STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 79 (2023)

Supporting information for article:

Competition of interactions and a new high-temperature phase of selenourea

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S1. Tables

Table S1 Crystallographic data of selenourea phases α and γ as a function of temperature.

		phase α	phase α	phase α	phase α	phase α
Temperature (K)		110	130	150	170	190
Formula weight		123.02	123.02	123.02	123.02	123.02
Wavelength (Å)		1.54184	1.54184	1.54184	1.54184	1.54184
Crystal system		trigonal	trigonal	trigonal	trigonal	trigonal
Space group		$P3_1$	$P3_1$	$P3_1$	$P3_1$	$P3_1$
Unit cell dimensions (Å,°)	*a*	15.1354(1)	15.14832(11)	15.16245(9)	15.17648(10)	15.1910(1)
	b	15.1354(1)	15.14832(11)	15.16245(9)	15.17648(10)	15.1910(1)
	c	12.9308(1)	12.93947(13)	12.94774(1)	12.95625(12)	12.9669(1)
	α	90	90	90	90	90
	β	90	90	90	90	90
	γ	120	120	120	120	120
Volume ($Å^3$)		2565.33(4)	2571.44(5)	2577.89(4)	2584.35(4)	2591.43(4)
Z/Z'		27/9	27/9	27/9	27/9	27/9
Calculated density (gcm^{-3})		2.150	2.145	2.140	2.134	2.128
Absorption coefficient (mm-1)		11.513	11.485	11.457	11.428	11.397
F(000)		1566	1566	1566	1566	1566
Crystal size (mm)		0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05
2θ-range for data collection (°)		6.744 to 144.822	6.738 to 144.804	6.732 to 144.704	6.726 to 144.414	6.718 to 144.91
Min/max indices: h, k, l		-18/16, -18/17, -14/13	-18/17, -18/18, -14/13	-16/18, -17/18, -13/14	-18/17, -18/18, -14/13	-18/17, -18/18, -14/13
Reflect. Collected/unique		6546/3849	6643/3884	7392/4445	7405/4459	6693/3945
Rint		0.0395	0.0322	0.0190	0.0195	0.0372
Data/restrains/parameters		3849/1/325	3884/1/326	4445/1/326	4459/1/326	3945/1/326
Goodness-of-fit on F2		1.123	1.118	1.126	1.106	1.084
Final *R*1/*wR*2 (I>2σ1)		0.0370/0.0995	0.0360/0.0979	0.0234/0.0650	0.0251/0.0686	0.0334/0.0921
*R*1/*wR*2 (all data)		0.0371/0.0996	0.0361/0.0980	0.0235/0.0650	0.0252/0.0687	0.0335/0.0922

Table S1 Continued. Crystallographic data of selenourea phases α and γ as a function of temperature.

		phase α	phase α	phase α	phase α	phase α
Temperature (K)		210	230	250	270	290
Formula weight		123.02	123.02	123.02	123.02	123.02
Wavelength (Å)		1.54184	1.54184	1.54184	1.54184	1.54184
Crystal system		trigonal	trigonal	trigonal	trigonal	trigonal
Space group		$P3_1$	$P3_1$	$P3_1$	$P3_1$	$P3_1$
Unit cell dimensions (Å,°)	*a*	15.2065(1)	15.2222(1)	15.23887(11)	15.2541(1)	15.2714(1)
	b	15.2065(1)	15.2222(1)	15.23887(11)	15.2541(1)	15.2714(1)
	c	12.9770(1)	12.9882(1)	12.99870(13)	13.0096(2)	13.0219(2)
	α	90	90	90	90	90
	β	90	90	90	90	90
	γ	120	120	120	120	120
Volume ($Å^3$)		2598.74(4)	2606.36(4)	2614.18(5)	2621.61(5)	2630.04(5)
Z/Z'		27/9	27/9	27/9	27/9	27/9
Calculated density (gcm^{-3})		2.122	2.116	2.110	2.104	2.097
Absorption coefficient (mm-1)		11.365	11.332	11.298	11.266	11.229
F(000)		1566	1566	1566	1566	1566
Crystal size (mm)		0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05
2θ-range for data collection (°)		6.712 to 144.914	6.706 to 144.576	6.698 to 144.696	6.692 to 144.616	6.684 to 144.898
Min/max indices: h, k, l		-18/16, -18/18, -14/13	-18/16, -18/18, -14/13	-18/18, -18/16, -14/13	-18/18, -18/16, -14/13	-12/15, -18/11, -13/11
Reflect. Collected/unique		6773/3970	6843/3976	6882/4004	6907/4032	3810/2709
Rint		0.0370	0.0312	0.0365	0.0358	0.0298
Data/restrains/parameters		3970/1/326	3976/1/326	4004/1/326	4032/1/326	2709/1/326
Goodness-of-fit on F2		1.127	1.089	1.089	1.042	1.059
Final *R*1/*wR*2 (I>2σ1)		0.0328/0.0949	0.0332/0.0900	0.0325/0.0897	0.0326/0.0894	0.0351/0.1011
*R*1/*wR*2 (all data)		0.0330/0.0950	0.0333/0.0901	0.0327/0.0899	0.0328/0.0896	0.0355/0.1015

Table S1 Continued. Crystallographic data of selenourea phases α and γ as a function of temperature.

