carried out for diselenide **2a** and mercuryselenolate complex **3c**. The study suggests that Hg…O/Se…O non-bonding interactions are present in the compounds.

The variable temperature ^{1}H NMR was recorded for compound.**2a.** Interestingly, at low temperature (-20° C) two methyl peaks were separate and distinct but as the temperature increases gradually from -20 °C to 0 °C, 20 °C and finally 40 °C the two methyl peaks gradually merge and finally give a single peak at 40°C. This shows the fluxional behavior of the diselenide **2a** caused due to the Se…O non-bonding interaction which lapse at elevated temperature and results in a single peak at 40°C (Fig. S1).
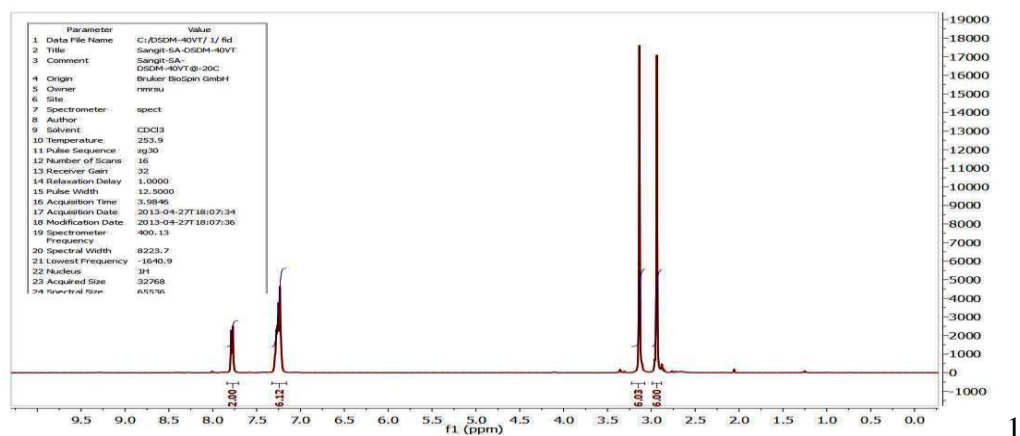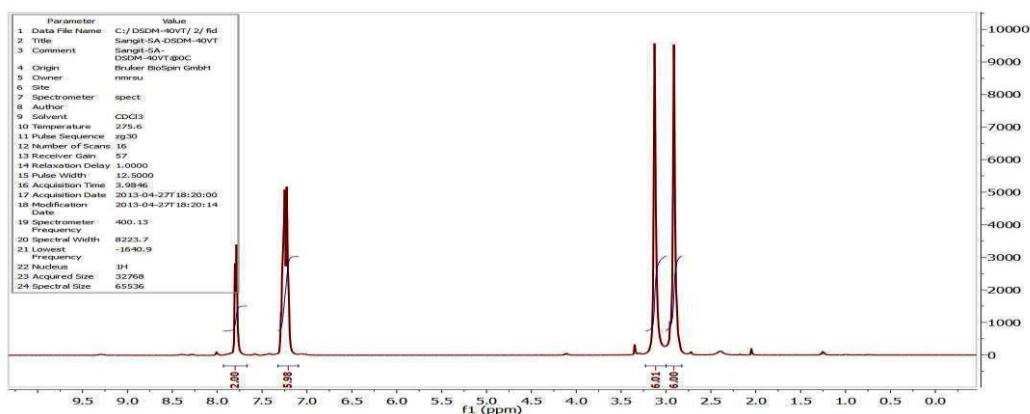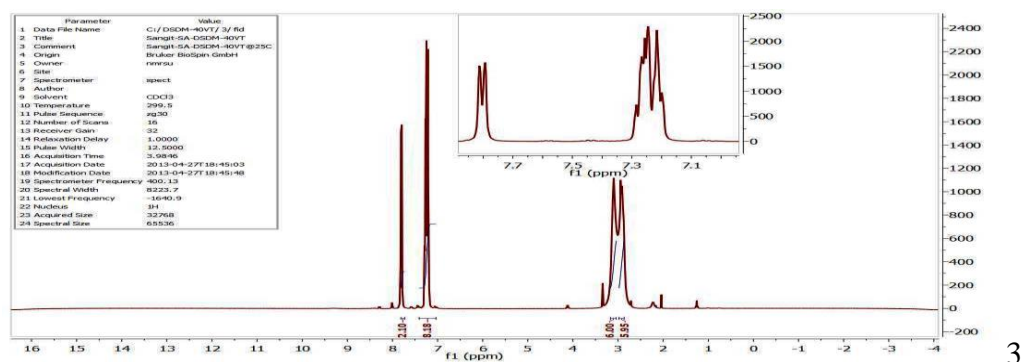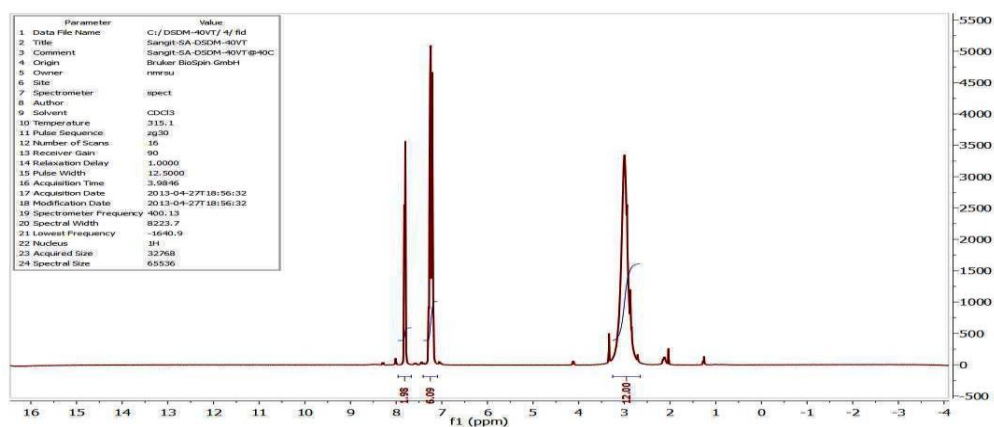
Fig S1. ^{1}H VT NMR of dimethyl diselenides (**2a**) at -20°C (1), 0°C (2), RT (3), 40°C (4)

The variable temperature ^{1}H NMR was recorded for compound **3c.** At low temperature (-40° C) two isopropyl peaks were separate and appeared as doublet of doublet (1.48 ppm) but as the temperature increases gradually from -0 °C to -20 °C, 0 °C, and finally 40 °C the two isopropyl peaks gradually merge and finally give a single peak (doublet) at room temperature which at 40 °C again shows little splitting of that doublet into doublet of doublet. This shows the that Hg…O non-bonding interaction are present in the complex which lapse at elevated temperature and results in a single peak at 40°C (Fig. S2).

40 °C

Room temperature

1

0 °C

-20 °C

-40 °C

2

3
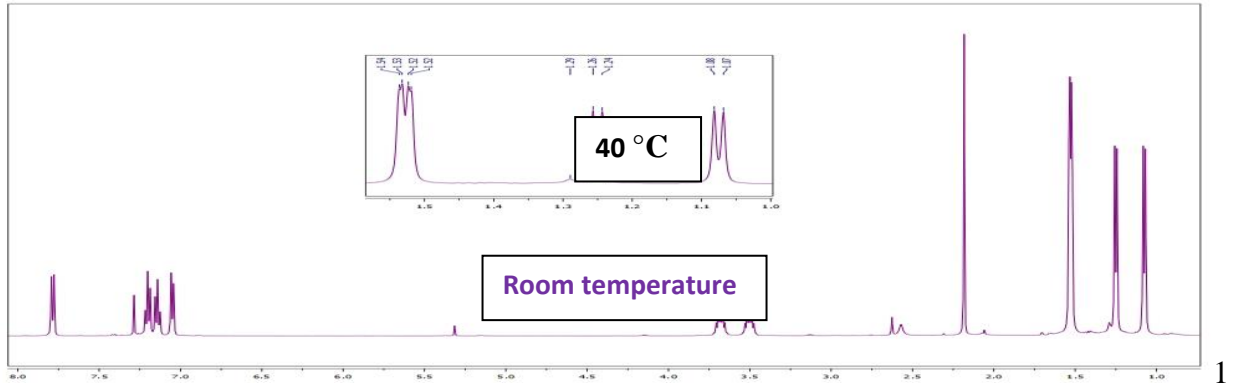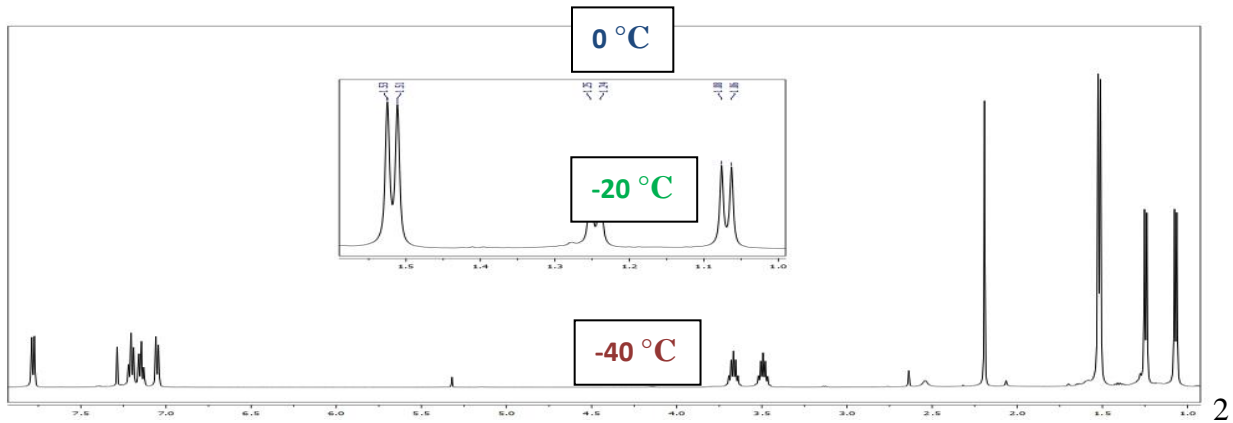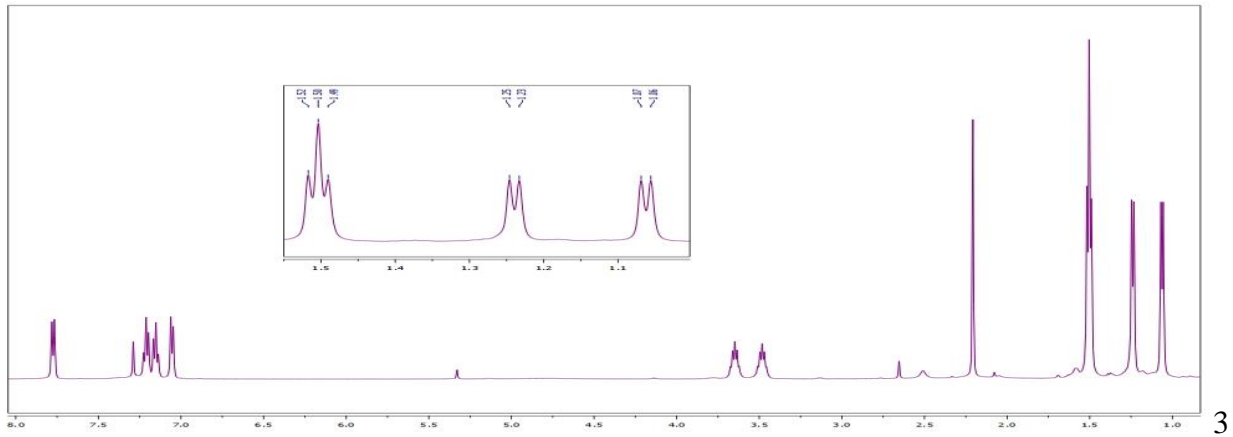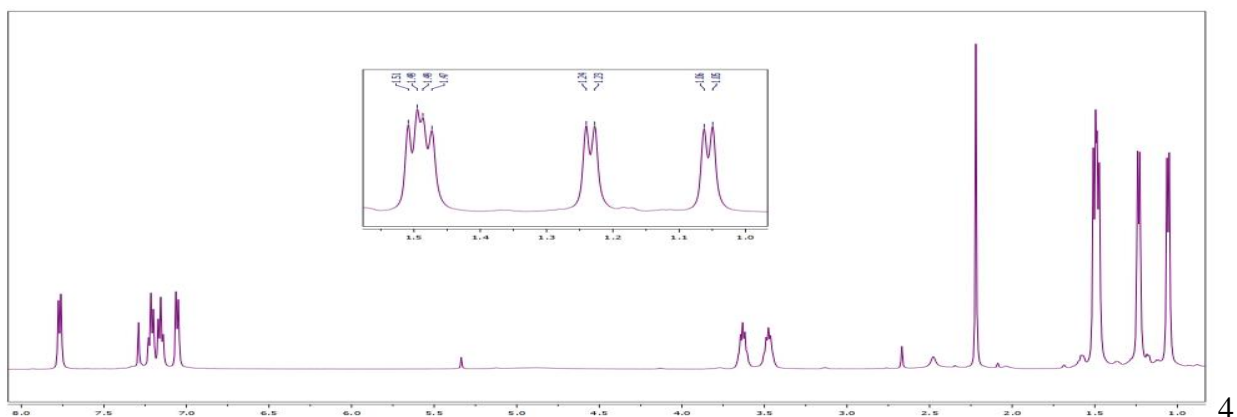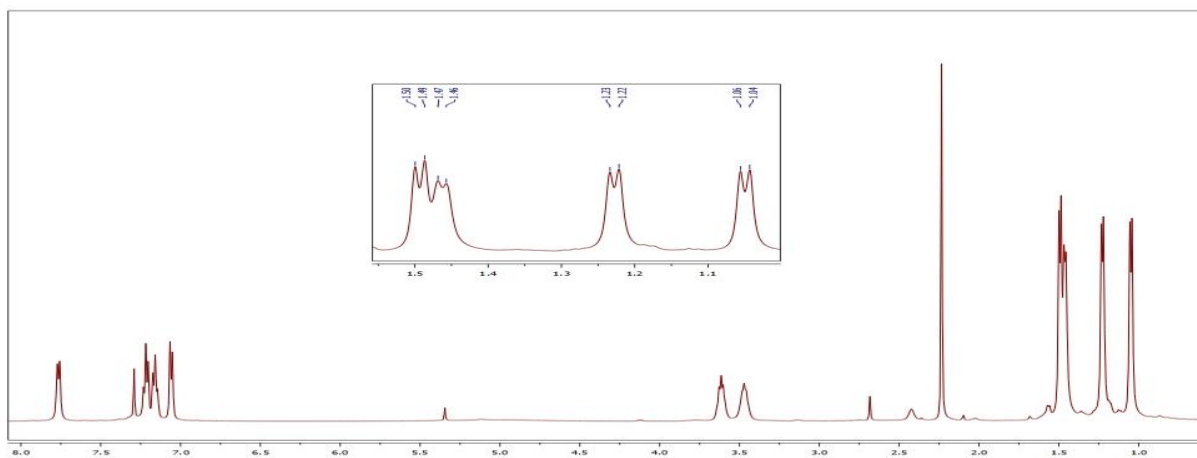
Fig S2. ^{1}H VT NMR of mercury selenolate **3c** at 40°C (1), RT (2), 0°C (3), RT (4), 40°C (5)

Thermal Studies. In order to understand the thermal stability and suitability of mercury selenolate complexes as a single source molecular precursor for the mercury selenides, thermogravimetric analysis (TGA) was carried out from 30−1000 °C at 10 °C/min under N_2 atmosphere. The mercury selenolate **3a** is thermally stable upto120°C and then decomposes in two stages. A large reaction interval of 230 °C suggests that this compound decomposes very slowly. DTG shows two peak maxima at 250 °C which corresponds to the 50% weight loss at this temperature and 350°C as the maximum rate of decomposition (Figure S3). In case of both **3a** and **3d**, the first step corresponds to the formation of RSeHg (for **3a** weight loss found 38.5%, calculated for RSeHg 34.69% and for **3d** weight loss found 35.3%, calculated for RSeHg 36.96%). The second step for **3a** involves complete decomposition and vaporization of RSeHg leaving empty pan behind. This suggests formation of volatile selenium containing intermediates

during the decomposition process. In contrast, second step in the TG curve of **3d** (weight loss found 88.79%, calculated for the Se 89.73%) leads to the formation of selenium residue (Figure S6). Similarly, mercury complexes **3c**, **3d**, and **3e** also underwent two-step decomposition each *via* a different pathway whereas mercury selenolate complex **3b** found to be highly unstable beyond 350 ˚C and decomposes in to selenium residue in single step (Figure S4).

The complex **3c** also shows two step decomposition but in a different way. Complex **3c** is stable up to 200 ^{0}C, then the first decomposition step occur and belongs to the formation of SeHg (for **3c** weight loss found 68.5%, calculated for HgSe 63.1%). The second step decomposition for the complex **3c** results in the formation of selenium residue (for **3c** weight loss found 12.0%, calculated for Selenium 10.2%) Figure S5.