		phase α	phase α	phase α	phase α	phase α
Temperature (K)		293	303	313	323	333
Formula weight		123.02	123.02	123.02	123.02	123.02
Wavelength (Å)		0.71073	1.54184	0.71073	0.71073	0.71073
Crystal system		trigonal	trigonal	trigonal	trigonal	trigonal
Space group		$P3_1$	$P3_1$	$P3_1$	$P3_1$	$P3_1$
Unit cell dimensions (Å,°)	*a*	15.2757(6)	15.2813(2)	15.2940(5)	15.3052(6)	15.3150(6)
	b	15.2757(6)	15.2813(2)	15.2940(5)	15.3052(6)	15.3150(6)
	c	13.0230(5)	13.0272(2)	13.0350(4)	13.0398(4)	13.0481(5)
	α	90	90	90	90	90
	β	90	90	90	90	90
	γ	120	120	120	120	120
Volume ($Å^3$)		2631.7(2)	2634.52(8)	2640.48(19)	2645.33(2)	2650.4(2)
Z/Z'		27/9	27/9	27/9	27/9	27/9
Calculated density (gcm^{-3})		2.113	2.094	2.089	2.090	2.086
Absorption coefficient (mm-1)		9.480	11.210	9.370	9.375	9.357
F(000)		1566	1566	1566	1566	1566
Crystal size (mm)		0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05
2θ-range for data collection (°)		6.178 to 58.112	6.68 to 144.332	6.152 to 57.988	6.152 to 58.014	6.148 to 57.972
Min/max indices: h, k, l		-18/20, -19/19, -17/16	-15/16, -18/14, -15/11	-20/20, -19/19, -17/17	-19/19, -20/20, -17/17	-20/20, -19/19, -17/17
Reflect. Collected/unique		18848/7257	7938/3791	28408/8231	28481/8247	28577/8258
Rint		0.0348	0.0327	0.0411	0.0391	0.0405
Data/restrains/parameters		7257/1/326	3791/1/326	8231/50/326	8247/107/326	8258/80/326
Goodness-of-fit on F2		1.092	1.074	1.081	1.047	1.055
Final *R*1/*wR*2 (I>2σ1)		0.0805/0.1312	0.0269/0.0745	0.0805/0.1309	0.0982/0.1626	0.0781/0.1341
*R*1/*wR*2 (all data)		0.1119/0.1428	0.0271/0.0749	0.1168/0.1436	0.1385/0.1788	0.1206/0.1493

Table S1 Continued. Crystallographic data of selenourea phases α and γ as a function of temperature.

		phase α	phase α	phase α	phase α
Temperature (K)		343	353	363	373
Formula weight		123.02	123.02	123.02	123.02
Wavelength (Å)		0.71073	0.71073	0.71073	0.71073
Crystal system		trigonal	trigonal	trigonal	trigonal
Space group		$P3_1$	$P3_1$	$P3_1$	$P3_1$
Unit cell dimensions (Å,°)	*a*	15.3269(7)	15.3389(7)	15.3505(7)	15.3619(8)
	b	15.3269(7)	15.3389(7)	15.3505(7)	15.3619(8)
	c	13.0553(5)	13.0642(6)	13.0706(6)	13.0768(6)
	α	90	90	90	90
	β	90	90	90	90
	γ	120	120	120	120
Volume ($Å^3$)		2655.99(3)	2662.0(3)	2667.3(3)	2672.5(3)
Z/Z'		27/9	27/9	27/9	27/9
Calculated density (gcm^{-3})		2.082	2.077	2.073	2.064
Absorption coefficient (mm-1)		9.337	9.316	9.298	9.257
F(000)		1566	1566	1566	1566
Crystal size (mm)		0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05	0.25·0.10·0.05
2θ-range for data collection (°)		6.144 to 57.936	6.138 to 58.076	6.134 to 58.04	6.124 to 57.956
Min/max indices: h, k, l		-20/20, -19/19, -17/17	-20/20, -19/19, -17/17	-20/20, -19/19, -17/17	-20/20, -19/19, -17/17
Reflect. Collected/unique		28565/8276	28618/8281	28681/8308	28736/8325
Rint		0.0410	0.0430	0.0438	0.0452
Data/restrains/parameters		8276/75/326	8281/61/326	8308/74/326	8325/93/326
Goodness-of-fit on F2		1.061	1.053	1.039	1.027
Final *R*1/*wR*2 (I>2σ1)		0.0782/0.1241	0.0757/0.1271	0.0754/0.1379	0.0746/0.1443
*R*1/*wR*2 (all data)		0.1235/0.1387	0.1260/0.1446	0.1310/0.1576	0.1364/0.1672

Table S1 Continued. Crystallographic data of selenourea phases α and γ as a function of temperature.