The complex **3e** underwent two-step decomposition (Figure S7). The first step is found to be sluggish till ~ 515 ˚C, a characteristic for the loss of one ligand forming RSeHg (weight loss found 31.9%, calculated weight loss 37.48%). The second step of decomposition corresponds to the loss of organic moiety with the formation of HgSe as inferred from the weight loss (weight loss found 70%, calculated for HgSe 65.1%).
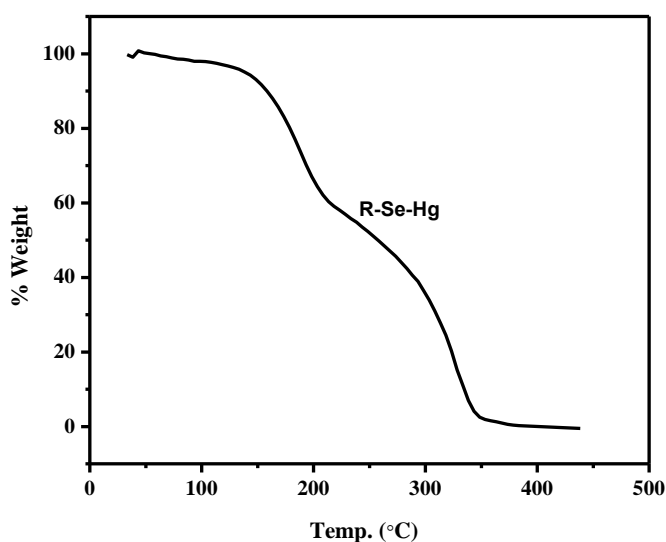
Figure S3. TG curve of **3a**
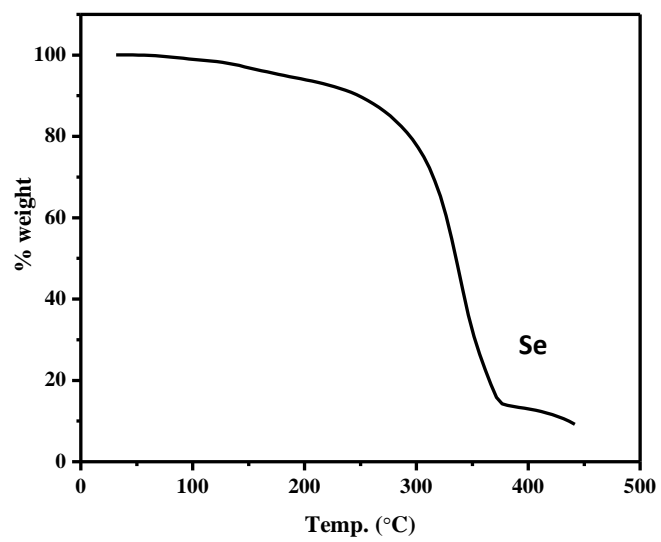
Figure S4. TG curve of **3b**
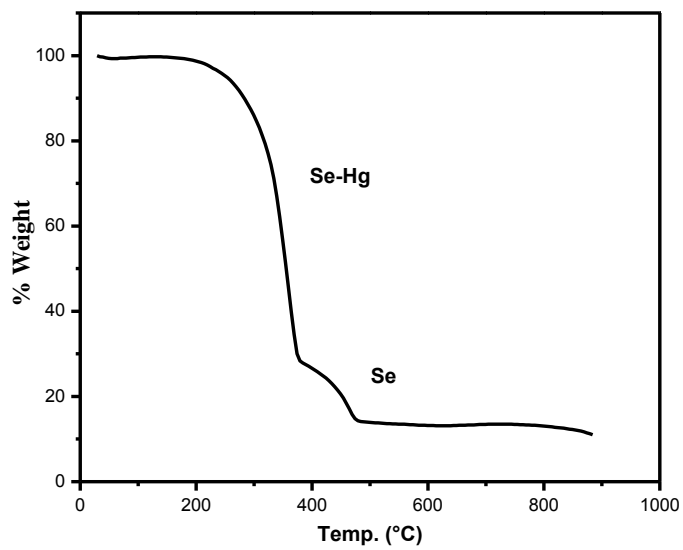
Figure S5. TG curve of **3c**
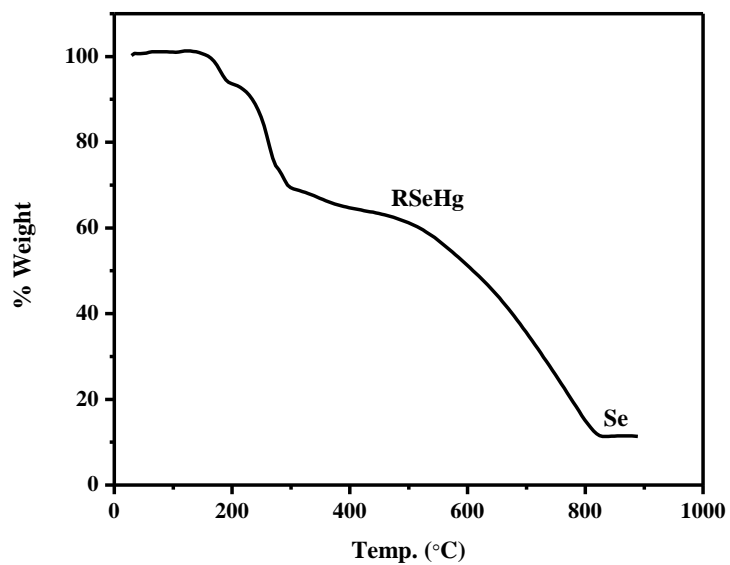
Figure S6. TG curve of **3d**
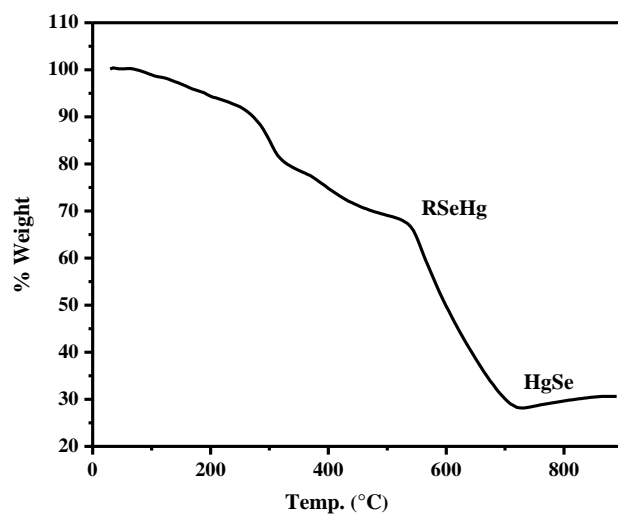
Figure S7. TG curve of **3e**

Figure S8 ^{1}H NMR spectrum of **2a**
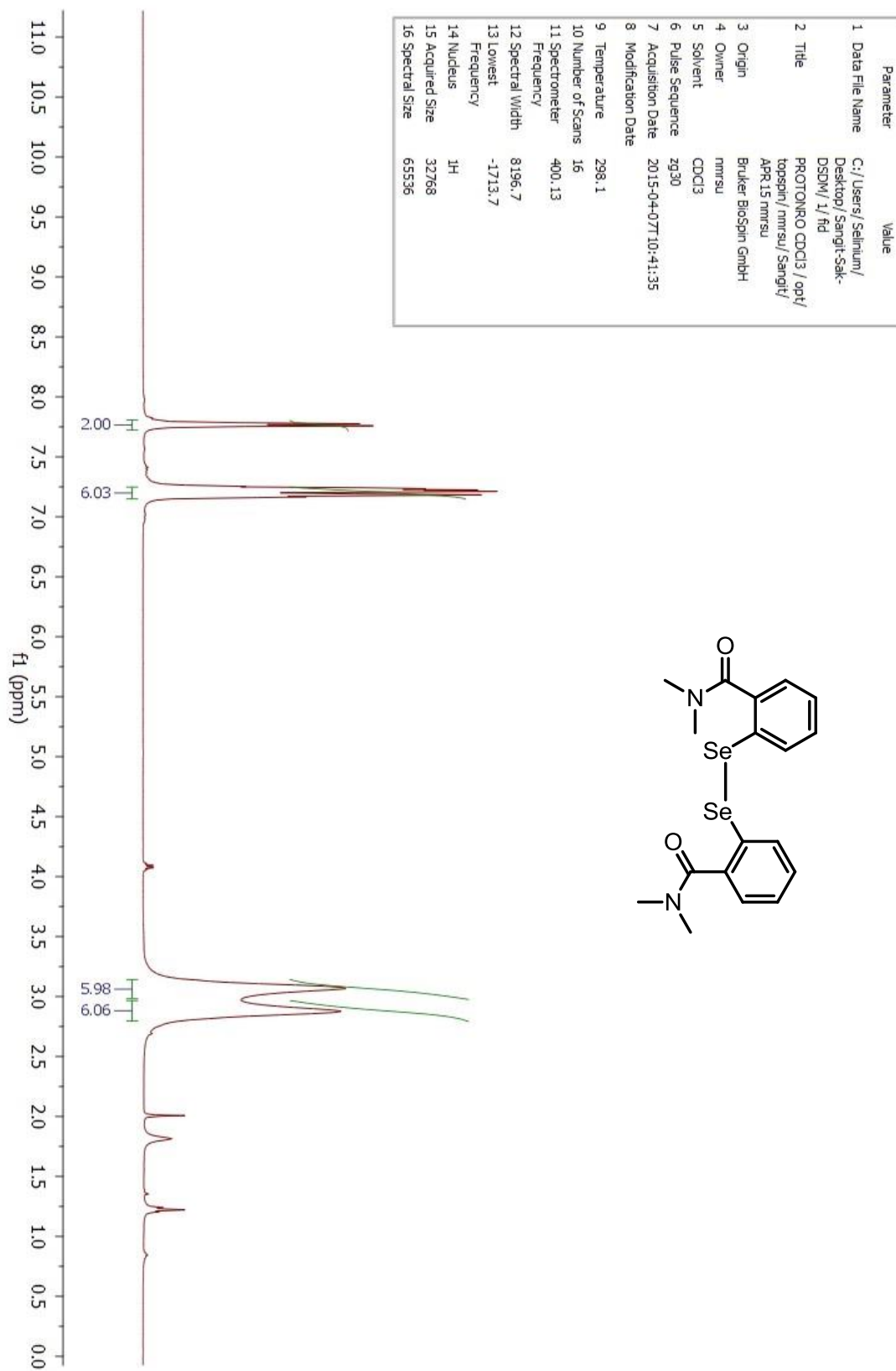
Figure S9 ^{13}C NMR spectrum of **2a**

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3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Solvent	CDCl3
6 Pulse Sequence	zgpg30
7 Acquisition Date	2015-04-07 20:07:00
8 Modification Date	
9 Temperature	298.2
10 Number of Scans	512
11 Spectrometer Frequency	100.61
12 Spectral Width	24038.5
13 Lowest Frequency	-1958.9
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

170.11

137.15
132.45
130.12
129.54
127.14
126.74

39.12
35.07

f1 (ppm)

Figure S10 ^{77}Se NMR spectrum of **2a**

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2	Title	Sangit-Sak-DSDM SE77ZG CDCl3/opt/ topspin/nmrsu/Sangit/ APR 15 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zg
7	Acquisition Date	2015-04-07T20:33:20
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	512
11	Spectrometer Frequency	76.31
12	Spectral Width	41666.7
13	Lowest Frequency	15414.3
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

—435.50

Figure S11 Mass spectrum of **2a**

Display Report

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Method	HRLCMS-20 Sept.m
Sample Name	Dr.S.Kumar-SA-DSDME-24
Comment	

Operator   IISERB
Instrument   microTOF-Q II 10330

Acquisition Parameter

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Bruker Compass DataAnalysis 4.0   printed: 2/20/2013 12:19:57 PM   Page 1 of 1
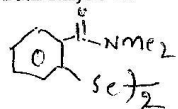
$m.wt = 455.99$

$C_{18}H_{20}N_2O_2Se_2$

Figure S12 ^{1}H NMR spectrum of **3a**
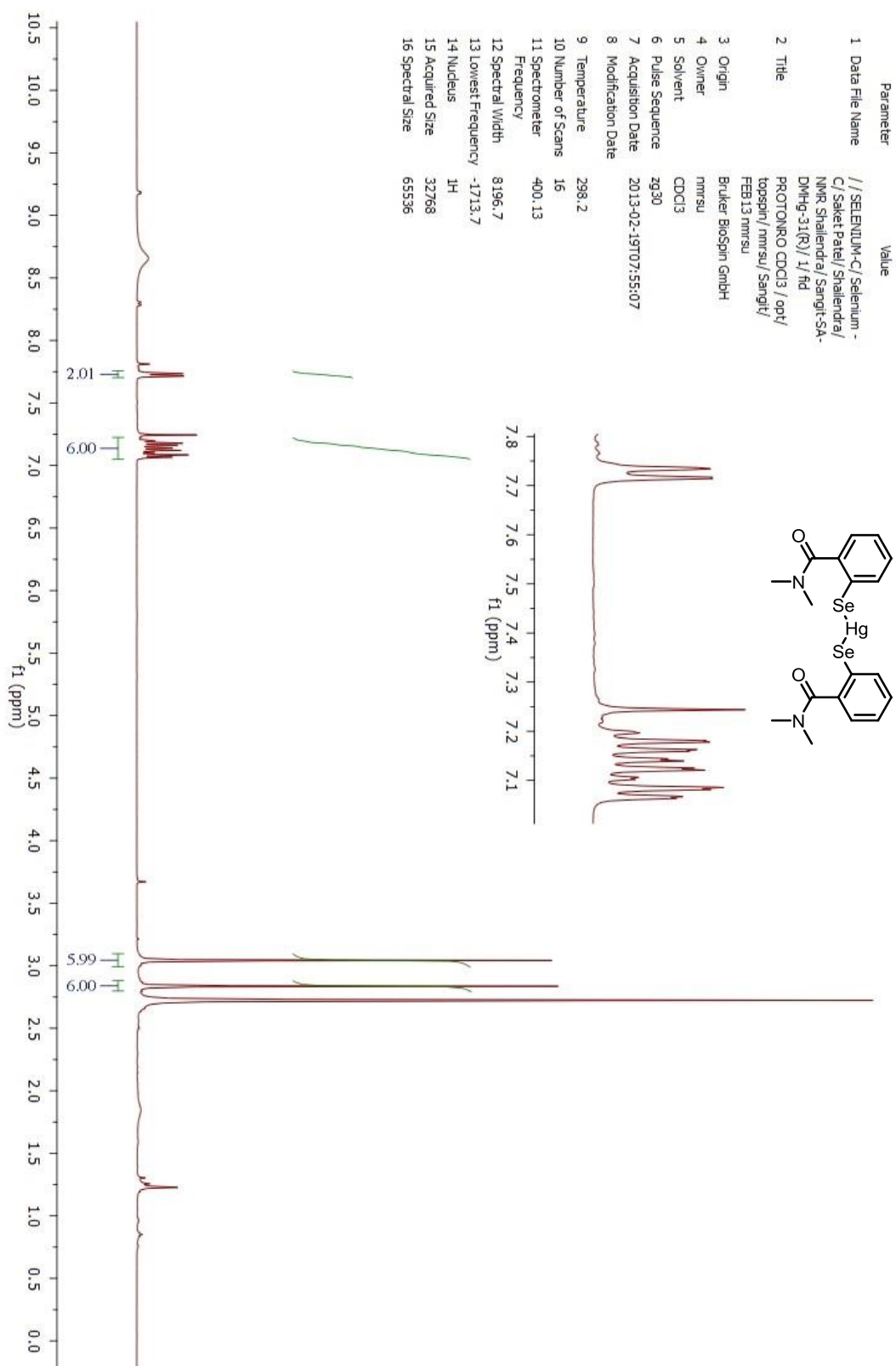
Figure S13 ^{13}C NMR spectrum of **3a**

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3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
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6	Pulse Sequence	zgpg30
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8	Modification Date	
9	Temperature	298.2
10	Number of Scans	148
11	Spectrometer Frequency	100.61
12	Spectral Width	24038.5
13	Lowest Frequency	-1958.9
14	Nucleus	13C
15	Acquired Size	32768
16	Spectral Size	65536

Figure S14 ^{77}Se NMR spectrum of **3a**

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3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zg
7	Acquisition Date	2013-02-26T04:21:16
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	1024
11	Spectrometer Frequency	76.31
12	Spectral Width	30864.2
13	Lowest Frequency	7461.1
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

—143.32

Figure S15 Mass spectrum of **3a**

Display Report

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Analysis Name   D:\Data\user data\2013\JAN\21 JAN\Dr.S.Kumar-SA-DMHg-31_1-C,1_01_5268.d
Method   HRLCMS-20 Sept.m   Operator   IISERB
Sample Name   Dr.S.Kumar-SA-DMHg-31   Instrument   micrOTOF-Q II 10330
Comment

Acquisition Parameter
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Bruker Compass DataAnalysis 4.0   printed: 2/20/2013 12:34:54 PM   Page 1 of 1
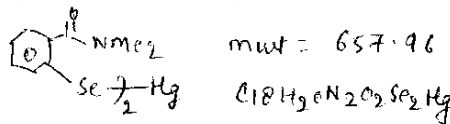
Figure S16 ^{1}H NMR spectrum of **2b**

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3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Solvent	DMSO
6 Pulse Sequence	zg30
7 Acquisition Date	2012-12-14T09:49:32
8 Modification Date	
9 Temperature	298.2
10 Number of Scans	32
11 Spectrometer Frequency	400.13
12 Spectral Width	8196.7
13 Lowest Frequency	-1713.7
14 Nucleus	1H
15 Acquired Size	32768
16 Spectral Size	65536

Figure S17 ^{13}C NMR spectrum of **2b**

	Parameter	Value
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4	Owner	nmrsu
5	Solvent	DMSO
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7	Acquisition Date	2012-12-14T11:00:10
8	Modification Date	
9	Temperature	298.3
10	Number of Scans	201
11	Spectrometer Frequency	100.61
12	Spectral Width	24038.5
13	Lowest Frequency	-1958.9
14	Nucleus	13C
15	Acquired Size	32768
16	Spectral Size	65536

168.79

138.29
132.23
130.47
128.95
127.90
126.46

14.36
13.10

f1 (ppm)

Figure S18 ^{77}Se NMR spectrum of **2b**

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5	Solvent	DMSO
6	Pulse Sequence	zg
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9	Temperature	298.2
10	Number of Scans	74
11	Spectrometer Frequency	76.31
12	Spectral Width	92592.6
13	Lowest Frequency	-509.8
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

—425.48

Figure S19 Mass spectrum of **2b**

Figure S20 ^{1}H NMR spectrum of **3b**

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9	Temperature	298.3
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12	Spectral Width	8196.7
13	Lowest Frequency	-1713.7
14	Nucleus	1H
15	Acquired Size	32768
16	Spectral Size	65536