		phase γ	phase γ
Temperature (K)		383	393
Formula weight		123.02	123.02
Wavelength (Å)		0.71073	0.71073
Crystal system		trigonal	trigonal
Space group		$P3_121$	$P3_121$
Unit cell dimensions (Å,°)	*a*	8.8551(4)	8.8607(4)
	b	8.8551(4)	8.8607(4)
	c	13.0694(7)	13.0716(7)
	α	90	90
	β	90	90
	γ	120	120
Volume ($Å^3$)		887.50(8)	888.78(9)
Z/Z'		9/3	9/3
Calculated density (gcm^{-3})		2.072	2.069
Absorption coefficient (mm-1)		9.292	9.279
F(000)		522	522
Crystal size (mm)		0.25·0.10·0.05	0.25·0.10·0.05
2θ-range for data collection (°)		6.16 to 57.724	6.156 to 57.71
Min/max indices: h, k, l		-11/11, -11/11, -17/16	-11/11, -11/11, -17/16
Reflect. Collected/unique		6352/1414	6391/1422
Rint		0.0243	0.0244
Data/restrains/parameters		1414/0/57	1422/0/57
Goodness-of-fit on F2		1.061	1.024
Final *R*1/*wR*2 (I>2σ1)		0.0285/0.0547	0.0294/0.0542
*R*1/*wR*2 (all data)		0.0430/0.0593	0.0451/0.0593

Table S2 The distances of NH···Se and NH···N in selenourea phases α and γ.

	H11B···Se2^{i}	**N11···Se2^{i}**	**N11H11B ···Se2^{i}**	**H11A··· Se7^{ii}**	**N11··· Se7^{ii}**	**N11H11A··· Se7^{ii}**
373	2.7880	3.581(2)	160.62	3.1281	3.790(3)	136.67
363	2.7906	3.581(1)	160.13	3.1280	3.797(2)	136.32
353	2.7819	3.591(1)	159.61	3.1255	3.796(2)	136.54
343	2.7894	3.580(2)	160.20	3.1240	3.794(2)	136.48
333	2.7767	3.582(1)	161.36	3.1277	3.797(1)	137.50
323	2.7619	3.575(4)	158.19	3.1218	3.805(3)	133.45
313	2.7791	3.587(1)	159.35	3.1225	3.798(2)	134.84
303	2.7690	3.5827(5)	160.91	3.1226	3.8145(5)	135.57
293	2.7471	3.579(2)	160.38	3.1226	3.798(2)	138.32
290	2.7662	3.5907(8)	161.10	3.1290	3.8117(7)	135.65
270	2.7658	3.5927(5)	161.77	3.1269	3.8008(7)	136.92
250	2.7605	3.5896(5)	162.39	3.1243	3.8018(5)	137.35
230	2.7609	3.5881(6)	161.84	3.1260	3.7933(5)	136.16
210	2.7628	3.5901(6)	161.86	3.1153	3.7890(6)	136.89
190	2.7563	3.5832(5)	161.77	3.1204	3.7891(5)	136.30
170	2.7464	3.5743(4)	162.02	3.1224	3.7904(4)	136.22
150	2.7486	3.5741(4)	161.37	3.1227	3.7855(4)	135.63
130	2.7441	3.5716(6)	161.90	3.1115	3.7764(6)	135.85
100	2.7407	3.5690(6)	161.53	3.1024	3.7703(6)	135.99

(i) = y-x,1-x,0.667+z; (ii) =x,y,-1+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H12B···Se3	**N12···Se3**	**N12H12B···Se3**	**H12A···Se7^{ii}**	**N12···Se7^{ii}**	**N12H12A···Se7^{ii}**
373	2.7899	3.636(2)	164.63	3.0055	3.702(5)	139.48
363	2.7848	3.639(3)	163.93	3.0161	3.711(5)	139.32
353	2.7805	3.632(3)	163.29	3.0130	3.713(4)	140.17
343	2.7856	3.631(2)	164.22	3.0131	3.713(4)	138.78
333	2.7890	3.630(6)	165.58	2.9975	3.718(5)	139.97
323	2.7936	3.630(3)	166.35	3.0067	3.712(2)	138.11
313	2.7992	3.638(3)	165.35	3.0136	3.706(5)	137.79
303	2.7890	3.6307(5)	166.48	3.0189	3.7291(5)	137.57
293	2.7860	3.637(3)	165.85	3.0200	3.719(5)	139.48
290	2.7916	3.6323(9)	166.11	3.0125	3.7284(9)	137.06
270	2.7942	3.6342(6)	165.88	3.0189	3.7105(6)	138.93
250	2.7906	3.6300(6)	165.64	3.0148	3.7098(6)	139.34
230	2.7815	3.6218(6)	165.94	3.0251	3.7090(6)	137.98
210	2.7728	3.6118(6)	165.49	3.0132	3.7033(6)	138.73
190	2.7751	3.6148(5)	165.73	3.0088	3.6948(6)	138.22
170	2.7618	3.6015(4)	165.74	3.0061	3.6931(5)	138.33
150	2.7608	3.6006(5)	165.78	3.0085	3.6893(5)	137.59
130	2.7671	3.6073(6)	165.93	2.9944	3.6771(7)	137.80
110	2.7665	3.6055(6)	165.50	2.9882	3.6729(6)	138.03

(ii) = x,y,-1+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H21B···Se1^{ii}	**N21···Se1^{ii}**	**H21BN21···Se1^{ii}**	**H21A···Se5^{iii}**	**N21···Se5^{iii}**	**H21AN21···Se5^{iii}**
373	2.7334	3.605(2)	166.45	2.9101	3.736(5)	144.71
363	2.7341	3.602(2)	165.37	2.9121	3.750(3)	143.79
353	2.7363	3.601(2)	164.19	2.9121	3.744(8)	143.04
343	2.7384	3.592(3)	167.17	2.9187	3.740(6)	147.38
333	2.7398	3.586(8)	168.18	2.9139	3.747(2)	142.35
323	2.7348	3.585(3)	170.23	2.9120	3.758(6)	147.82
313	2.7359	3.581(2)	167.70	2.9164	3.746(2)	145.44
303	2.7340	3.5785(5)	167.53	2.9188	3.7423(5)	147.56
293	2.7199	3.577(2)	166.96	2.9190	3.738(2)	146.63
290	2.7377	3.5817(8)	167.35	2.9183	3.7387(8)	147.81
270	2.7315	3.5779(6)	168.28	2.9172	3.7316(6)	148.43
250	2.7321	3.5784(6)	168.30	2.9128	3.7238(6)	148.58
230	2.7263	3.5733(6)	168.59	2.9159	3.7166(6)	148.54
210	2.7132	3.5603(7)	168.60	2.9130	3.7150(6)	148.74
190	2.7128	3.5600(6)	168.66	2.9140	3.7055(6)	148.64
170	2.7140	3.5609(5)	168.49	2.9166	3.6987(4)	148.72
150	2.7080	3.5555(5)	168.77	2.9188	3.6929(5)	149.05
130	2.7108	3.5593(6)	169.28	2.9138	3.6831(6)	149.88
110	2.7047	3.5532(6)	169.22	2.9106	3.6793(6)	149.78

(ii) = x,y,-1+z; (iii) = x,y,1+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H22B···Se3	**N22···Se3**	**H22BN22···Se3**	**H22A···Se5^{iii}**	**N22···Se5^{iii}**	**H22AN22···Se5^{iii}**
373	2.7277	3.573(2)	173.20	2.7297	3.573(2)	145.76
363	2.7295	3.571(3)	170.64	2.7269	3.571(3)	144.35
353	2.7234	3.577(3)	171.97	2.7267	3.565(3)	143.48
343	2.7276	3.570(2)	171.42	2.7301	3.562(2)	148.63
333	2.7227	3.576(3)	167.35	2.7263	3.568(2)	144.05
323	2.7256	3.579(4)	166.91	2.7207	3.566(4)	150.77
313	2.7203	3.573(5)	166.83	2.7203	3.566(3)	149.48
303	2.7230	3.5862(5)	171.73	2.7217	3.5642(6)	155.93
293	2.7183	3.566(4)	169.68	2.7182	3.507(2)	153.15
290	2.7264	3.578(1)	170.79	2.7253	3.5610(9)	156.60
270	2.7248	3.5762(7)	170.70	2.7294	3.5426(6)	158.28
250	2.7266	3.5772(7)	170.27	2.7167	3.5322(6)	158.81
230	2.7270	3.5758(7)	169.40	2.7099	3.5267(6)	159.09
210	2.7277	3.5763(7)	169.31	2.7051	3.5240(7)	159.61
190	2.7106	3.5567(6)	168.17	2.7085	3.5239(6)	158.77
170	2.7112	3.5575(5)	168.25	2.6928	3.5101(5)	159.23
150	2.7120	3.5577(5)	167.99	2.6879	3.5061(5)	159.42
130	2.6994	3.5442(7)	167.62	2.6862	3.5054(6)	159.66
110	2.6897	3.5338(7)	167.34	2.6876	3.5072(6)	159.76

(iii) = x,+y,1+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H23B···Se2	**N23···Se2**	**H23BN23···Se2**	**H23A···Se6**	**N23···Se6**	**N23H23A···Se6**
373	2.7993	3.623(6)	158.40	2.9399	3.711(7)	153.82
363	2.7955	3.625(5)	157.51	2.9431	3.716(6)	154.22
353	2.7993	3.625(5)	156.73	2.9428	3.719(5)	154.80
343	2.7992	3.624(5)	156.50	2.9411	3.723(6)	153.88
333	2.8036	3.625(6)	155.79	2.9395	3.719(6)	153.41
323	2.8120	3.619(9)	152.85	2.9492	3.692(2)	155.46
313	2.8109	3.628(5)	154.93	2.9437	3.715(6)	153.80
303	2.8198	3.6253(5)	158.89	2.9300	3.7122(5)	152.15
293	2.8403	3.629(2)	153.22	2.9434	3.700(2)	154.78
290	2.8419	3.6255(9)	156.24	2.9424	3.7047(8)	152.17
270	2.8149	3.6290(6)	158.56	2.9417	3.7153(6)	150.66
250	2.8147	3.6274(6)	158.22	2.9416	3.7133(6)	150.31
230	2.8066	3.6155(6)	157.37	2.9483	3.7171(6)	149.85
210	2.7978	3.6124(7)	158.65	2.9444	3.7109(6)	149.45
190	2.7947	3.6073(6)	158.20	2.9485	3.7104(6)	148.71
170	2.7962	3.6077(5)	157.94	2.9421	3.7063(4)	149.07
150	2.7920	3.6034(5)	157.90	2.9420	3.7038(5)	148.68
130	2.7865	3.5978(6)	157.87	2.9419	3.7015(6)	148.35
110	2.7796	3.5935(7)	158.47	2.9454	3.6999(6)	147.53