Figure S21 ^{13}C NMR spectrum of **3b**

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9 Temperature	298.3
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11 Spectrometer Frequency	100.61
12 Spectral Width	24038.5
13 Lowest Frequency	-1958.9
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

—172.10
—142.14
—137.59
128.65
126.71
125.44
123.61
—43.17
—39.15
14.06
12.90

Figure S22 ^{77}Se NMR spectrum of **3b**

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9	Temperature	298.2
10	Number of Scans	512
11	Spectrometer Frequency	76.31
12	Spectral Width	45454.5
13	Lowest Frequency	166.0
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

—143.90

Figure S23 Mass spectrum of **3b**

Figure S24 ^{1}H NMR spectrum of **2c**

	Parameter	Value
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10	Number of Scans	16
11	Spectrometer Frequency	400.13
12	Spectral Width	8196.7
13	Lowest Frequency	-1713.7
14	Nucleus	1H
15	Acquired Size	32768
16	Spectral Size	65536

Figure S25 ^{13}C NMR spectrum of **2c**

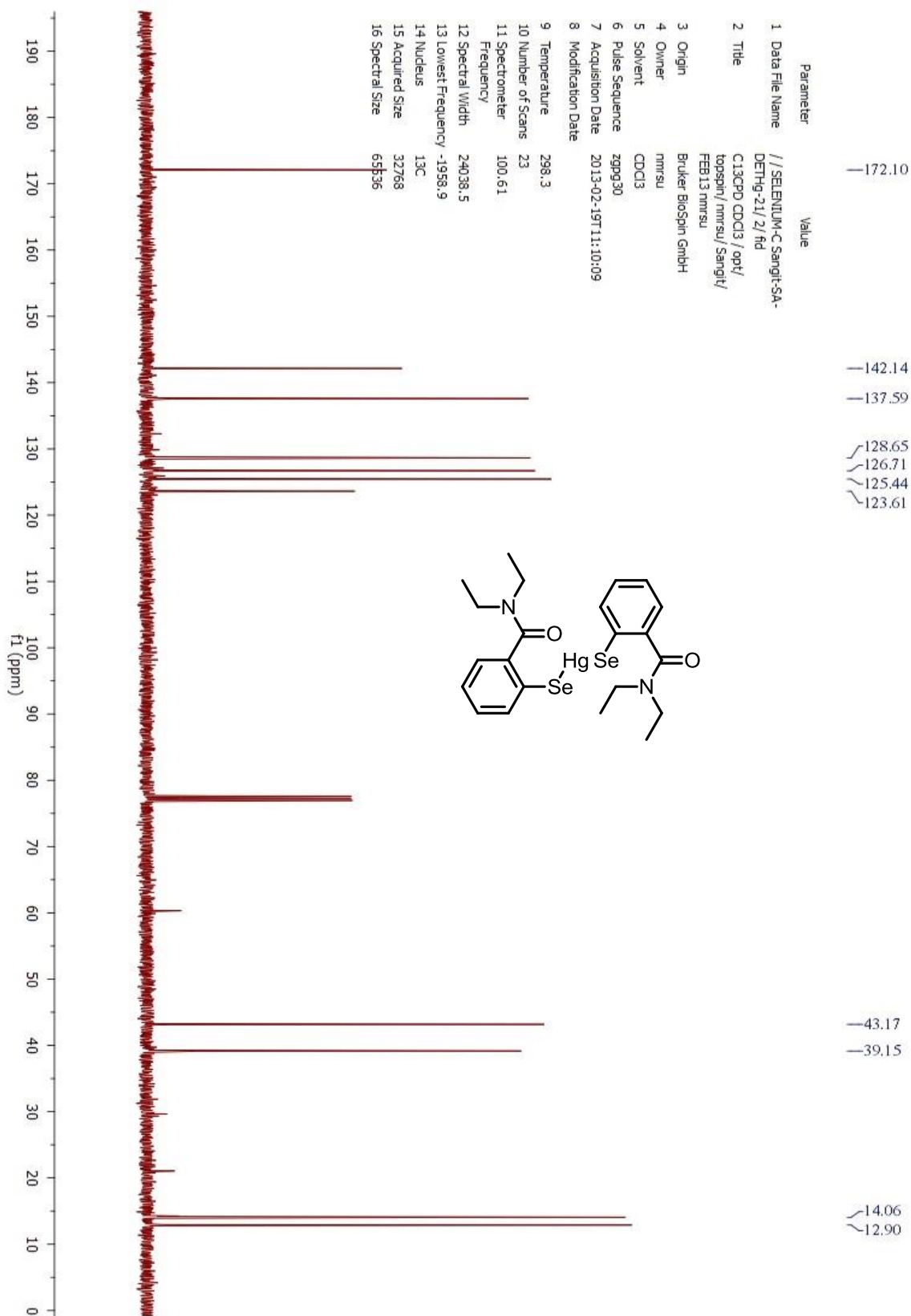| Parameter	Value
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3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Solvent	CDCl3
6 Pulse Sequence	zgpg30
7 Acquisition Date	2015-02-10T22:26:37
8 Modification Date	
9 Temperature	298.2
10 Number of Scans	300
11 Spectrometer Frequency	100.61
12 Spectral Width	24038.5
13 Lowest Frequency	-1958.9
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

−169.27

−138.99
131.73
129.46
128.79
126.85
125.06

−20.77

f1 (ppm)

Figure S26 ^{77}Se NMR spectrum of **2c**

	Parameter	Value
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11	Spectrometer Frequency	76.31
12	Spectral Width	75757.6
13	Lowest Frequency	276.6
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

—414.72

Figure S27 Mass spectrum of **2c**

Figure S28 ^{1}H NMR spectrum of **3c**

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9 Temperature	298.3
10 Number of Scans	16
11 Spectrometer Frequency	400.13
12 Spectral Width	8196.7
13 Lowest Frequency	-1713.7
14 Nucleus	1H
15 Acquired Size	32768
16 Spectral Size	65536

S30

Figure S29 ^{13}C NMR spectrum of **3c**

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4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zgpg30
7	Acquisition Date	2015-03-05T03:23:29
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	512
11	Spectrometer Frequency	100.61
12	Spectral Width	24038.5
13	Lowest Frequency	-1958.9
14	Nucleus	13C
15	Acquired Size	32768
16	Spectral Size	65536

Figure S30 ⁷⁷Se NMR spectrum of **3c**

Parameter		Value
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		4/ fid
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		topspin/ nmrsu/ Sangit/
		MAR 15 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zg
7	Acquisition Date	2015-03-06T01:33:19
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	3000
11	Spectrometer	76.31
	Frequency	
12	Spectral Width	34090.9
13	Lowest	3940.0
	Frequency	
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

—135.48

Figure S31 Mass spectrum of **3c**

Figure S32. ^{1}H NMR of **4a**

	Parameter	Value
1	Data File Name	1:/ Ananda/ Se-Allyl/ 1/ fid
2	Title	PROTONRO DMSO/ opt/ topspin/ nmrsu/ Sangit/ NOV13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg30
7	Acquisition Date	2013-11-12T14:31:48
8	Modification Date	
9	Temperature	298.7
10	Number of Scans	16
11	Spectrometer Frequency	400.13
12	Spectral Width	8196.7
13	Lowest Frequency	-1713.7
14	Nucleus	1H
15	Acquired Size	32768
16	Spectral Size	65536

Figure S33. ^{13}C NMR of **4a**

	Parameter	Value
1	Data File Name	1:/ Ananda / Se-Allyl / 2/ fid
2	Title	Sangit-AH-JS-02-hexane C13CPD DMSO / opt / topspin / nmrsu / Sangit / NOV 13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zgpg30
7	Acquisition Date	2013-11-12T16:26:36
8	Modification Date	
9	Temperature	298.3
10	Number of Scans	2000
11	Spectrometer Frequency	100.61
12	Spectral Width	24038.5
13	Lowest Frequency	-1958.9
14	Nucleus	13C
15	Acquired Size	32768
16	Spectral Size	65536

165.23
148.05
146.53
134.57
129.34
127.90
125.69
122.42
118.41
46.14

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Figure S34. ^{77}Se NMR of **4a**

−866.08

	Parameter	Value
1	Data File Name	1:/ Ananda/ Se-Allyl/ 3/ fid
2	Title	Sangit-AH-JS-02-hexane SE77ZG DMSO / opt/ topspin/ nmrsu/ Sangit/ NOV13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg
7	Acquisition Date	2013-11-12T17:54:12
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	2000
11	Spectrometer Frequency	76.31
12	Spectral Width	62500.0
13	Lowest Frequency	14536.5
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S35. Mass spectrum of **4a**

Figure S36. ^{1}H NMR of **4b**

Parameter	Value
1 Data File Name	/ / SELENIUM-C/ Selenium -C/ Saket Patel/ Shailendra/ NMR Shailendra/ AH-60 butyl Se-N/ 1/ fid
2 Title	PROTON RO CDCl3 / opt/ topspin/ nmrsu/ Sangit/ FEB 14 nmrsu
3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Solvent	CDCl3
6 Pulse Sequence	zg30
7 Acquisition Date	2014-02-11T08:21:43
8 Modification Date	
9 Temperature	298.2
10 Number of Scans	16
11 Spectrometer Frequency	400.13
12 Spectral Width	8196.7
13 Lowest Frequency	-1713.7
14 Nucleus	1H
15 Acquired Size	32768
16 Spectral Size	65536

Figure S37. ^{13}C NMR of **4b**

Parameter	Value
1 Data File Name	// SELENIUM-C/ Selenium -C/ Saket Patel/ Shailendra/ NMR Shailendra/ AH-60 butyl Se-N/ 2/ fid
2 Title	Sangit-AH-60 C13CPD CDCl3 / opt/ topspin/ nmrsu/ Sangit/ FEB14 nmrsu
3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Solvent	CDCl3
6 Pulse Sequence	zgpg30
7 Acquisition Date	2014-02-12T21:40:25
8 Modification Date	
9 Temperature	298.2
10 Number of Scans	512
11 Spectrometer Frequency	100.61
12 Spectral Width	24038.5
13 Lowest Frequency	-1958.9
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

—165.60

146.82
145.51

128.72
125.71
125.30
123.93

—44.94

—32.55

—19.84

—13.66

Figure S38. ^{77}Se NMR of **4b**

—891.70

	Parameter	Value
1	Data File Name	// SELENIUM-C/ Selenium -C/ Saket Patel/ Shailendra/ NMR Shailendra/ A.H-60 butyl Se- N/ 3/ fid
2	Title	Sangt-A.H-60 SE77G CDCl3 / opt/ topspin/ nmrsu/ Sangt/ FEB14 nmrsu
		Bruker BioSpin GmbH
	nmrsu	
		CDCl3
	equence	zg
	ion Date	2014-02-12T22:07:19
	ature	298.2
	of Scans	512
	meter Frequency	76.31
	lWidth	38265.3
	Frequency	38100.5
	d Size	32768
	Size	65536

Figure S39. Mass spectrum of **4b**

Figure S40. ^{1}H NMR of **2d**

	Parameter	Value
1	Data File Name	//SELENIUM-C/ Selenium -C/ Saket Patel/ Shailendra/ NMR diselenide/ AH -49 Allyl
2	Title	PROTON RO DMSO / opt/ topspin/ nmrsu/ Sangit/ FEB 14 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg30
7	Acquisition Date	2014-02-21T09:24:01
8	Modification Date	
9	Temperature	298.1
10	Number of Scans	16
11	Spectrometer Frequency	400.13
12	Spectral Width	8196.7
13	Lowest Frequency	-1713.7
14	Nucleus	1H
15	Acquired Size	32768
16	Spectral Size	65536

Figure S41. ^{13}C NMR of **2d**

Parameter	Value
1 Data File Name	/ / SELENIUM-C / Selenium -
	C / Saket Patel / Shailendra /
	NMR Shailendra / AH-49
2 Title	Allyl diselenide / 3 / fid
	Sangit-AH-49-R-
	C13CPD DMSO / opt /
	topspin / nmrsu / Sangit /
	JAN14 nmrsu
3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Solvent	DMSO
6 Pulse Sequence	zgpg30
7 Acquisition Date	2014-01-10T16:23:47
8 Modification Date	
9 Temperature	298.2
10 Number of Scans	2000
11 Spectrometer	100.61
Frequency	
12 Spectral Width	24038.5
13 Lowest Frequency	-1958.9
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

—169.36

—143.43
—139.13
—134.89

123.07
122.67

—116.38

139.22
139.13

42.28
40.53
40.32
40.11
39.90
39.69
39.48
39.27

Figure S42. ^{77}Se NMR of **2d**

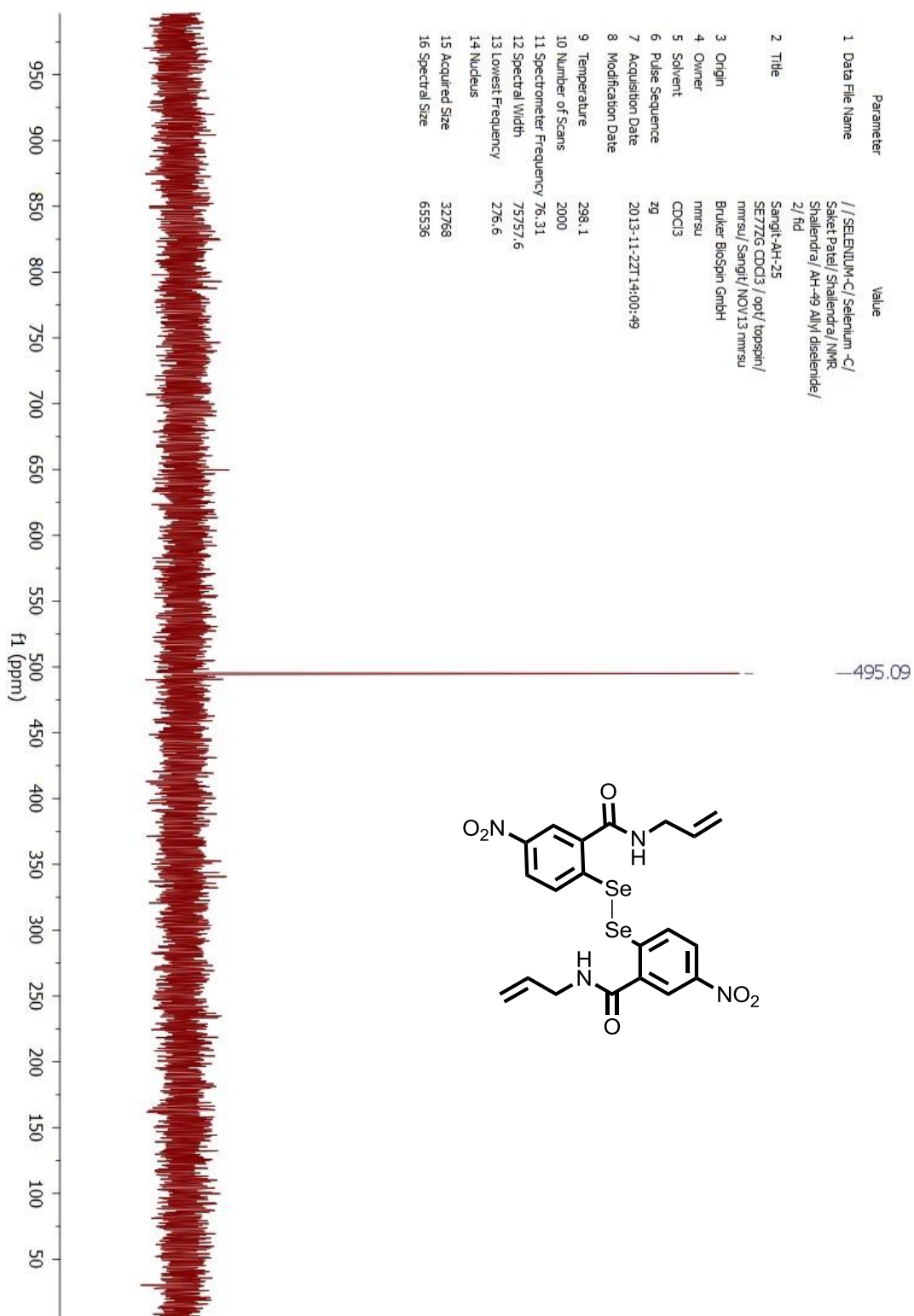|	Parameter	Value
1	Data File Name	//SELENIUM-C/Selenium -C/ Saket Patel/Shailendra/NMR Shailendra/AH-49 Allyl diselenide/ 2/fid
2	Title	Sangit-AH-25 SE77ZG CDCl3 /opt/ topspin/ nmrsu/ Sangit/ NOV13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zg
7	Acquisition Date	2013-11-22T14:00:49
8	Modification Date	
9	Temperature	298.1
10	Number of Scans	2000
11	Spectrometer Frequency	76.31
12	Spectral Width	75757.6
13	Lowest Frequency	276.6
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

—495.09

S44

Figure S43. Mass spectrum of **2d**

Figure S44. ^{1}H NMR of **2e**

Figure S45. ^{13}C NMR of **2e**

Parameter		Value
1	Data File Name	//SELENIUM-C/Selenium-C/ Saket Patel/Selenium-C/ Shailendra/AH-66 NMR diselenide/2/fid
2	Title	Sangit-AH-61 C13CPD DMSO/opt/topspin/ nmrsu/Sangit/FEB14 nmrsu
3	Origin	nmrsu
4	Owner	Bruker BioSpin GmbH
5	Solvent	DMSO
6	Pulse Sequence	zgpg30
7	Acquisition Date	2014-02-28T02:58:20
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	512
11	Spectrometer Frequency	100.61
12	Spectral Width	24038.5
13	Lowest Frequency	-1958.9
14	Nucleus	13C
15	Acquired Size	32768
16	Spectral Size	65536

S47

Figure S46. ^{77}Se NMR of **2e**

	Parameter	Value
1	Data File Name	/ / SELENIUM -C / Selenium -C / Saket Patel / Shailendra / NMR Shailendra / AH-66 butyl diselenide / 3 / fid
2	Title	Sangit-AH-61 SE77ZG DMSO / opt / topspin / nmrsu / Sangit / FEB 14 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg
7	Acquisition Date	2014-02-28T03:25:15
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	512
11	Spectrometer Frequency	76.31
12	Spectral Width	38265.3
13	Lowest Frequency	7576.1
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S47. ^{1}H NMR of **3d**

	Parameter	Value
1	Data File Name	/ / SELENIUM-C / Selenium - C / Saket Patel / Shailendra / NMR Shailendra / AH-38 Allyl Hg-Se / 1 / fid
2	Title	PROTON RO DMSO / opt / topspin / nmrsu / Sangit / DEC13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg30
7	Acquisition Date	2013-12-24T11:15:22
8	Modification Date	
9	Temperature	298.5
10	Number of Scans	16
11	Spectrometer Frequency	400.13
12	Spectral Width	8196.7
13	Lowest Frequency	-1713.7
14	Nucleus	1H
15	Acquired Size	32768
16	Spectral Size	65536

Figure S48. ^{13}C NMR of **3d**

Parameter		Value
1	Data File Name	// SELENIUM-C/ Selenium - C/ Saket Patel/ Shailendra/ NMR_Shailendra/ AH-38 Ally/ Hg-Se/ 3/ fid
2	Title	Sangit-AH-38 C13CPD CDCl3 / opt/ topspin/ nmrsu/ Sangit/ DEC13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zgpg30
7	Acquisition Date	2013-12-27 01:20:01
8	Modification Date	
9	Temperature	298.1
10	Number of Scans	3000
11	Spectrometer Frequency	100.61
12	Spectral Width	24038.5
13	Lowest Frequency	-1958.9
14	Nucleus	13C
15	Acquired Size	32768
16	Spectral Size	65536

S50

Figure S49. ^{77}Se NMR of **3d**

	Parameter	Value
1	Data File Name	// SELENIUM-C/ Selenium -C/ Saket Patel/ Shailendra/ NMR Shailendra/ AH-38 Allyl Hg-Se/ 2/ fid
2	Title	Sangit-AH-38 SE77ZG DMSO / opt/ topspin/ nmrsu/ Sangit/ DEC13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg
7	Acquisition Date	2013-12-25T09:40:28
8	Modification Date	
9	Temperature	298.6
10	Number of Scans	2000
11	Spectrometer Frequency	76.31
12	Spectral Width	113636.4
13	Lowest Frequency	-37740.5
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

—218.12

Figure S50. Mass spectrum of **3d**

Figure S51. ^{1}H NMR of **3e**

Figure S52. ^{13}C NMR of **3e**

	Parameter	Value
1	Data File Name	/ / SELENIUM-C/ AH-67-Butyl Hg-Se/ 2/ fid
2	Title	C13CPD DMSO / opt/ topspin/ nmrsu/ Sangit/ FEB 14 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zgpg30
7	Acquisition Date	2014-02-19T02:32:24
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	1024
11	Spectrometer Frequency	100.61
12	Spectral Width	24038.5
13	Lowest Frequency	-1958.9
14	Nucleus	13C
15	Acquired Size	32768
16	Spectral Size	65536

—168.07

—144.83
—143.02
—142.50
—138.25

—122.59
—121.76

—31.44

—20.18

—14.16

f1 (ppm)

Figure S53. ^{77}Se NMR of **3e**

Parameter		Value
1	Data File Name	/ / SELENIUM-C/ Selenium -C/ Saket Patel/ Shailendra/ NMR
2	Title	Shailendra/ AH-67-Butyl Hg-Se/ 3/ fid
		Sangit-AH-67-repeat
		SE77ZG DMSO / opt/ topspin/
		nmrsu/ Sangit/ FEB14 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg
7	Acquisition Date	2014-02-19T03:15:37
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	1000
11	Spectrometer Frequency	76.31
12	Spectral Width	75757.6
13	Lowest Frequency	276.6
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

—211.67

Figure S54. Mass spectrum of **3e**

UV-Visible spectra of mercury selenolates (3a, 3c, 3d, 3e) in acetonitrile
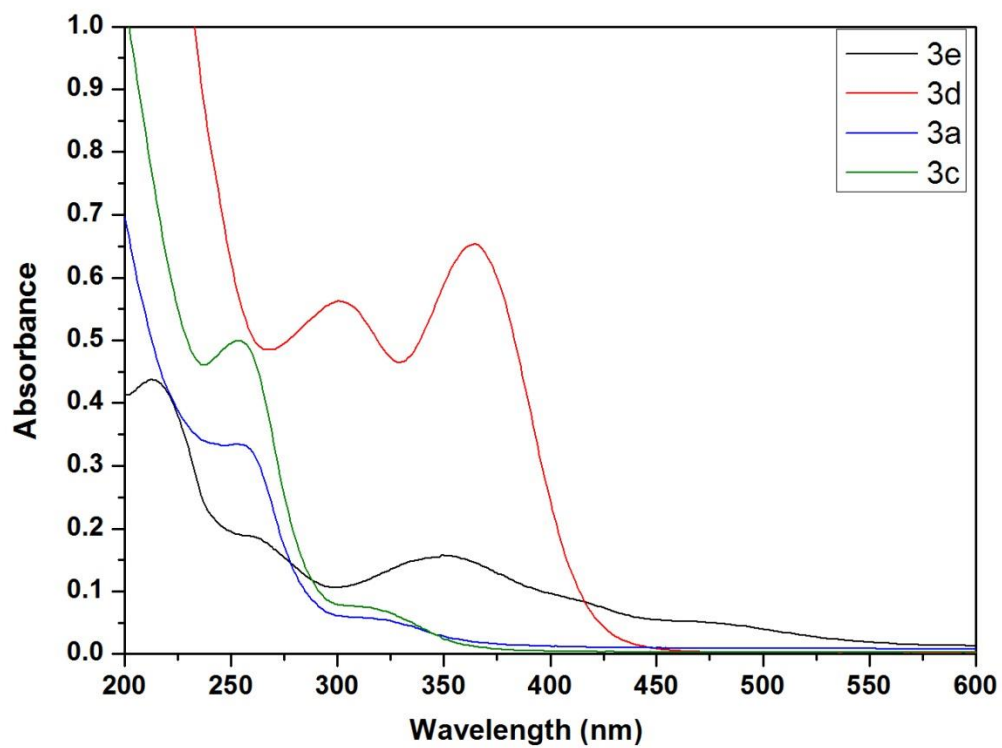
Crystal structure description

Crystal Structure of bis(*N*,*N*-dimethylbenzamide) diselenide 2a with 50% ellipsoidal probability (CCDC No.- 1059010)
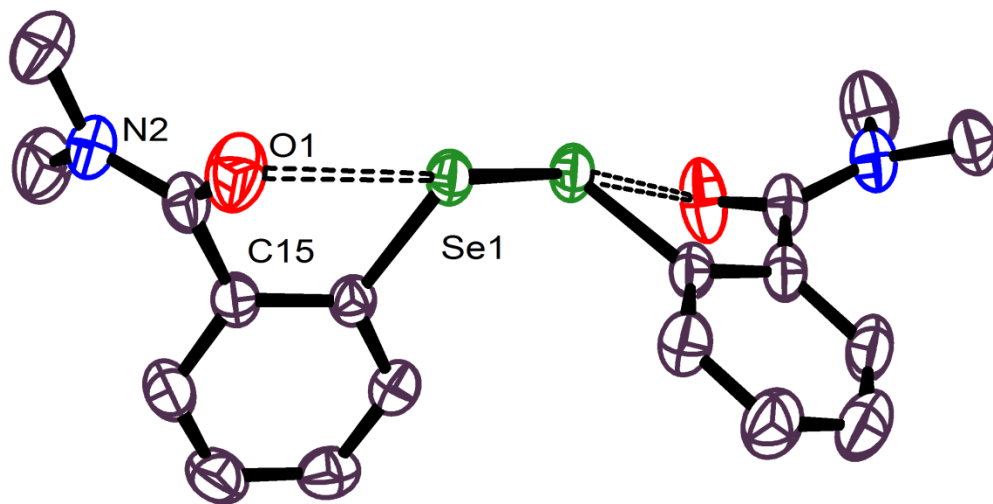
Packing diagram for 2a
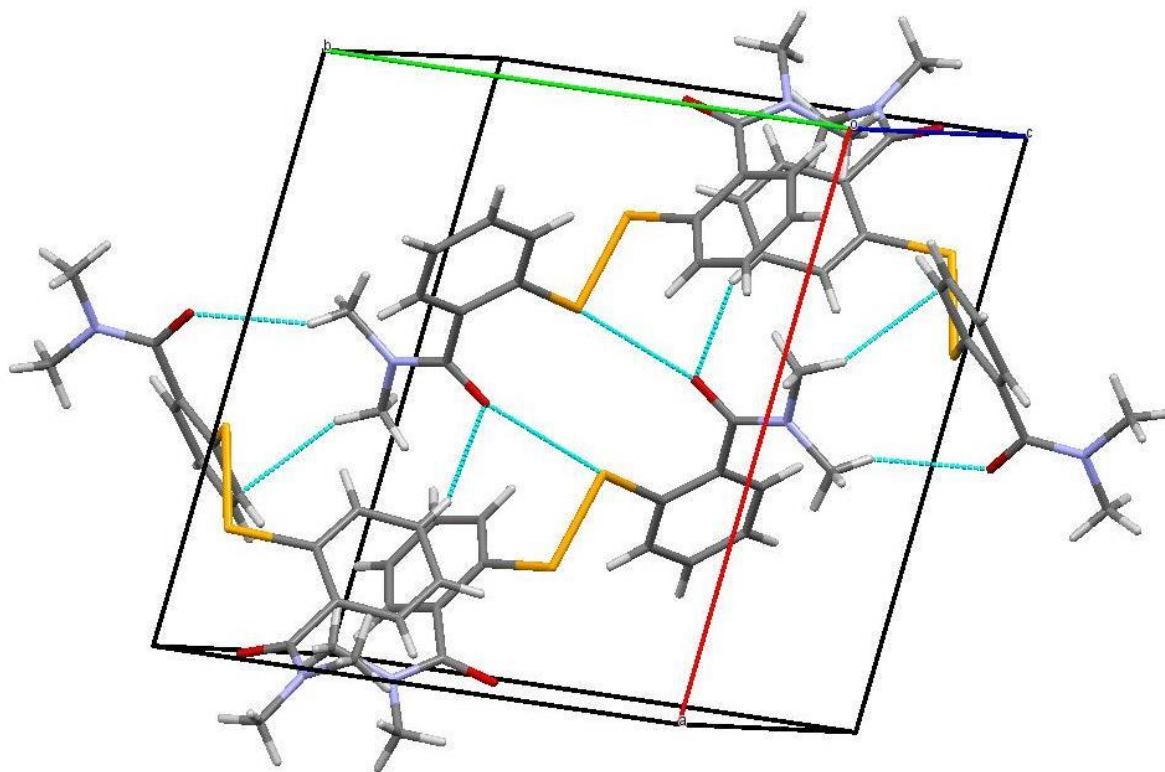
Table 1. Crystal data and structure refinement for 2a

Identification code	SAMSDM
Empirical formula	$C_{18} H_{20} N_2 O_2 Se_2$
Formula weight	454.28
Temperature	298 (2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P\,2_1/c$
Unit cell dimensions	a = 14.2781 (7) Å α= 90 °.
	b = 12.1561 (6) Å β= 113.62 °.
	c = 11.4422 (5) Å γ = 90 °.
Volume	1819.58 (15) Å^3
Z	4
Density (calculated)	1.658 g/cm^3
Absorption coefficient	4.076 mm^{-1}
F(000)	904
Theta range for data collection	2.23 to 29.56 °.
Index ranges	-22<=h<=18, -19<=k<=16, -17<=l<=18
Reflections collected	26969
Independent reflections	7496 [R(int) = 0.0466]
Completeness to theta = 25.242°	95.7 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7496 / 0 / 221
Goodness-of-fit on F^2	1.012
Final R indices [I>2sigma(I)]	R1 = 0.0363, wR2 = 0.0803
R indices (all data)	R1 = 0.0771, wR2 = 0.0919
Extinction coefficient	n/a
Largest diff. peak and hole	0.569 and -0.452 e.Å^{-3}

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 2a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	Uiso*/Ueq
Se1	0.63360 (2)	0.47574 (2)	0.62884 (2)	0.03734 (6)
Se2	0.79678 (2)	0.52563 (2)	0.65017 (2)	0.04029 (6)
O1	0.45954 (11)	0.35325 (12)	0.61730 (14)	0.0581 (4)
O2	0.99804 (12)	0.59398 (12)	0.71361 (18)	0.0657 (4)
C8	0.66744 (13)	0.40791 (12)	0.79424 (15)	0.0315 (3)
C1	0.80845 (14)	0.67467 (14)	0.71526 (16)	0.0369 (4)
C2	0.74021 (15)	0.71649 (16)	0.76001 (19)	0.0465 (5)
H2	0.6835	0.6750	0.7531	0.056*
C3	0.75442 (19)	0.82008 (17)	0.8156 (2)	0.0590 (6)
H3	0.7080	0.8473	0.8466	0.071*
C4	0.8376 (2)	0.88220 (18)	0.8246 (2)	0.0661 (7)
H4	0.8484	0.9507	0.8639	0.079*
C5	0.90460 (17)	0.84312 (16)	0.7754 (2)	0.0532 (5)
H5	0.9593	0.8866	0.7792	0.064*
C6	0.89151 (14)	0.73861 (14)	0.71964 (17)	0.0396 (4)
C7	0.97092 (14)	0.68949 (15)	0.68175 (19)	0.0426 (4)
N1	1.01426 (12)	0.74999 (13)	0.61970 (15)	0.0467 (4)
C9	1.09851 (18)	0.7017 (2)	0.5965 (3)	0.0696 (7)
H9A	1.1038	0.6249	0.6177	0.104*
H9B	1.1611	0.7381	0.6484	0.104*
H9C	1.0863	0.7102	0.5082	0.104*
C10	0.97565 (18)	0.85530 (17)	0.5572 (2)	0.0572 (6)
H10A	0.9055	0.8639	0.5451	0.086*
H10B	0.9805	0.8570	0.4759	0.086*
H10C	1.0156	0.9141	0.6096	0.086*

C11	0.74728 (14)	0.44452 (15)	0.90303 (18)	0.0392 (4)
H11	0.7886	0.5013	0.8965	0.047*
C12	0.76723 (16)	0.39907 (17)	1.02069 (18)	0.0466 (5)
H12	0.8218	0.4243	1.0926	0.056*
C13	0.70529 (17)	0.31544 (19)	1.03081 (19)	0.0528 (5)
H13	0.7172	0.2851	1.1101	0.063*
C14	0.62546 (16)	0.27681 (17)	0.92261 (18)	0.0483 (5)
H14	0.5841	0.2206	0.9302	0.058*
C15	0.60634 (13)	0.32058 (14)	0.80356 (16)	0.0350 (4)
C16	0.51829 (14)	0.28383 (15)	0.68629 (18)	0.0398 (4)
N2	0.50572 (14)	0.17657 (13)	0.65818 (17)	0.0503 (4)
C18	0.5783 (2)	0.08980 (17)	0.7237 (3)	0.0697 (7)
H18A	0.6406	0.1221	0.7828	0.105*
H18B	0.5923	0.0466	0.6624	0.105*
H18C	0.5497	0.0436	0.7691	0.105*
C19	0.4198 (2)	0.1432 (2)	0.5427 (2)	0.0757 (8)
H19A	0.3667	0.1975	0.5212	0.114*
H19B	0.3941	0.0736	0.5568	0.114*
H19C	0.4418	0.1364	0.4741	0.114*

* Hydrogens are treated anisotropically

Table 3. Selected bond lengths [Å] for 2a.

Se1—C8	1.9396 (16)	C9—H9C	0.9600
Se1—Se2	2.3237 (3)	C10—H10A	0.9600
Se2—C1	1.9404 (17)	C10—H10B	0.9600
O1—C16	1.228 (2)	C10—H10C	0.9600
O2—C7	1.232 (2)	C11—C12	1.375 (3)
C8—C11	1.382 (2)	C11—H11	0.9300

C8—C15	1.405 (2)	C12—C13	1.382 (3)
C1—C2	1.367 (3)	C12—H12	0.9300
C1—C6	1.402 (2)	C13—C14	1.386 (3)
C2—C3	1.389 (3)	C13—H13	0.9300
C2—H2	0.9300	C14—C15	1.384 (2)
C3—C4	1.376 (3)	C14—H14	0.9300
C3—H3	0.9300	C15—C16	1.493 (2)
C4—C5	1.375 (3)	C16—N2	1.338 (2)
C4—H4	0.9300	N2—C19	1.455 (3)
C5—C6	1.400 (3)	N2—C18	1.458 (3)
C5—H5	0.9300	C18—H18A	0.9600
C6—C7	1.491 (3)	C18—H18B	0.9600
C7—N1	1.334 (2)	C18—H18C	0.9600
N1—C9	1.455 (3)	C19—H19A	0.9600
N1—C10	1.462 (2)	C19—H19B	0.9600
C9—H9A	0.9600	C19—H19C	0.9600
C9—H9B	0.9600		

Table 4. Selected Bond angles [°] for 2a.