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H13B···Se1	**N13···Se1**	**H13BN13···Se1**	**H13A···Se6**	**N13···Se6**	**H13AN13···Se6**
373	2.6938	3.513(7)	169.70	2.7138	3.546(8)	163.35
363	2.6909	3.512(7)	170.68	2.7107	3.547(7)	164.51
353	2.6965	3.516(7)	169.62	2.7190	3.553(7)	164.59
343	2.6955	3.514(6)	169.62	2.7130	3.553(7)	162.90
333	2.6870	3.517(7)	169.25	2.7176	3.558(7)	162.68
323	2.6822	3.511(5)	169.20	2.6943	3.543(5)	165.17
313	2.6835	3.514(8)	170.39	2.7128	3.544(9)	163.04
303	2.6835	3.5129(5)	169.65	2.7321	3.5580(5)	161.46
293	2.6691	3.519(2)	170.04	2.7314	3.545(5)	163.61
290	2.6759	3.5141(9)	169.09	2.7268	3.5514(8)	161.11
270	2.6705	3.5191(6)	169.23	2.7322	3.5520(6)	159.88
250	2.6683	3.5172(6)	169.43	2.7250	3.5442(6)	159.70
230	2.6694	3.5203(7)	170.42	2.7153	3.5383(6)	160.66
210	2.6628	3.5130(7)	170.05	2.7202	3.5375(6)	159.23
190	2.6587	3.5089(6)	170.08	2.7153	3.5313(6)	158.92
170	2.6510	3.5029(5)	170.98	2.7059	3.5222(5)	158.96
150	2.6503	3.5021(5)	170.88	2.7021	3.5172(5)	158.68
130	2.6547	3.5083(7)	171.98	2.6896	3.5065(6)	159.12
110	2.6471	3.4998(6)	171.40	2.6992	3.5109(6)	157.90

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H14B···Se6	**N14···Se6**	**H14BN14···Se6**	**H14A···Se3^{iv}**	**N14···Se3^{iv}**	**N14H14A···Se3^{iv}**
373	2.8600	3.613(7)	154.01	2.8147	3.607(4)	144.07
363	2.8606	3.607(3)	152.83	2.8188	3.608(2)	141.15
353	2.8585	3.615(2)	152.83	2.8191	3.605(2)	143.53
343	2.8618	3.627(2)	153.03	2.8155	3.605(3)	145.27
333	2.8618	3.627(2)	151.40	2.8189	3.602(6)	147.22
323	2.8620	3.628(3)	147.71	2.8242	3.596(5)	146.98
313	2.8617	3.628(3)	149.26	2.8143	3.602(5)	143.54
303	2.8546	3.6413(5)	152.88	2.8248	3.6024(5)	151.22
293	2.8483	3.636(2)	153.03	2.8196	3.605(2)	147.59
290	2.8562	3.635(9)	151.40	2.8298	3.6019(9)	150.27
270	2.8607	3.6378(6)	151.17	2.8078	3.5867(6)	151.44
250	2.8653	3.6347(6)	149.85	2.8083	3.5819(6)	150.50
230	2.8565	3.6271(7)	150.04	2.8073	3.5764(6)	149.73
210	2.8708	3.6383(7)	149.55	2.7902	3.5642(6)	150.53
190	2.8658	3.6315(6)	149.23	2.7883	3.5603(6)	150.20
170	2.8597	3.6267(5)	149.45	2.7767	3.5511(5)	150.59
150	2.8582	3.6231(4)	149.09	2.7743	3.5452(5)	149.98
130	2.8590	3.6241(7)	149.14	2.7585	3.5332(6)	150.62
110	2.8643	3.6265(7)	148.66	2.7494	3.5247(6)	150.71

(iv) = y-x,1-x,-0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H24A···Se9^{v}	**N24···Se9^{v}**	**N24H24A···Se9^{v}**	**H24B···Se5^{vi}**	**N24···Se5^{vi}**	**N24H24B···Se5^{vi}**
373	2.9746	3.621(2)	141.96	2.7865	3.560(2)	156.09
363	2.9762	3.618(2)	145.52	2.7880	3.562(5)	156.18
353	2.9690	3.616(2)	143.27	2.7839	3.565(6)	155.66
343	2.9735	3.613(2)	141.01	2.7824	3.562(6)	153.28
333	2.9701	3.611(2)	139.78	2.7858	3.569(2)	148.64
323	2.9770	3.625(2)	141.67	2.7854	3.569(3)	144.11
313	2.9771	3.640(2)	142.77	2.7882	3.562(2)	150.50
303	2.9707	3.6354(5)	136.82	2.7838	3.5669(5)	152.14
293	2.9697	3.636(7)	136.77	2.7844	3.574(2)	148.05
290	2.9694	3.6384(9)	137.30	2.7958	3.5741(9)	151.30
270	2.9693	3.6384(6)	136.13	2.7975	3.5700(6)	150.29
250	2.9520	3.6322(6)	137.43	2.8018	3.5719(6)	149.88
230	2.9473	3.6333(6)	138.11	2.7960	3.5693(6)	150.43
210	2.9370	3.6199(6)	137.73	2.7981	3.5647(7)	149.30
190	2.9382	3.6227(6)	137.92	2.8058	3.5704(6)	148.97
170	2.9401	3.6207(4)	137.46	2.8040	3.5678(5)	148.83
150	2.9308	3.6168(4)	138.10	2.7980	3.5678(7)	148.62
130	2.9330	3.6150(6)	137.61	2.8035	3.5635(6)	148.23
110	2.9267	3.6078(6)	137.49	2.8191	3.5737(6)	147.38