C8—Se1—Se2	99.28 (5)	H10A—C10—H10B	109.5
C1—Se2—Se1	102.26 (5)	N1—C10—H10C	109.5
C11—C8—C15	119.21 (16)	H10A—C10—H10C	109.5
C11—C8—Se1	122.35 (13)	H10B—C10—H10C	109.5
C15—C8—Se1	118.41 (12)	C12—C11—C8	121.66 (18)
C2—C1—C6	119.99 (17)	C12—C11—H11	119.2
C2—C1—Se2	121.76 (14)	C8—C11—H11	119.2

C6—C1—Se2	118.21 (14)	C11—C12—C13	119.27 (19)
C1—C2—C3	120.9 (2)	C11—C12—H12	120.4
C1—C2—H2	119.6	C13—C12—H12	120.4
C3—C2—H2	119.6	C12—C13—C14	119.93 (18)
C4—C3—C2	119.7 (2)	C12—C13—H13	120.0
C4—C3—H3	120.2	C14—C13—H13	120.0
C2—C3—H3	120.2	C15—C14—C13	121.08 (18)
C5—C4—C3	120.1 (2)	C15—C14—H14	119.5
C5—C4—H4	120.0	C13—C14—H14	119.5
C3—C4—H4	120.0	C14—C15—C8	118.79 (16)
C4—C5—C6	120.8 (2)	C14—C15—C16	122.18 (16)
C4—C5—H5	119.6	C8—C15—C16	118.87 (15)
C6—C5—H5	119.6	O1—C16—N2	121.59 (18)
C5—C6—C1	118.43 (19)	O1—C16—C15	118.98 (16)
C5—C6—C7	121.16 (18)	N2—C16—C15	119.43 (18)
C1—C6—C7	119.89 (16)	C16—N2—C19	118.3 (2)
O2—C7—N1	121.28 (19)	C16—N2—C18	125.62 (18)
O2—C7—C6	118.47 (17)	C19—N2—C18	115.6 (2)
N1—C7—C6	120.18 (16)	N2—C18—H18A	109.5
C7—N1—C9	117.91 (17)	N2—C18—H18B	109.5

C7—N1—C10	125.35 (17)	H18A—C18—H18B	109.5
C9—N1—C10	116.18 (17)	N2—C18—H18C	109.5
N1—C9—H9A	109.5	H18A—C18—H18C	109.5
N1—C9—H9B	109.5	H18B—C18—H18C	109.5
H9A—C9—H9B	109.5	N2—C19—H19A	109.5
N1—C9—H9C	109.5	N2—C19—H19B	109.5
H9A—C9—H9C	109.5	H19A—C19—H19B	109.5
H9B—C9—H9C	109.5	N2—C19—H19C	109.5
N1—C10—H10A	109.5	H19A—C19—H19C	109.5
N1—C10—H10B	109.5	H19B—C19—H19C	109.5

Table 5. Anisotropic displacement parameters (Å^2) for 2a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2 a^{*2} U^{11} + ... + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U11	U22	U33	U12	U13	U23
Se1	0.03870 (11)	0.03357 (10)	0.03694 (10)	−0.00830 (7)	0.01222 (8)	0.00188 (7)
Se2	0.04531 (12)	0.03006 (10)	0.05242 (13)	−0.00619 (7)	0.02684 (10)	−0.00080 (8)
O1	0.0452 (8)	0.0494 (8)	0.0654 (9)	−0.0070 (7)	0.0072 (7)	0.0071 (7)
O2	0.0553 (9)	0.0426 (8)	0.1093 (13)	0.0100 (7)	0.0435 (9)	0.0290 (9)
C8	0.0341 (9)	0.0258 (7)	0.0369 (8)	0.0018 (6)	0.0167 (7)	0.0004 (6)
C1	0.0392 (10)	0.0281 (8)	0.0400 (9)	−0.0027 (7)	0.0121 (8)	0.0048 (7)
C2	0.0469 (11)	0.0363 (9)	0.0595 (12)	−0.0011 (8)	0.0246 (10)	0.0005 (9)

C3	0.0696 (16)	0.0403 (11)	0.0754 (15)	0.0045 (11)	0.0376 (13)	−0.0037 (11)
C4	0.0857 (19)	0.0356 (10)	0.0817 (17)	−0.0085 (11)	0.0384 (15)	−0.0108 (11)
C5	0.0587 (13)	0.0339 (9)	0.0627 (13)	−0.0135 (9)	0.0199 (11)	0.0007 (9)
C6	0.0387 (10)	0.0301 (8)	0.0441 (10)	−0.0047 (7)	0.0104 (8)	0.0074 (7)
C7	0.0346 (10)	0.0345 (9)	0.0533 (11)	−0.0041 (8)	0.0120 (9)	0.0093 (8)
N1	0.0408 (9)	0.0397 (8)	0.0591 (10)	−0.0026 (7)	0.0193 (8)	0.0121 (8)
C9	0.0536 (14)	0.0704 (16)	0.0979 (19)	−0.0005 (13)	0.0439 (14)	0.0197 (15)
C10	0.0707 (15)	0.0428 (11)	0.0547 (12)	−0.0067 (11)	0.0216 (11)	0.0139 (10)
C11	0.0399 (10)	0.0332 (8)	0.0441 (10)	−0.0012 (7)	0.0163 (8)	−0.0031 (8)
C12	0.0499 (12)	0.0480 (11)	0.0371 (10)	0.0050 (9)	0.0124 (9)	−0.0033 (9)
C13	0.0659 (14)	0.0560 (12)	0.0398 (10)	0.0031 (11)	0.0248 (10)	0.0082 (9)
C14	0.0574 (13)	0.0441 (10)	0.0517 (11)	−0.0045 (9)	0.0307 (10)	0.0072 (9)
C15	0.0376 (9)	0.0307 (8)	0.0402 (9)	−0.0009 (7)	0.0193 (8)	0.0016 (7)
C16	0.0398 (10)	0.0379 (9)	0.0467 (10)	−0.0098 (8)	0.0226 (9)	0.0010 (8)
N2	0.0600 (11)	0.0381 (8)	0.0554 (10)	−0.0170 (8)	0.0257 (9)	−0.0060 (8)
C18	0.098 (2)	0.0333 (10)	0.0871 (17)	−0.0030 (12)	0.0463 (15)	0.0008 (12)
C19	0.0816 (19)	0.0716 (16)	0.0731 (16)	−0.0411 (15)	0.0302 (14)	−0.0241 (14)

Crystal Structure of bis(*N,N*-diisopropylbenzamide) diselenide 2c with 50% ellipsoidal probability (CCDC No.- 1059009)
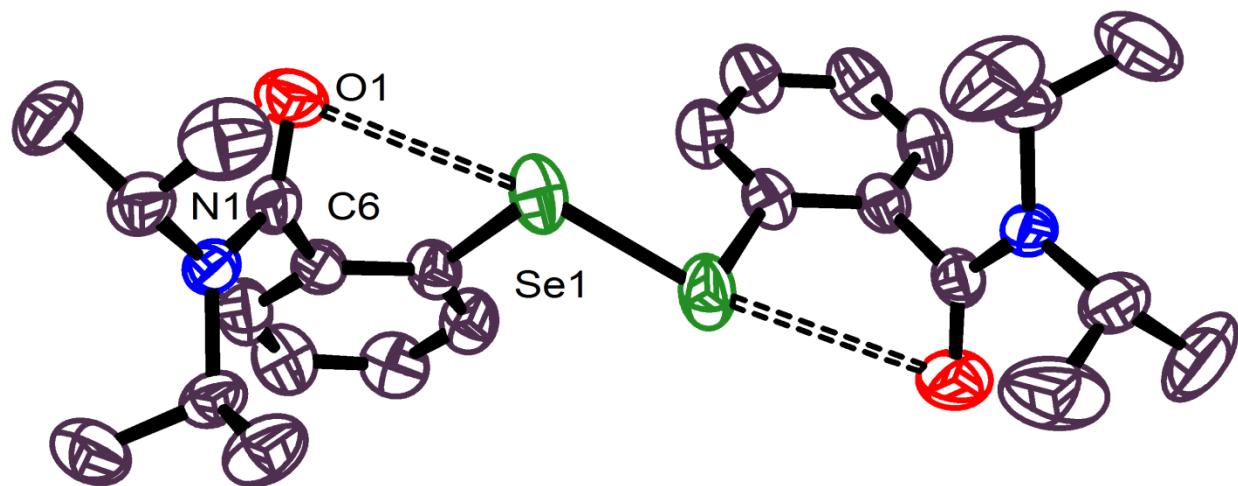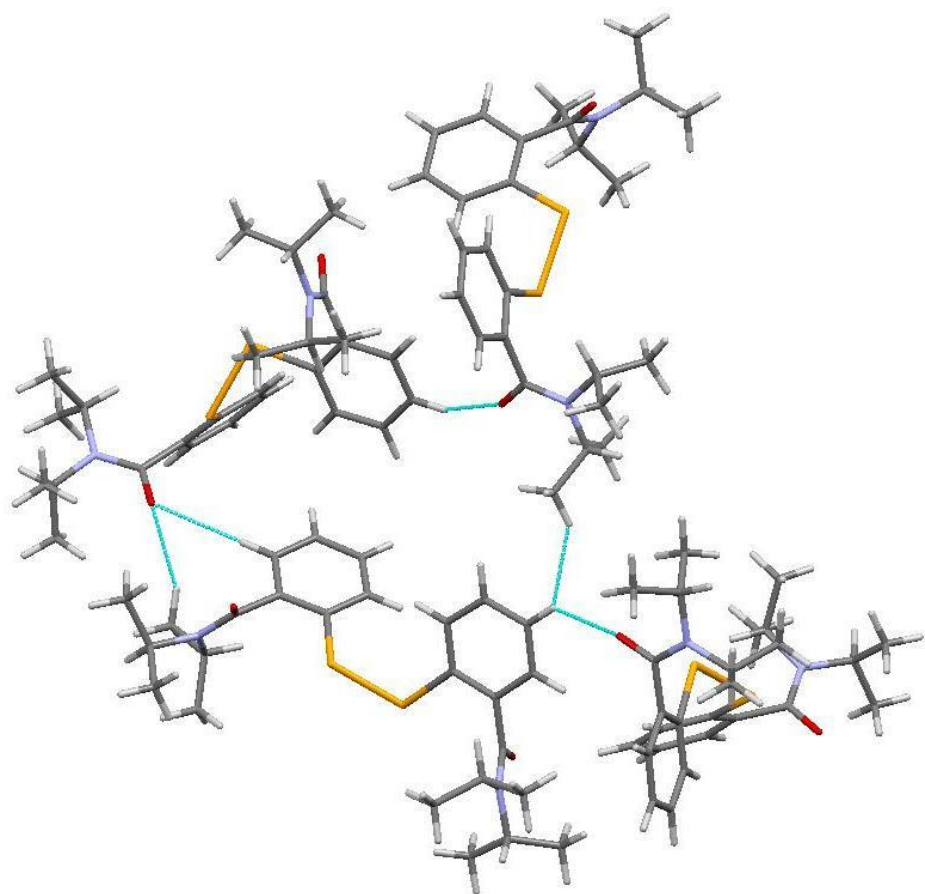

Packing diagram for 2c

Table 6. Crystal data and structure refinement for 2c

Identification code	**Saket_DS**
Empirical formula	$C_{26} H_{36} N_2 O_2 Se_2$
Formula weight	566.49
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P b c a
Unit cell dimensions	a = 19.2091(7) Å $\quad \alpha = 90°$.
	b = 9.3046(3) Å $\quad \beta = 90°$.
	c = 30.9426(11) Å $\quad \gamma = 90°$.
Volume	5530.5(3) $Å^3$
Z	8
Density (calculated)	1.361 g/cm^3
Absorption coefficient	2.697 mm^{-1}
F(000)	2320
Theta range for data collection	2.120 to 25.718°.
Index ranges	-23<=h<=23, -11<=k<=11, -37<=l<=36
Reflections collected	56260
Independent reflections	5260 [R(int) = 0.1038]
Completeness to theta = 25.242°	100.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5260 / 0 / 297
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0452, wR2 = 0.0909
R indices (all data)	R1 = 0.0856, wR2 = 0.1053
Extinction coefficient	n/a
Largest diff. peak and hole	0.900 and -0.718 $e.Å^{-3}$

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2c. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(1)	4078(1)	6454(1)	4078(1)	65(1)
Se(2)	4962(1)	6980(1)	3595(1)	68(1)
N(2)	5974(1)	10327(3)	3267(1)	44(1)
O(1)	2963(1)	5273(3)	4687(1)	68(1)
N(1)	3562(1)	3274(3)	4877(1)	47(1)
O(2)	6039(2)	8278(3)	2881(1)	81(1)
C(1)	3686(2)	4727(4)	3832(1)	47(1)
C(6)	3346(2)	3804(4)	4114(1)	45(1)
C(19)	4919(2)	9245(4)	2975(1)	47(1)
C(20)	5694(2)	9253(4)	3039(1)	49(1)
C(7)	3282(2)	4177(4)	4585(1)	48(1)
C(8)	4070(2)	2153(4)	4757(1)	54(1)
C(14)	4502(2)	8273(4)	3196(1)	50(1)
C(21)	5553(2)	11417(4)	3491(1)	60(1)
C(11)	3409(2)	3445(4)	5342(1)	59(1)
C(5)	3017(2)	2593(4)	3949(1)	60(1)
C(2)	3724(2)	4393(4)	3395(1)	58(1)
C(15)	3789(2)	8252(4)	3127(1)	62(1)
C(4)	3050(2)	2286(5)	3516(1)	69(1)
C(24)	6734(2)	10414(5)	3320(2)	67(1)
C(16)	3500(2)	9168(4)	2829(1)	67(1)
C(18)	4609(2)	10148(4)	2674(1)	59(1)
C(17)	3903(2)	10111(4)	2602(1)	67(1)
C(3)	3411(2)	3171(5)	3241(1)	67(1)
C(12)	2626(2)	3320(5)	5426(2)	80(1)
C(10)	4764(2)	2405(5)	4980(2)	76(1)

C(9)	3793(2)	652(5)	4842(2)	83(1)
C(13)	3724(3)	4803(5)	5533(2)	86(1)
C(22)	5646(3)	11353(7)	3975(2)	111(2)
C(23)	5686(3)	12908(5)	3312(2)	109(2)
C(25)	7093(2)	10657(7)	2892(2)	120(2)
C(26)	7023(3)	9150(6)	3572(2)	119(2)

Table 8. Selected bond lengths [Å] for 2c.

Se1—C1	1.932 (4)	C4—H4	0.95
Se1—Se2	2.3147 (6)	C24—C25	1.509 (6)
Se2—C14	1.936 (3)	C24—C26	1.516 (7)
N2—C20	1.338 (4)	C24—H24	1
N2—C21	1.470 (4)	C16—C17	1.366 (6)
N2—C24	1.472 (4)	C16—H16	0.95
O1—C7	1.231 (4)	C18—C17	1.375 (5)
N1—C7	1.347 (4)	C18—H18	0.95
N1—C8	1.476 (4)	C17—H17	0.95
N1—C11	1.477 (4)	C3—H3	0.95
O2—C20	1.225 (4)	C12—H12A	0.98
C1—C6	1.389 (5)	C12—H12B	0.98
C1—C2	1.390 (5)	C12—H12C	0.98
C6—C5	1.389 (5)	C10—H10A	0.98
C6—C7	1.502 (5)	C10—H10B	0.98
C19—C18	1.388 (5)	C10—H10C	0.98
C19—C14	1.390 (5)	C9—H9A	0.98
C19—C20	1.500 (5)	C9—H9B	0.98
C8—C9	1.517 (6)	C9—H9C	0.98
C8—C10	1.521 (5)	C13—H13A	0.98
C8—H8	1	C13—H13B	0.98

C14—C15	1.385 (5)	C13—H13C	0.98
C21—C22	1.510 (6)	C22—H22A	0.98
C21—C23	1.515 (6)	C22—H22B	0.98
C21—H21	1	C22—H22C	0.98
C11—C13	1.520 (6)	C23—H23A	0.98
C11—C12	1.531 (5)	C23—H23B	0.98
C11—H11	1	C23—H23C	0.98
C5—C4	1.374 (5)	C25—H25A	0.98
C5—H5	0.95	C25—H25B	0.98
C2—C3	1.372 (5)	C25—H25C	0.98
C2—H2	0.95	C26—H26A	0.98
C15—C16	1.372 (5)	C26—H26B	0.98
C15—H15	0.95	C26—H26C	0.98
C4—C3	1.372 (6)		

Table 9. Selected bond angles [°] for 2c.

C1—Se1—Se2	101.94 (11)	C26—C24—H24	106.4
C14—Se2—Se1	101.99 (11)	C17—C16—C15	121.0 (4)
C20—N2—C21	122.9 (3)	C17—C16—H16	119.5
C20—N2—C24	119.9 (3)	C15—C16—H16	119.5
C21—N2—C24	117.1 (3)	C17—C18—C19	121.2 (4)
C7—N1—C8	122.3 (3)	C17—C18—H18	119.4
C7—N1—C11	120.5 (3)	C19—C18—H18	119.4
C8—N1—C11	117.0 (3)	C16—C17—C18	119.4 (4)
C6—C1—C2	120.0 (3)	C16—C17—H17	120.3
C6—C1—Se1	116.7 (3)	C18—C17—H17	120.3
C2—C1—Se1	123.3 (3)	C4—C3—C2	120.3 (4)
C1—C6—C5	118.9 (3)	C4—C3—H3	119.9

C1—C6—C7	120.4 (3)	C2—C3—H3	119.9
C5—C6—C7	120.4 (3)	C11—C12—H12A	109.5
C18—C19—C14	118.4 (3)	C11—C12—H12B	109.5
C18—C19—C20	120.8 (3)	H12A—C12—H12B	109.5
C14—C19—C20	120.7 (3)	C11—C12—H12C	109.5
O2—C20—N2	123.1 (3)	H12A—C12—H12C	109.5
O2—C20—C19	118.7 (3)	H12B—C12—H12C	109.5
N2—C20—C19	118.2 (3)	C8—C10—H10A	109.5
O1—C7—N1	122.9 (3)	C8—C10—H10B	109.5
O1—C7—C6	118.7 (3)	H10A—C10—H10B	109.5
N1—C7—C6	118.3 (3)	C8—C10—H10C	109.5
N1—C8—C9	112.0 (3)	H10A—C10—H10C	109.5
N1—C8—C10	110.9 (3)	H10B—C10—H10C	109.5
C9—C8—C10	111.8 (3)	C8—C9—H9A	109.5
N1—C8—H8	107.3	C8—C9—H9B	109.5
C9—C8—H8	107.3	H9A—C9—H9B	109.5
C10—C8—H8	107.3	C8—C9—H9C	109.5
C15—C14—C19	120.2 (3)	H9A—C9—H9C	109.5
C15—C14—Se2	122.8 (3)	H9B—C9—H9C	109.5
C19—C14—Se2	117.0 (3)	C11—C13—H13A	109.5
N2—C21—C22	112.0 (4)	C11—C13—H13B	109.5
N2—C21—C23	111.5 (4)	H13A—C13—H13B	109.5
C22—C21—C23	112.3 (4)	C11—C13—H13C	109.5
N2—C21—H21	106.9	H13A—C13—H13C	109.5
C22—C21—H21	106.9	H13B—C13—H13C	109.5
C23—C21—H21	106.9	C21—C22—H22A	109.5
N1—C11—C13	112.8 (3)	C21—C22—H22B	109.5
N1—C11—C12	110.6 (3)	H22A—C22—H22B	109.5

C13—C11—C12	112.9 (4)	C21—C22—H22C	109.5
N1—C11—H11	106.7	H22A—C22—H22C	109.5
C13—C11—H11	106.7	H22B—C22—H22C	109.5
C12—C11—H11	106.7	C21—C23—H23A	109.5
C4—C5—C6	120.5 (4)	C21—C23—H23B	109.5
C4—C5—H5	119.8	H23A—C23—H23B	109.5
C6—C5—H5	119.8	C21—C23—H23C	109.5
C3—C2—C1	120.0 (4)	H23A—C23—H23C	109.5
C3—C2—H2	120	H23B—C23—H23C	109.5
C1—C2—H2	120	C24—C25—H25A	109.5
C16—C15—C14	119.7 (4)	C24—C25—H25B	109.5
C16—C15—H15	120.1	H25A—C25—H25B	109.5
C14—C15—H15	120.1	C24—C25—H25C	109.5
C3—C4—C5	120.3 (4)	H25A—C25—H25C	109.5
C3—C4—H4	119.9	H25B—C25—H25C	109.5
C5—C4—H4	119.9	C24—C26—H26A	109.5
N2—C24—C25	111.4 (4)	C24—C26—H26B	109.5
N2—C24—C26	112.2 (4)	H26A—C26—H26B	109.5
C25—C24—C26	113.6 (4)	C24—C26—H26C	109.5
N2—C24—H24	106.4	H26A—C26—H26C	109.5
C25—C24—H24	106.4	H26B—C26—H26C	109.5

Table 10. Anisotropic displacement parameters (Å^2x 10^3) for 2c. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2a^{*2}U^{11} + ... + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(1)	81(1)	60(1)	54(1)	12(1)	-6(1)	-18(1)
Se(2)	54(1)	67(1)	84(1)	33(1)	-11(1)	-8(1)

N(2)	45(2)	43(2)	44(2)	-9(1)	5(1)	-1(1)
O(1)	85(2)	56(2)	64(2)	11(1)	10(2)	26(2)
N(1)	45(2)	50(2)	46(2)	11(1)	8(1)	10(1)
O(2)	73(2)	66(2)	105(3)	-42(2)	8(2)	1(2)
C(1)	48(2)	47(2)	46(2)	13(2)	-5(2)	2(2)
C(6)	42(2)	46(2)	48(2)	12(2)	-1(2)	7(2)
C(19)	55(2)	42(2)	43(2)	-2(2)	-2(2)	-6(2)
C(20)	60(2)	41(2)	46(2)	0(2)	9(2)	-5(2)
C(7)	46(2)	48(2)	51(2)	12(2)	6(2)	3(2)
C(8)	43(2)	67(3)	51(2)	9(2)	4(2)	16(2)
C(14)	57(2)	42(2)	51(2)	7(2)	-3(2)	-3(2)
C(21)	48(2)	61(2)	70(3)	-23(2)	5(2)	4(2)
C(11)	63(2)	67(3)	46(2)	14(2)	11(2)	17(2)
C(5)	56(2)	58(2)	65(3)	14(2)	0(2)	-6(2)
C(2)	58(2)	67(3)	48(2)	15(2)	-2(2)	0(2)
C(15)	55(2)	61(3)	70(3)	15(2)	-9(2)	-8(2)
C(4)	77(3)	65(3)	64(3)	-1(2)	-11(2)	-8(2)
C(24)	46(2)	70(3)	86(3)	-28(2)	4(2)	-1(2)
C(16)	62(3)	59(2)	80(3)	10(2)	-22(2)	-3(2)
C(18)	73(3)	56(2)	48(2)	9(2)	-4(2)	-15(2)
C(17)	85(3)	55(2)	61(3)	12(2)	-24(2)	-3(2)
C(3)	79(3)	71(3)	50(2)	0(2)	-9(2)	6(2)
C(12)	71(3)	97(3)	71(3)	20(3)	31(2)	13(3)

C(10)	52(2)	107(4)	68(3)	5(3)	0(2)	18(2)
C(9)	83(3)	59(3)	106(4)	11(3)	-4(3)	19(2)
C(13)	94(4)	101(4)	63(3)	-12(3)	-3(3)	10(3)
C(22)	110(4)	156(5)	68(3)	-49(4)	20(3)	4(4)
C(23)	113(4)	51(3)	162(6)	-16(3)	-7(4)	15(3)
C(25)	69(3)	153(5)	137(5)	-44(4)	52(3)	-33(3)
C(26)	89(4)	106(4)	163(6)	-24(4)	-46(4)	39(3)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2x 10^3) for 2c.

	x	y	z	U(eq)
H(8)	4152	2237	4439	65
H(21)	5054	11186	3431	72
H(11)	3634	2617	5494	70
H(5)	2768	1973	4138	72
H(2)	3968	5011	3203	70
H(15)	3502	7606	3284	74
H(4)	2821	1458	3405	83
H(24)	6827	11288	3499	81
H(16)	3011	9146	2781	80
H(18)	4889	10804	2516	71
H(17)	3697	10735	2395	80
H(3)	3443	2937	2942	80
H(12A)	2390	4179	5317	120
H(12B)	2543	3231	5738	120

H(12C)	2444	2468	5278	120
H(10A)	4929	3379	4916	114
H(10B)	5105	1704	4875	114
H(10C)	4707	2294	5293	114
H(9A)	3741	506	5154	124
H(9B)	4120	-59	4725	124
H(9C)	3339	539	4701	124
H(13A)	3635	4831	5844	129
H(13B)	3513	5647	5396	129
H(13C)	4227	4808	5481	129
H(22A)	5544	10379	4078	167
H(22B)	5328	12036	4114	167
H(22C)	6128	11604	4049	167
H(23A)	6168	13191	3374	163
H(23B)	5366	13594	3448	163
H(23C)	5611	12904	2999	163
H(25A)	7592	10804	2941	179
H(25B)	6896	11510	2752	179
H(25C)	7024	9817	2706	179
H(26A)	6788	9089	3853	179
H(26B)	7524	9283	3617	179
H(26C)	6942	8260	3410	179

Crystal structure of bis[2-(*N*-allyl-5-nitrobenzamide)] diselenide 2d with 40% ellipsoidal probability (CCDC No.- 1019634)
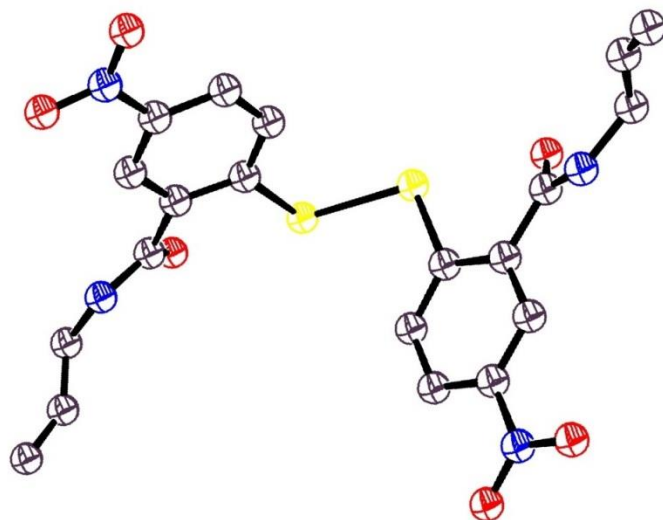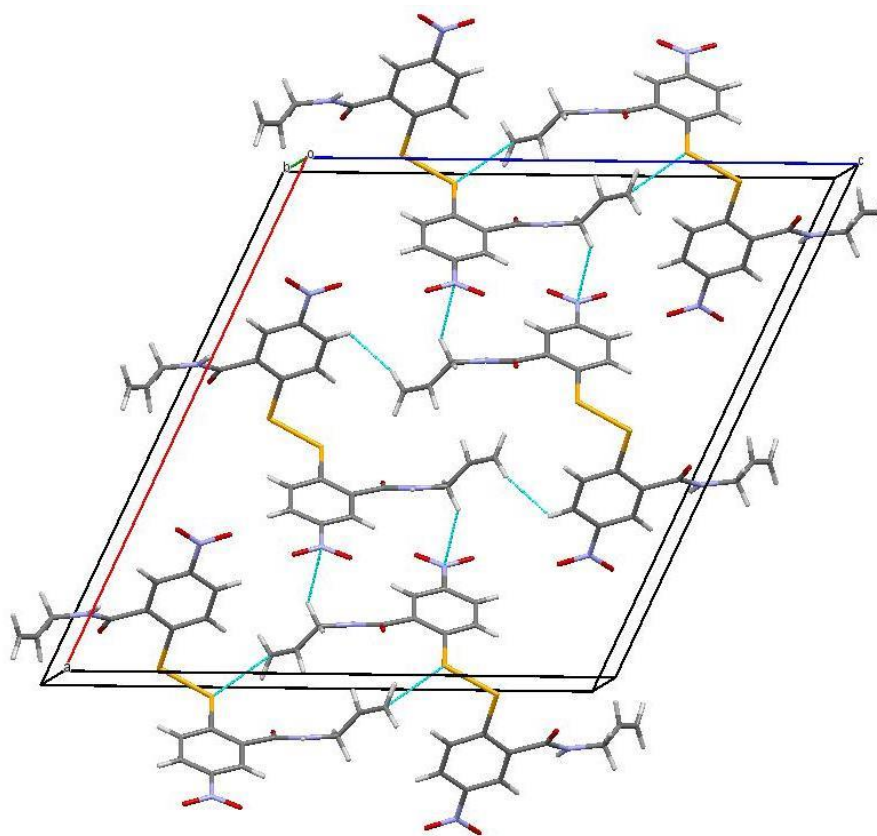

Packing diagram of 2d

Table 12. Crystal data and structure refinement for 2d

Identification code	Try_Ajay
Empirical formula	$C_{20} H_{18} N_4 O_6 Se_2$
Formula weight	568.30
Temperature	159(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C 2/c
Unit cell dimensions	a = 22.461(3) Å $\quad$ α= 90°.
	b = 4.8135(6) Å $\quad$ β= 115.883(3)°.
	c = 21.823(3) Å $\quad$ γ = 90°.
Volume	2122.7(5) Å^3
Z	4
Density (calculated)	1.778 g/cm^3
Absorption coefficient	3.530 mm^{-1}
F(000)	1128
Theta range for data collection	3.468 to 25.791°.
Index ranges	-27<=h<=27, -5<=k<=5, -26<=l<=26
Reflections collected	18455
Independent reflections	2027 [R(int) = 0.0745]
Completeness to theta = 25.242°	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2027 / 0 / 145
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.0844
R indices (all data)	R1 = 0.0603, wR2 = 0.0927
Extinction coefficient	n/a
Largest diff. peak and hole	1.077 and -1.043 e.Å^{-3}

Table 13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2x 10^3) for t Try_Ajay. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(1)	4728(1)	12030(1)	6905(1)	23(1)
O(3)	4037(2)	11631(6)	5505(2)	28(1)
O(2)	2317(2)	2141(7)	5754(2)	40(1)
C(6)	3712(2)	8168(9)	6069(2)	20(1)
O(1)	2386(2)	2706(9)	6762(2)	53(1)
N(2)	3823(2)	7340(8)	5035(2)	31(1)
C(1)	4032(2)	9343(9)	6723(2)	20(1)
C(5)	3226(2)	6182(9)	5937(2)	22(1)
N(1)	2553(2)	3277(8)	6314(2)	33(1)
C(7)	3875(2)	9178(9)	5512(2)	22(1)
C(2)	3840(2)	8562(10)	7222(2)	30(1)
C(4)	3056(2)	5423(9)	6450(2)	26(1)
C(3)	3349(2)	6611(11)	7091(2)	34(1)
C(10)	4360(3)	4732(12)	3902(3)	45(1)
C(8)	3884(4)	8067(12)	4420(3)	62(2)
C(9)	4306(5)	6595(15)	4267(4)	97(3)

Table 14. Selected bond lengths [Å] for Try_Ajay.

Se1—C1	1.931 (4)	C5—H3	0.95
Se1—Se1′	2.3390 (9)	N1—C4	1.463 (5)
O3—C7	1.238 (5)	C2—C3	1.381 (6)
O2—N1	1.228 (5)	C2—H1	0.95
C6—C5	1.383 (6)	C4—C3	1.383 (6)
C6—C1	1.406 (6)	C3—H2	0.95
C6—C7	1.497 (6)	C10—C9	1.240 (8)
O1—N1	1.223 (5)	C10—H8	0.95
N2—C7	1.331 (5)	C10—H7	0.95
N2—C8	1.451 (6)	C8—C9	1.337 (9)
N2—H4	0.88	C8—H8A	0.99
C1—C2	1.388 (6)	C8—H8B	0.99
C5—C4	1.382 (6)	C9—H6	0.95

Table 15. Selected Bond angles [°] for Try_Ajay.

C1—Se1—Se1′	102.25 (12)	C3—C2—H1	119.5
C5—C6—C1	119.9 (4)	C1—C2—H1	119.5
C5—C6—C7	120.3 (4)	C5—C4—C3	122.3 (4)
C1—C6—C7	119.7 (4)	C5—C4—N1	118.9 (4)
C7—N2—C8	123.4 (4)	C3—C4—N1	118.8 (4)
C7—N2—H4	118.3	C2—C3—C4	118.3 (4)
C8—N2—H4	118.3	C2—C3—H2	120.8
C2—C1—C6	119.4 (4)	C4—C3—H2	120.8
C2—C1—Se1	121.4 (3)	C9—C10—H8	120
C6—C1—Se1	119.2 (3)	C9—C10—H7	120
C4—C5—C6	119.0 (4)	H8—C10—H7	120
C4—C5—H3	120.5	C9—C8—N2	117.8 (5)

C6—C5—H3	120.5	C9—C8—H8A	107.9
O1—N1—O2	123.2 (4)	N2—C8—H8A	107.9
O1—N1—C4	118.4 (4)	C9—C8—H8B	107.9
O2—N1—C4	118.4 (4)	N2—C8—H8B	107.9
O3—C7—N2	123.4 (4)	H8A—C8—H8B	107.2
O3—C7—C6	119.8 (4)	C10—C9—C8	145.3 (10)
N2—C7—C6	116.8 (4)	C10—C9—H6	107.4
C3—C2—C1	121.1 (4)	C8—C9—H6	107.4

Symmetry transformations used to generate equivalent atoms:

Symmetry code: (i) −x+1, y, −z+3/2.