(v) = 1-y,1+x-y,0.333+z; (vi) = 1-y,x-y,0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H15B···Se4^{vi}	**N15···Se4^{vi}**	**N15H15B···Se4^{vi}**	**H15A···Se8^{vii}**	**N15···Se8^{vii}**	**N15H15A···Se8^{vii}**
373	2.7933	3.606(5)	160.65	3.0804	3.749(6)	145.18
363	2.7872	3.600(5)	160.78	3.0839	3.753(2)	143.80
353	2.7939	3.606(4)	160.50	3.0857	3.742(5)	143.47
343	2.7715	3.598(5)	161.77	3.0850	3.741(6)	143.46
333	2.7703	3.596(5)	161.53	3.0859	3.748(6)	142.92
323	2.7595	3.584(9)	161.19	3.0882	3.745(2)	147.30
313	2.7774	3.604(5)	161.64	3.0866	3.753(6)	143.51
303	2.7998	3.6032(6)	159.15	3.0820	3.7562(5)	141.90
293	2.7381	3.596(6)	161.08	3.0710	3.751(2)	143.96
290	2.7845	3.5891(8)	159.40	3.0748	3.7504(9)	142.06
270	2.7882	3.5905(6)	158.91	3.0842	3.7495(6)	140.85
250	2.7835	3.5866(6)	158.09	3.0849	3.7466(6)	140.45
230	2.7852	3.5906(6)	157.57	3.0771	3.7385(6)	139.40
210	2.7862	3.5871(6)	157.62	3.0887	3.7441(7)	138.73
190	2.7815	3.5820(6)	155.53	3.0814	3.7366(6)	138.69
170	2.7764	3.5791(5)	154.98	3.0710	3.7248(4)	137.92
150	2.7804	3.5817(5)	155.70	3.0726	3.7236(5)	137.21
130	2.7795	3.5824(6)	156.03	3.0639	3.7151(6)	136.22
110	2.7849	3.5823(7)	154.91	3.0655	3.7171(6)	135.99

(vi) = 1-y,x-y,0.333+z; (vii) = 1-y,1+x-y,-0.667+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H25A···Se8^{vii}	**N25···Se8^{vii}**	**N25H25A···Se8^{vii}**	**H25B···Se6**	**N25···Se6**	**N25H25B···Se6**
373	3.0045	3.686(4)	141.53	2.8069	3.631(3)	167.32
363	3.0045	3.682(3)	140.98	2.8016	3.636(3)	167.37
353	3.0044	3.696(3)	140.20	2.8007	3.622(3)	166.19
343	3.0071	3.691(3)	140.61	2.8010	3.636(3)	167.65
333	3.0009	3.692(4)	140.24	2.8045	3.632(4)	167.46
323	3.0001	3.691(2)	144.08	2.8045	3.637(8)	171.55
313	3.0005	3.692(4)	140.26	2.8027	3.637(4)	167.58
303	3.0013	3.6890(5)	138.42	2.8071	3.6334(5)	161.64
293	3.0055	3.684(6)	141.03	2.8024	3.641(6)	169.47
290	2.9910	3.6804(9)	138.61	2.8163	3.6422(9)	161.54
270	2.9847	3.6679(6)	137.85	2.8182	3.6427(6)	161.14
250	2.9810	3.6611(6)	137.45	2.8180	3.6421(6)	161.05
230	2.9819	3.6572(6)	136.88	2.8107	3.6338(6)	160.78
210	2.9733	3.6488(7)	136.90	2.8073	3.6292(7)	160.47
190	2.9599	3.6362(6)	136.97	2.8036	3.6349(6)	160.31
170	2.9723	3.6426(5)	136.28	2.8094	3.6216(5)	160.53
150	2.9662	3.6351(5)	136.09	2.8014	3.6223(5)	160.21
130	2.9523	3.6203(7)	135.97	2.8037	3.6262(6)	160.62
110	2.9426	3.6123(4)	136.39	2.8043	3.6268(5)	160.48