Table 16. Anisotropic displacement parameters ($Å^2$x 10^3)for Try_Ajay. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(1)	21(1)	20(1)	22(1)	4(1)	4(1)	-1(1)
O(3)	38(2)	20(2)	26(2)	3(1)	13(1)	0(1)
O(2)	34(2)	42(2)	40(2)	-13(2)	12(2)	-17(2)
C(6)	19(2)	19(2)	21(2)	2(2)	7(2)	6(2)
O(1)	47(2)	71(3)	49(2)	-4(2)	29(2)	-28(2)
N(2)	48(2)	23(2)	28(2)	5(2)	23(2)	3(2)
C(1)	17(2)	21(2)	22(2)	2(2)	7(2)	1(2)
C(5)	18(2)	24(2)	20(2)	-1(2)	4(2)	3(2)
N(1)	23(2)	35(2)	40(2)	1(2)	13(2)	-5(2)
C(7)	19(2)	23(2)	21(2)	5(2)	4(2)	6(2)
C(2)	29(2)	36(3)	22(2)	-4(2)	9(2)	-8(2)

C(4)	20(2)	27(3)	30(2)	1(2)	10(2)	-4(2)
C(3)	31(2)	47(3)	26(2)	-2(2)	16(2)	-9(2)
C(10)	57(3)	50(4)	31(3)	0(3)	23(3)	4(3)
C(8)	127(6)	35(3)	50(3)	13(3)	63(4)	17(4)
C(9)	193(9)	57(5)	107(6)	46(4)	128(7)	50(5)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($\mathring{A}^2$x 10^3) for Try_Ajay.

	x	y	z	U(eq)
H(4)	3748	5592	5097	37
H(3)	3012	5352	5499	27
H(1)	4050	9382	7661	36
H(2)	3215	6098	7433	40
H(8)	3975	3825	3578	54
H(7)	4784	4210	3947	54
H(8A)	3440	7915	4032	74
H(8B)	4017	10043	4456	74
H(6)	4740	7233	4554	116

Crystal structure of bis((2-(dimethylcarbamoyl)phenyl)selanyl)mercury 3a with 50% ellipsoidal probability (CCDC No. 1059007)
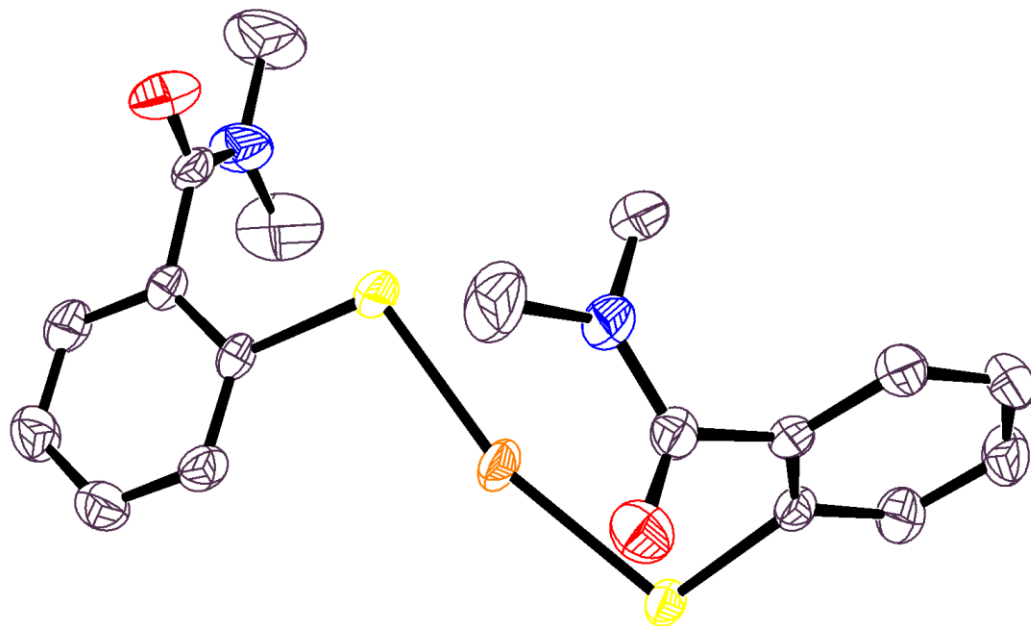
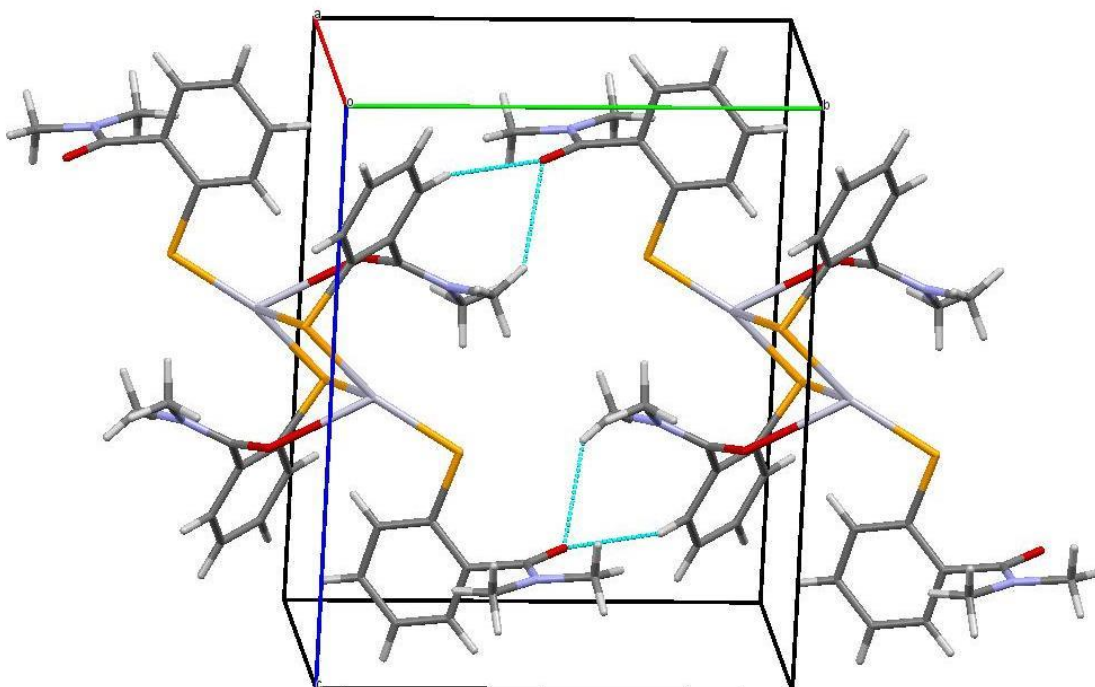

Crystal Structure of 3a with 50% ellipsoidal probability

Table 18. Crystal data and structure refinement for 3a

Identification code	Saket_01
Empirical formula	$C_{18} H_{20} Hg N_2 O_2 Se_2$
Formula weight	654.87
Temperature	300(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\bar{1}$
Unit cell dimensions	a = 6.4927(2) Å α= 92.694(2)°.
	b = 11.3302(5) Å β= 101.312(2)°.
	c = 13.9409(6) Å γ = 97.023(2)°.
Volume	995.42(7) Å^3
Z	2
Density (calculated)	2.185 g/cm^3
Absorption coefficient	11.401 mm^{-1}
F(000)	612
Theta range for data collection	2.266 to 25.758°.
Index ranges	-7<=h<=7, -13<=k<=13, -17<=l<=17
Reflections collected	17547
Independent reflections	3794 [R(int) = 0.0448]
Completeness to theta = 25.242°	99.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3794 / 0 / 230
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0223, wR2 = 0.0513
R indices (all data)	R1 = 0.0265, wR2 = 0.0528
Extinction coefficient	n/a
Largest diff. peak and hole	0.902 and -0.859 e.Å^{-3}

Table 19. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2x 10^3) for 3a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Hg(1)	2986(1)	1129(1)	5458(1)	36(1)
Se(1)	2093(1)	-458(1)	4110(1)	27(1)
Se(2)	3518(1)	3027(1)	6463(1)	41(1)
O(1)	6755(4)	1000(3)	3621(2)	41(1)
N(1)	5726(6)	2779(3)	3951(3)	39(1)
O(2)	4598(5)	5400(3)	8269(3)	54(1)
C(2)	3333(6)	1323(3)	2787(3)	25(1)
C(1)	1823(6)	418(3)	2947(3)	25(1)
C(7)	5401(6)	1686(3)	3499(3)	29(1)
C(6)	39(6)	50(4)	2218(3)	36(1)
C(16)	3322(6)	4538(3)	8349(3)	31(1)
C(15)	5130(6)	1520(3)	7994(3)	35(1)
N(2)	1289(6)	4610(3)	8310(3)	52(1)
C(4)	1250(7)	1480(4)	1179(3)	42(1)
C(11)	4078(6)	3350(3)	8535(3)	27(1)
C(3)	3012(7)	1854(3)	1899(3)	36(1)
C(10)	4296(5)	2571(3)	7774(3)	25(1)
C(8)	4147(8)	3596(4)	3865(3)	50(1)
C(5)	-232(7)	573(4)	1334(3)	42(1)
C(14)	5720(7)	1246(4)	8955(3)	43(1)

C(13)	5522(7)	2025(4)	9712(3)	46(1)
C(12)	4698(7)	3079(4)	9502(3)	39(1)
C(9)	7795(9)	3241(5)	4550(4)	66(2)
C(18)	-289(8)	3575(6)	8311(6)	93(2)
C(17)	525(11)	5759(5)	8140(6)	94(2)

Table 20. Selected bond lengths [Å] for 3a.

Hg1—Se2	2.4605 (4)	C4—C5	1.374 (6)
Hg1—Se1	2.4697 (4)	C4—H4	0.95
Se1—C1	1.930 (3)	C11—C10	1.388 (5)
Se2—C10	1.911 (4)	C11—C12	1.389 (5)
O1—C7	1.235 (4)	C3—H3	0.95
N1—C7	1.337 (5)	C8—H8A	0.98
N1—C8	1.455 (5)	C8—H8B	0.98
N1—C9	1.457 (6)	C8—H8C	0.98
O2—C16	1.225 (5)	C5—H5	0.95
C2—C1	1.387 (5)	C14—C13	1.380 (6)
C2—C3	1.392 (5)	C14—H14	0.95
C2—C7	1.504 (5)	C13—C12	1.388 (6)
C1—C6	1.389 (5)	C13—H13	0.95
C6—C5	1.382 (6)	C12—H12	0.95
C6—H6	0.95	C9—H9A	0.98
C16—N2	1.323 (5)	C9—H9B	0.98
C16—C11	1.505 (5)	C9—H9C	0.98
C15—C14	1.379 (6)	C18—H18A	0.98
C15—C10	1.390 (5)	C18—H18B	0.98
C15—H15	0.95	C18—H18C	0.98

N2—C18	1.460 (7)	C17—H17A	0.98
N2—C17	1.462 (6)	C17—H17B	0.98
C4—C3	1.374 (6)	C17—H17C	0.98

Table 21. Selected Bond angles [°] for 3a.

Se2—Hg1—Se1	165.235 (14)	C15—C10—Se2	122.9 (3)
C1—Se1—Hg1	103.33 (10)	N1—C8—H8A	109.5
C10—Se2—Hg1	103.53 (10)	N1—C8—H8B	109.5
C7—N1—C8	124.4 (4)	H8A—C8—H8B	109.5
C7—N1—C9	120.1 (4)	N1—C8—H8C	109.5
C8—N1—C9	115.5 (4)	H8A—C8—H8C	109.5
C1—C2—C3	119.1 (3)	H8B—C8—H8C	109.5
C1—C2—C7	122.6 (3)	C4—C5—C6	120.0 (4)
C3—C2—C7	118.2 (3)	C4—C5—H5	120
C2—C1—C6	119.6 (3)	C6—C5—H5	120
C2—C1—Se1	124.1 (3)	C15—C14—C13	120.2 (4)
C6—C1—Se1	116.1 (3)	C15—C14—H14	119.9
O1—C7—N1	122.5 (4)	C13—C14—H14	119.9
O1—C7—C2	120.0 (3)	C14—C13—C12	119.6 (4)
N1—C7—C2	117.4 (3)	C14—C13—H13	120.2
C5—C6—C1	120.4 (4)	C12—C13—H13	120.2
C5—C6—H6	119.8	C13—C12—C11	120.3 (4)
C1—C6—H6	119.8	C13—C12—H12	119.9
O2—C16—N2	122.7 (4)	C11—C12—H12	119.9
O2—C16—C11	119.5 (4)	N1—C9—H9A	109.5
N2—C16—C11	117.7 (3)	N1—C9—H9B	109.5
C14—C15—C10	120.7 (4)	H9A—C9—H9B	109.5
C14—C15—H15	119.6	N1—C9—H9C	109.5

C10—C15—H15	119.6		H9A—C9—H9C	109.5	
C16—N2—C18	123.5 (4)		H9B—C9—H9C	109.5	
C16—N2—C17	118.6 (4)		N2—C18—H18A	109.5	
C18—N2—C17	117.5 (4)		N2—C18—H18B	109.5	
C3—C4—C5	119.9 (4)		H18A—C18—H18B	109.5	
C3—C4—H4	120.1		N2—C18—H18C	109.5	
C5—C4—H4	120.1		H18A—C18—H18C	109.5	
C10—C11—C12	120.1 (3)		H18B—C18—H18C	109.5	
C10—C11—C16	121.7 (3)		N2—C17—H17A	109.5	
C12—C11—C16	118.1 (3)		N2—C17—H17B	109.5	
C4—C3—C2	121.0 (4)		H17A—C17—H17B	109.5	
C4—C3—H3	119.5		N2—C17—H17C	109.5	
C2—C3—H3	119.5		H17A—C17—H17C	109.5	
C11—C10—C15	119.1 (3)		H17B—C17—H17C	109.5	
C11—C10—Se2	118.0 (3)				

Table 22. Anisotropic displacement parameters ($\mathring{A}^2$x 10^3) for 3a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a*^2U^{11} + ... + 2\ h\ k\ a*\ b*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Hg(1)	52(1)	34(1)	21(1)	-6(1)	7(1)	1(1)
Se(1)	34(1)	26(1)	21(1)	-1(1)	7(1)	-1(1)
Se(2)	66(1)	30(1)	24(1)	-5(1)	3(1)	8(1)
O(1)	36(2)	43(2)	43(2)	7(1)	7(1)	7(1)
N(1)	45(2)	30(2)	36(2)	-1(1)	-2(2)	-6(2)
O(2)	63(2)	30(2)	69(2)	-1(2)	24(2)	-3(2)

C(2)	30(2)	23(2)	24(2)	-2(1)	7(2)	7(2)
C(1)	28(2)	26(2)	22(2)	-3(1)	6(1)	5(2)
C(7)	34(2)	27(2)	24(2)	4(2)	8(2)	-3(2)
C(6)	32(2)	40(2)	33(2)	-2(2)	1(2)	1(2)
C(16)	41(2)	25(2)	26(2)	-8(2)	7(2)	2(2)
C(15)	38(2)	32(2)	34(2)	-6(2)	9(2)	9(2)
N(2)	38(2)	42(2)	79(3)	2(2)	10(2)	17(2)
C(4)	58(3)	42(2)	27(2)	9(2)	3(2)	18(2)
C(11)	23(2)	30(2)	28(2)	-4(2)	6(1)	0(2)
C(3)	52(3)	31(2)	28(2)	5(2)	11(2)	7(2)
C(10)	21(2)	28(2)	24(2)	-4(1)	6(1)	-3(1)
C(8)	80(3)	29(2)	38(2)	-2(2)	7(2)	9(2)
C(5)	39(2)	50(3)	30(2)	-3(2)	-7(2)	9(2)
C(14)	48(3)	42(2)	42(3)	5(2)	7(2)	17(2)
C(13)	57(3)	53(3)	28(2)	4(2)	6(2)	16(2)
C(12)	48(3)	42(2)	28(2)	-9(2)	11(2)	7(2)
C(9)	69(3)	56(3)	54(3)	-2(2)	-13(3)	-23(3)
C(18)	33(3)	81(4)	167(8)	10(5)	25(4)	3(3)
C(17)	82(5)	68(4)	136(7)	16(4)	8(4)	46(4)

Table 23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 3a.

	x	y	z	U(eq)

H(6)	-1002	-567	2327	43
H(15)	5296	986	7478	41
H(4)	1056	1847	575	50
H(3)	4026	2485	1790	44
H(8A)	4524	4239	3460	75
H(8B)	4098	3934	4519	75
H(8C)	2754	3164	3559	75
H(5)	-1443	307	834	50
H(14)	6265	518	9095	52
H(13)	5946	1841	10374	55
H(12)	4558	3618	10021	47
H(9A)	7697	3291	5243	99
H(9B)	8256	4036	4359	99
H(9C)	8824	2705	4451	99
H(18A)	410	2855	8378	140
H(18B)	-1340	3493	7694	140
H(18C)	-997	3682	8863	140
H(17A)	-345	5931	8616	141
H(17B)	-329	5729	7474	141
H(17C)	1737	6387	8215	141

Crystal structure of bis((2-(diisopropylcarbamoyl)phenyl)selanyl)mercury 3c (CCDC No. 1059008)
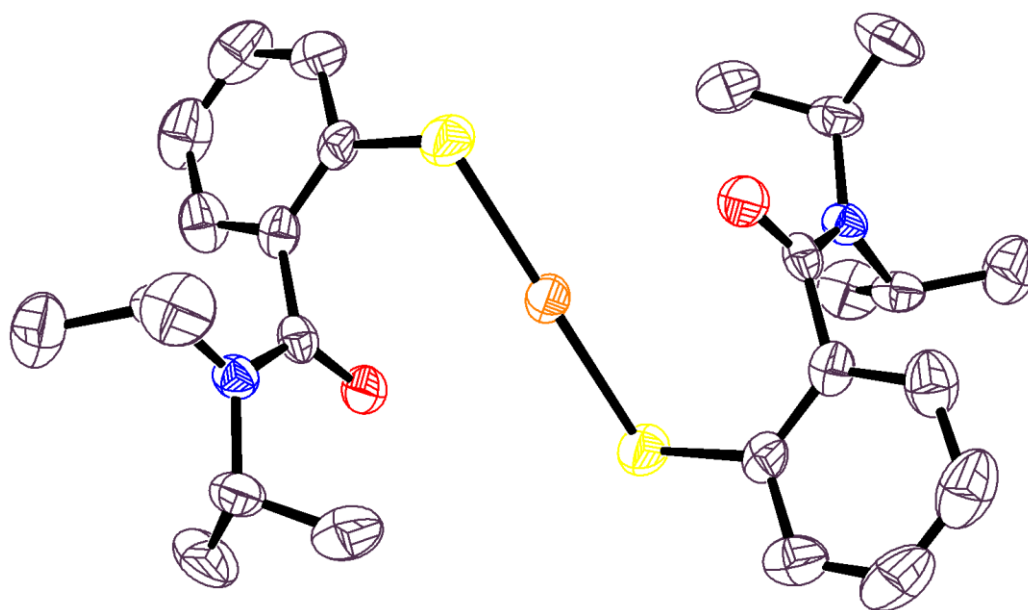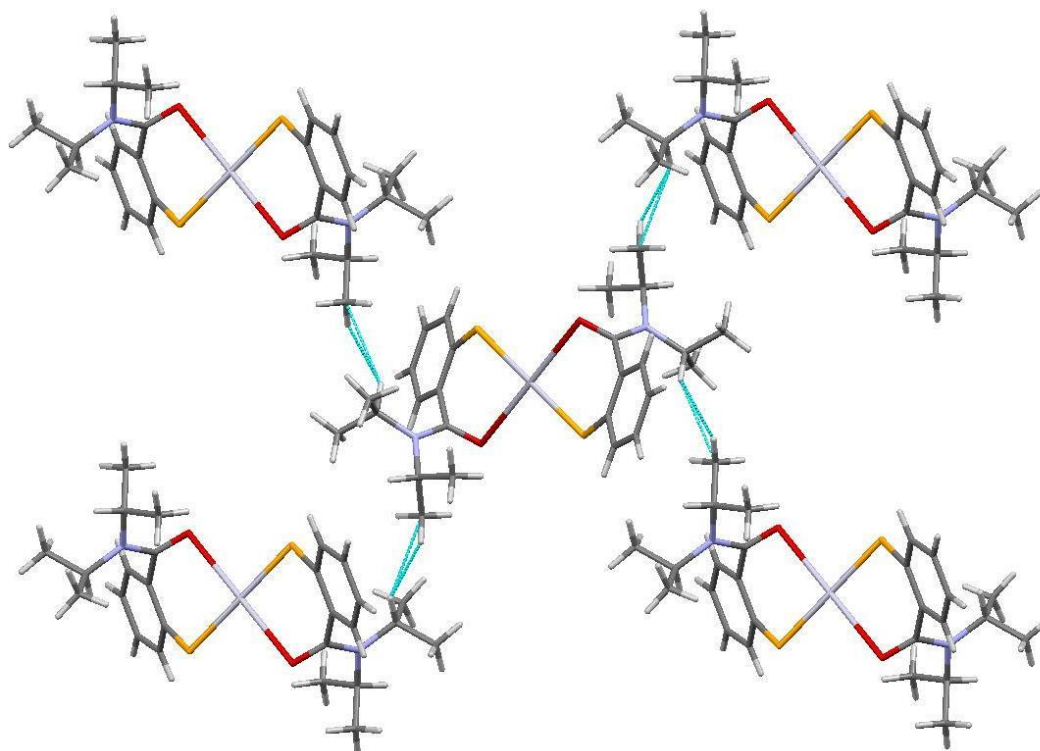

Packing diagram for 3c

Table 24. Crystal data and structure refinement for 3c

Identification code	Saket_02
Empirical formula	$C_{26} H_{36} Hg N_2 O_2 Se_2$
Formula weight	767.08
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P 2_1/c$
Unit cell dimensions	a = 7.5402(6) Å $\quad$ α= 90°.
	b = 13.4630(8) Å $\quad$ β= 99.456(3)°.
	c = 14.1093(12) Å $\quad$ γ = 90°.
Volume	1412.83(19) Å^3
Z	2
Density (calculated)	1.803 g/cm^3
Absorption coefficient	8.047 mm^{-1}
F(000)	740
Theta range for data collection	2.739 to 25.721°.
Index ranges	-9<=h<=9, -16<=k<=16, -16<=l<=17
Reflections collected	12457
Independent reflections	2695 [R(int) = 0.0501]
Completeness to theta = 25.242°	100.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2695 / 0 / 155
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0267, wR2 = 0.0472
R indices (all data)	R1 = 0.0461, wR2 = 0.0521
Extinction coefficient	n/a
Largest diff. peak and hole	0.496 and -0.349 e.Å^{-3}

Table 25. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($\mathring{A}^2$x 10^3) for 3c. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Hg(1)	0	5000	5000	39(1)
Se(1)	1594(1)	3748(1)	6052(1)	51(1)
O(1)	1121(3)	6490(2)	6416(2)	45(1)
N(1)	4110(4)	6259(2)	6831(2)	33(1)
C(6)	2020(5)	5258(3)	7572(3)	36(1)
C(7)	2398(5)	6047(2)	6878(3)	32(1)
C(1)	1525(5)	4282(3)	7307(3)	35(1)
C(11)	4576(5)	7139(2)	6297(3)	44(1)
C(8)	5613(5)	5630(3)	7292(3)	40(1)
C(5)	2062(6)	5540(3)	8520(3)	52(1)
C(10)	6738(6)	5258(3)	6570(4)	64(1)
C(2)	1077(5)	3629(3)	7995(3)	50(1)
C(13)	3973(6)	8094(3)	6722(4)	69(2)
C(12)	3927(7)	7071(3)	5221(3)	69(1)
C(4)	1662(6)	4882(4)	9201(4)	67(1)
C(3)	1184(6)	3933(4)	8941(4)	65(1)
C(9)	6741(6)	6143(4)	8134(3)	71(2)

Table 26. Selected bond lengths [Å] for 3c.

Hg1—Se1i	2.4301 (4)	C5—H5	0.95
Hg1—Se1	2.4301 (4)	C10—H10A	0.98
Se1—C1	1.919 (4)	C10—H10B	0.98
O1—C7	1.225 (4)	C10—H10C	0.98
N1—C7	1.334 (4)	C2—C3	1.386 (6)
N1—C11	1.477 (4)	C2—H2	0.95
N1—C8	1.478 (4)	C13—H13A	0.98
C6—C5	1.385 (6)	C13—H13B	0.98
C6—C1	1.401 (5)	C13—H13C	0.98
C6—C7	1.504 (5)	C12—H12A	0.98
C1—C2	1.392 (5)	C12—H12B	0.98
C11—C13	1.519 (5)	C12—H12C	0.98
C11—C12	1.520 (6)	C4—C3	1.361 (6)
C11—H11	1	C4—H4	0.95
C8—C9	1.510 (5)	C3—H3	0.95
C8—C10	1.513 (6)	C9—H9A	0.98
C8—H8	1	C9—H9B	0.98
C5—C4	1.377 (6)	C9—H9C	0.98

Table 27. Selected bond angles [°] for 3c.

Se1i—Hg1—Se1	179.999 (13)	H10A—C10—H10B	109.5
C1—Se1—Hg1	102.58 (10)	C8—C10—H10C	109.5
C7—N1—C11	120.7 (3)	H10A—C10—H10C	109.5
C7—N1—C8	122.3 (3)	H10B—C10—H10C	109.5
C11—N1—C8	117.1 (3)	C3—C2—C1	120.2 (4)
C5—C6—C1	118.6 (4)	C3—C2—H2	119.9
C5—C6—C7	117.3 (3)	C1—C2—H2	119.9

C1—C6—C7	124.0 (4)	C11—C13—H13A	109.5
O1—C7—N1	123.5 (3)	C11—C13—H13B	109.5
O1—C7—C6	118.3 (3)	H13A—C13—H13B	109.5
N1—C7—C6	118.2 (3)	C11—C13—H13C	109.5
C2—C1—C6	119.4 (4)	H13A—C13—H13C	109.5
C2—C1—Se1	117.0 (3)	H13B—C13—H13C	109.5
C6—C1—Se1	123.5 (3)	C11—C12—H12A	109.5
N1—C11—C13	111.4 (4)	C11—C12—H12B	109.5
N1—C11—C12	113.4 (3)	H12A—C12—H12B	109.5
C13—C11—C12	112.2 (4)	C11—C12—H12C	109.5
N1—C11—H11	106.4	H12A—C12—H12C	109.5
C13—C11—H11	106.4	H12B—C12—H12C	109.5
C12—C11—H11	106.4	C3—C4—C5	119.6 (5)
N1—C8—C9	112.1 (3)	C3—C4—H4	120.2
N1—C8—C10	111.6 (4)	C5—C4—H4	120.2
C9—C8—C10	112.0 (4)	C4—C3—C2	120.5 (5)
N1—C8—H8	106.9	C4—C3—H3	119.7
C9—C8—H8	106.9	C2—C3—H3	119.7
C10—C8—H8	106.9	C8—C9—H9A	109.5
C4—C5—C6	121.6 (4)	C8—C9—H9B	109.5
C4—C5—H5	119.2	H9A—C9—H9B	109.5
C6—C5—H5	119.2	C8—C9—H9C	109.5
C8—C10—H10A	109.5	H9A—C9—H9C	109.5
C8—C10—H10B	109.5	H9B—C9—H9C	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1

Table 28. Anisotropic displacement parameters ($Å^2$x 10^3) for 3c. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Hg(1)	40(1)	41(1)	34(1)	0(1)	2(1)	1(1)
Se(1)	68(1)	38(1)	45(1)	-1(1)	0(1)	13(1)
O(1)	34(2)	41(2)	55(2)	5(1)	-7(1)	-1(1)
N(1)	28(2)	31(2)	39(2)	0(2)	6(1)	-1(1)
C(6)	25(2)	50(2)	33(2)	-2(2)	6(2)	0(2)
C(7)	34(2)	31(2)	32(2)	-11(2)	5(2)	0(2)
C(1)	20(2)	46(2)	38(2)	5(2)	-1(2)	3(2)
C(11)	37(2)	33(2)	62(3)	8(2)	6(2)	-5(2)
C(8)	31(2)	33(2)	56(3)	9(2)	9(2)	1(2)
C(5)	46(3)	67(3)	45(3)	-10(2)	11(2)	-6(2)
C(10)	45(3)	66(3)	84(4)	-2(3)	19(3)	18(2)
C(2)	30(2)	52(3)	67(3)	19(2)	8(2)	-1(2)
C(13)	63(3)	31(2)	109(5)	-12(3)	2(3)	-3(2)
C(12)	86(4)	64(3)	59(4)	19(3)	17(3)	-9(3)
C(4)	55(3)	109(4)	39(3)	4(3)	16(2)	0(3)
C(3)	53(3)	98(4)	51(3)	28(3)	26(3)	5(3)
C(9)	54(3)	92(4)	61(4)	2(3)	-8(3)	0(3)

Table 29. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 3c.

	x	y	z	U(eq)
H(11)	5919	7165	6388	53
H(8)	5068	5032	7552	48
H(5)	2375	6204	8704	63
H(10A)	5947	5000	6003	96
H(10B)	7537	4728	6861	96
H(10C)	7459	5806	6380	96
H(2)	696	2973	7816	60
H(13A)	2657	8111	6636	103
H(13B)	4407	8665	6396	103
H(13C)	4465	8122	7409	103
H(12A)	4306	6435	4981	103
H(12B)	4444	7617	4897	103
H(12C)	2612	7117	5091	103
H(4)	1719	5089	9849	80
H(3)	922	3476	9412	78
H(9A)	7276	6744	7910	107
H(9B)	7697	5694	8430	107
H(9C)	5980	6323	8608	107

Table 30. Crystal data and structure refinement for 3d.

Identification code	shelx_arun191015
Empirical formula	$C_{20} H_{22} Hg N_4 O_6 Se_2$
Formula weight	772.92
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\bar{1}$
Unit cell dimensions	a = 8.9938(5) Å $\quad$ α= 100.352(3)°.
	b = 10.4786(6) Å $\quad$ β= 98.708(3)°.
	c = 13.1186(7) Å $\quad$ γ = 99.288(3)°.
Volume	1179.35(11) Å^3
Z	2
Density (calculated)	2.177 g/cm^3
Absorption coefficient	9.656 mm^{-1}
F(000)	732
Crystal size	0.2 x 0.19 x 0.16 mm^3
Theta range for data collection	1.606 to 25.242°.
Reflections collected	5605
Independent reflections	3709 [R(int) = 0.039]
Completeness to theta = 25.242°	99.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5605 / 72 / 362
Goodness-of-fit on F^2	1.021
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.0722
R indices (all data)	R1 = 0.0751, wR2 = 0.0857
Extinction coefficient	n/a
Largest diff. peak and hole	1.116 and -1.052 e.Å^{-3}

Table 31. Selected bond lengths [Å] for shelx_arun191015.

Hg1—Se1	2.4549 (6)	C13—C14	1.370 (9)
Hg1—Se2	2.4519 (7)	C13—H13	0.87 (5)
Se1—C19	1.927 (5)	C14—C15	1.361 (9)
Se2—C12	1.922 (6)	C14—H14	0.94 (7)
O3—C8	1.237 (6)	C5—H5	0.87 (6)
N3B—H3B	0.8600	C20—H20A	0.9700
N3B—C8	1.37 (3)	C20—H20B	0.9700
N3B—C1B	1.47 (3)	C20—C21	1.356 (11)
O2—N1	1.217 (7)	C21—H21A	0.9700
C8—C2	1.496 (7)	C21—H21B	0.9700
C8—N3A	1.29 (2)	C21—C11	1.246 (11)
C3—C2	1.388 (7)	C11—H11A	0.9600
C3—C4	1.372 (7)	C11—H11B	0.9600
C3—H3	0.92 (5)	C11—H11C	0.9600
C2—C19	1.388 (7)	C1A—H1AA	0.9700
O9—C1	1.210 (7)	C1A—H1AB	0.9700
C19—C6	1.385 (7)	C1A—C2A	1.46 (2)
N2—O7	1.205 (8)	C1A—N3A	1.46 (2)
N2—C15	1.470 (8)	C1B—H1BA	0.9700
N2—O8	1.204 (8)	C1B—H1BB	0.9700

C12—C17	1.383 (8)	C1B—C2B	1.52 (3)
C12—C13	1.387 (8)	C2A—H2AA	0.9700
N1—O1	1.212 (7)	C2A—H2AB	0.9700
N1—C4	1.470 (7)	C2A—C3AB	1.47 (3)
C6—C5	1.374 (9)	C2B—H2BA	0.9700
C6—H6	0.91 (6)	C2B—H2BB	0.9700
C4—C5	1.369 (8)	C2B—C3AA	1.41 (4)
C17—C16	1.388 (9)	C3AB—H3AA	0.9600
C17—C1	1.512 (8)	C3AB—H3AB	0.9600
N4—H4	0.8600	C3AB—H3AC	0.9600
N4—C1	1.285 (8)	C3AA—H3AD	0.9600
N4—C20	1.457 (8)	C3AA—H3AE	0.9600
C16—C15	1.366 (8)	C3AA—H3AF	0.9600
C16—H16	0.89 (6)	N3A—H3A	0.8600

Table 32. Selected bond angles [°] for shelx_arun191015.

Se2—Hg1—Se1	171.88 (2)	C14—C15—C16	122.0 (6)
C19—Se1—Hg1	99.96 (15)	N4—C20—H20A	108.7
C12—Se2—Hg1	97.25 (16)	N4—C20—H20B	108.7
C8—N3B—H3B	95.5	H20A—C20—H20B	107.6
C8—N3B—C1B	122 (3)	C21—C20—N4	114.3 (7)
C1B—N3B—H3B	99.4	C21—C20—H20A	108.7

O3—C8—N3B	122.9 (17)	C21—C20—H20B	108.7
O3—C8—C2	121.7 (5)	C20—C21—H21A	102.0
O3—C8—N3A	122.5 (13)	C20—C21—H21B	102.0
N3B—C8—C2	114.4 (17)	H21A—C21—H21B	104.7
N3A—C8—C2	115.2 (13)	C11—C21—C20	140.3 (13)
C2—C3—H3	121 (3)	C11—C21—H21A	102.0
C4—C3—C2	119.2 (6)	C11—C21—H21B	102.0
C4—C3—H3	120 (3)	C21—C11—H11A	109.5
C3—C2—C8	118.1 (5)	C21—C11—H11B	109.5
C19—C2—C8	122.3 (4)	C21—C11—H11C	109.5
C19—C2—C3	119.6 (5)	H11A—C11—H11B	109.5
C2—C19—Se1	123.2 (4)	H11A—C11—H11C	109.5
C6—C19—Se1	117.2 (4)	H11B—C11—H11C	109.5
C6—C19—C2	119.6 (5)	H1AA—C1A—H1AB	108.0
O7—N2—C15	118.9 (7)	C2A—C1A—H1AA	109.4
O8—N2—O7	122.9 (7)	C2A—C1A—H1AB	109.4
O8—N2—C15	118.2 (7)	N3A—C1A—H1AA	109.4
C17—C12—Se2	122.7 (4)	N3A—C1A—H1AB	109.4
C17—C12—C13	118.9 (5)	N3A—C1A—C2A	111.3 (15)
C13—C12—Se2	118.3 (5)	N3B—C1B—H1BA	109.3
O2—N1—C4	118.5 (6)	N3B—C1B—H1BB	109.3

O1—N1—O2	123.3 (6)	N3B—C1B—C2B	111.5 (19)
O1—N1—C4	118.2 (6)	H1BA—C1B—H1BB	108.0
C19—C6—H6	118 (4)	C2B—C1B—H1BA	109.3
C5—C6—C19	120.7 (6)	C2B—C1B—H1BB	109.3
C5—C6—H6	121 (4)	C1A—C2A—H2AA	108.6
C3—C4—N1	119.0 (6)	C1A—C2A—H2AB	108.6
C5—C4—C3	121.9 (5)	C1A—C2A—C3AB	115 (2)
C5—C4—N1	119.1 (5)	H2AA—C2A—H2AB	107.6
C12—C17—C16	119.6 (5)	C3AB—C2A—H2AA	108.6
C12—C17—C1	122.0 (6)	C3AB—C2A—H2AB	108.6
C16—C17—C1	118.4 (6)	C1B—C2B—H2BA	110.4
C1—N4—H4	117.6	C1B—C2B—H2BB	110.4
C1—N4—C20	124.7 (6)	H2BA—C2B—H2BB	108.6
C20—N4—H4	117.6	C3AA—C2B—C1B	106 (2)
C17—C16—H16	122 (4)	C3AA—C2B—H2BA	110.4
C15—C16—C17	119.5 (6)	C3AA—C2B—H2BB	110.4
C15—C16—H16	118 (4)	C2A—C3AB—H3AA	109.5
C12—C13—H13	119 (3)	C2A—C3AB—H3AB	109.5
C14—C13—C12	121.5 (7)	C2A—C3AB—H3AC	109.5
C14—C13—H13	120 (3)	H3AA—C3AB—H3AB	109.5
C13—C14—H14	121 (4)	H3AA—C3AB—H3AC	109.5

C15—C14—C13	118.4 (6)	H3AB—C3AB—H3AC	109.5
C15—C14—H14	120 (4)	C2B—C3AA—H3AD	109.5
O9—C1—C17	119.7 (6)	C2B—C3AA—H3AE	109.5
O9—C1—N4	123.7 (6)	C2B—C3AA—H3AF	109.5
N4—C1—C17	116.5 (5)	H3AD—C3AA—H3AE	109.5
C6—C5—H5	117 (4)	H3AD—C3AA—H3AF	109.5
C4—C5—C6	118.9 (6)	H3AE—C3AA—H3AF	109.5
C4—C5—H5	124 (4)	C8—N3A—C1A	124 (2)
C16—C15—N2	119.3 (6)	C8—N3A—H3A	118.1
C14—C15—N2	118.7 (6)	C1A—N3A—H3A	118.1