(vii) = 1-y,1+x-y,-0.667+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H16B···Se5	**N16···Se5**	**N16H16B···Se5**	**H16A^{viii}···Se2**	**N16···Se2^{viii}**	**N16H16A···Se2^{viii}**
373	2.8015	3.601(2)	162.53	2.9712	3.740(4)	153.31
363	2.7912	3.608(2)	161.69	2.9798	3.730(5)	152.96
353	2.7895	3.599(3)	161.30	2.9797	3.731(4)	152.06
343	2.7738	3.597(3)	161.38	2.9781	3.740(6)	152.01
333	2.7689	3.595(4)	161.61	2.9749	3.742(2)	151.30
323	2.7847	3.596(5)	160.19	2.9769	3.742(6)	150.79
313	2.7753	3.585(3)	159.98	2.9749	3.744(2)	151.61
303	2.7620	3.5725(5)	160.07	2.9775	3.7416(5)	150.10
293	2.7789	3.571(5)	159.01	2.9736	3.742(2)	151.49
290	2.7469	3.5659(8)	159.68	2.9702	3.7436(8)	149.98
270	2.7510	3.5718(6)	160.14	2.9782	3.7391(5)	149.59
250	2.7460	3.5681(6)	160.48	2.9740	3.7327(6)	149.23
230	2.7508	3.5719(6)	160.21	2.9667	3.7262(6)	148.35
210	2.7407	3.5634(6)	160.62	2.9821	3.7321(6)	147.88
190	2.7395	3.5609(5)	160.29	2.9757	3.7274(5)	147.14
170	2.7385	3.5589(5)	160.03	2.9802	3.7254(4)	146.15
150	2.7372	3.5580(5)	160.13	2.9805	3.7220(4)	145.60
130	2.7263	3.5465(6)	159.96	2.9853	3.7249(6)	145.34
110	2.7206	3.5438(6)	160.79	2.9891	3.7237(6)	144.82

(viii) = 2-y,1+x-y,0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H26A···Se2^{viii}	**N26···Se2^{viii}**	**N26H26A···Se2^{viii}**	**H26B···Se4**	**N26···Se4**	**N26H26A···Se4**
373	2.7135	3.557(2)	156.12	2.6620	3.537(5)	167.58
363	2.7205	3.554(3)	157.27	2.6615	3.538(5)	168.28
353	2.7160	3.544(2)	156.75	2.6722	3.538(3)	168.03
343	2.7159	3.545(3)	157.32	2.6701	3.538(5)	168.86
333	2.7160	3.5352(4)	157.39	2.6591	3.539(5)	169.89
323	2.7120	3.531(6)	157.27	2.6601	3.538(7)	169.02
313	2.7147	3.531(3)	156.84	2.6586	3.535(4)	168.36
303	2.7117	3.5306(5)	159.61	2.6756	3.5303(5)	170.65
293	2.7202	3.537(5)	158.81	2.6765	3.533(6)	168.23
290	2.7162	3.533(8)	159.19	2.6746	3.5278(9)	171.72
270	2.7097	3.5259(6)	158.96	2.6831	3.5351(6)	171.00
250	2.7109	3.5245(6)	158.33	2.6759	3.5273(6)	170.66
230	2.7000	3.513396)	158.26	2.6769	3.5291(6)	171.13
210	2.7023	3.5103(6)	157.05	2.6724	3.5239(7)	170.72
190	2.6984	3.5055(5)	156.84	2.6695	3.5215(6)	171.01
170	2.6968	3.5015(4)	156.33	2.6701	3.5220(5)	171.00
150	2.6984	3.5000(4)	155.68	2.6674	3.5187(5)	170.66
130	2.6956	3.4965(6)	155.51	2.6699	3.5202(6)	170.12
110	2.6977	3.4945(6)	154.58	2.6675	3.5196(6)	170.98

(viii) = 2-y,1+x-y,0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H17B^{viii}···Se7	**N17···Se7^{viii}**	**N17H17B···Se7^{viii}**	**H17A···Se5^{ix}**	**N17···Se5^{ix}**	**N17H17A···Se5^{ix}**
373	2.6509	3.511(5)	163.22	2.6311	3.504(5)	145.50
363	2.6517	3.514(5)	164.60	2.6382	3.504(4)	144.50
353	2.6473	3.512(5)	163.88	2.6306	3.505(5)	146.25
343	2.6461	3.513(5)	164.83	2.6381	3.487(8)	148.36
333	2.6501	3.514(5)	165.24	2.6210	3.499(4)	150.12
323	2.6482	3.511(5)	166.86	2.6324	3.502(8)	149.77
313	2.6464	3.5168(6)	165.96	2.6355	3.498(7)	149.90
303	2.6694	3.5190(5)	169.76	2.6342	3.4556(5)	157.76
293	2.6547	3.5190(5)	167.69	2.6217	3.459(5)	154.68
290	2.6547	3.5096(6)	170.21	2.6313	3.4455(8)	158.41
270	2.6536	3.5052(8)	169.38	2.6289	3.4459(6)	159.06
250	2.6523	3.5024(5)	169.78	2.6189	3.4363(6)	159.17
230	2.6552	3.5020(8)	168.73	2.6317	3.4470(6)	158.65
210	2.6489	3.5073(7)	169.18	2.6168	3.4340(6)	159.13
190	2.6484	3.5073(5)	168.66	2.6172	3.4373(5)	159.84
170	2.6476	3.4949(5)	168.63	2.6162	3.4382(4)	160.31
150	2.6428	3.4999(5)	168.54	2.6140	3.435894)	160.26
130	2.6478	3.4936(6)	168.01	2.6070	3.4275(6)	159.93
110	2.6375	3.4831(6)	168.03	2.6065	3.4260(6)	159.18

(viii) = 2-y,1+x-y,0.333+z; (ix) = 1+y-x,1-x,-0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H27A···Se5^{ix}	**N27···Se5^{ix}**	**N27H27A···Se5^{ix}**	**H27B···Se7^{viii}**	**N27···Se7^{viii}**	**N27H27B···Se7^{viii}**
373	3.6474	4.283(4)	124.06	2.6675	3.518(9)	162.59
363	3.6354	4.272(8)	124.82	2.6606	3.513(8)	163.31
353	3.6237	4.268(6)	124.12	2.6640	3.515(8)	164.96
343	3.6132	4.257(6)	125.51	2.6653	3.512(9)	165.68
333	3.5962	4.244(5)	126.48	2.6790	3.513(9)	166.58
323	3.5806	4.240(9)	127.75	2.6635	3.510(7)	167.36
313	3.5945	4.227(5)	126.08	2.6639	3.517(9)	168.71
303	3.5662	4.2137(6)	130.48	2.6661	3.5161(6)	169.96
293	3.5735	4.218(7)	128.13	2.6726	3.515(3)	166.75
290	3.5533	4.2017(9)	130.56	2.6748	3.5245(9)	169.82
270	3.5325	4.1903(6)	130.59	2.6704	3.5226(6)	171.12
250	3.5260	4.1826(6)	131.45	2.6707	3.5228(7)	171.10
230	3.5204	4.1739(7)	132.10	2.6685	3.5105(7)	171.01
210	3.5145	4.1699(7)	133.30	2.6624	3.5151(7)	171.41
190	3.5066	4.1624(6)	132.34	2.6705	3.5125(6)	171.02
170	3.5117	4.1655(5)	133.12	2.6566	3.5085(5)	170.95
150	3.5031	4.1584(5)	133.28	2.6538	3.5064(5)	171.34
130	3.4883	4.1443(6)	132.33	2.6552	3.5081(7)	171.51
110	3.4990	4.1499(6)	134.91	2.6480	3.5018(7)	171.38

(viii) = 2-y,1+x-y,0.333+z; (ix) = 1+y-x,1-x,-0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H18B···Se8^{vii}	**N18···Se8^{vii}**	**N18H18B···Se8^{vii}**	**H18A···Se4**	**N18···Se4**	**N18H18A···Se4**
373	2.6651	3.504(6)	165.33	3.0360	3.760(6)	149.15
363	2.6594	3.491(6)	162.92	3.0304	3.758(6)	148.04
353	2.6602	3.504(6)	167.05	3.0323	3.746(7)	150.37
343	2.6622	3.508(7)	164.27	3.0391	3.765(5)	146.30
333	2.6534	3.501(7)	164.92	3.0358	3.766(7)	150.08
323	2.6667	3.502(9)	167.87	3.0336	3.757(5)	147.21
313	2.6695	3.508(2)	165.33	3.0320	3.744(8)	148.78
303	2.6662	3.5018(5)	164.29	3.0299	3.7481(5)	146.80
293	2.6779	3.503(5)	167.67	3.0337	3.745(6)	144.74
290	2.6807	3.5060(9)	164.22	3.0334	3.7335(8)	143.02
270	2.6680	3.5039(6)	164.34	3.0355	3.7463(6)	143.12
250	2.6638	3.5019(6)	165.10	3.0380	3.7385(6)	142.07
230	2.6590	3.5004(6)	166.27	3.0319	3.7338(6)	140.24
210	2.6605	3.4997(6)	165.51	3.0290	3.7281(6)	139.89
190	2.6439	3.4833(6)	165.55	3.0314	3.7312(6)	139.98
170	2.6358	3.4764(5)	166.00	3.0280	3.7281(5)	140.00
150	2.6373	3.4799(5)	166.70	3.0165	3.7175(5)	140.11
130	2.6310	3.4755(6)	167.44	3.0070	3.7113(6)	140.53
110	2.6295	3.4722(6)	166.85	3.0065	3.7079(6)	140.41

(vii) = 1-y,1+x-y,-0.667+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H28A···Se4	**N28···Se4**	**N28H28A···Se4**	**H28B···Se8^{vii}**	**N28···Se8^{vii}**	**N28H28B···Se8^{vii}**
373	2.9228	3.712(7)	151.60	2.6267	3.490(7)	171.59
363	2.9460	3.719(7)	150.48	2.6213	3.468(7)	168.48
353	2.8549	3.712(6)	151.31	2.6298	3.476(6)	168.33
343	2.9179	3.717(8)	149.89	2.6217	3.483(6)	170.49
333	2.8799	3.720(6)	152.49	2.6250	3.481(6)	167.86
323	2.8399	3.714(7)	152.32	2.6216	3.474(7)	170.65
313	2.8589	3.713(6)	154.34	2.6235	3.474(3)	170.20
303	3.0047	3.7118(6)	149.87	2.6286	3.4715(6)	166.80
293	2.8880	3.714(7)	147.81	2.6254	3.470(4)	169.89
290	3.0072	3.7111(9)	146.46	2.6299	3.479(1)	165.44
270	2.9843	3.6960(7)	145.46	2.6279	3.4790(7)	166.16
250	2.9749	3.6869(6)	145.48	2.6298	3.4720(7)	166.54
230	2.9708	3.6813(7)	144.27	2.6265	3.4673(7)	166.06
210	2.9534	3.6682(7)	143.82	2.6257	3.4691(7)	167.01
190	2.9407	3.6594(6)	142.34	2.6281	3.4721/(6)	167.29
170	2.9278	3.6474(5)	142.44	2.6232	3.4672(5)	167.23
150	2.9170	3.6385(5)	142.67	2.6152	3.4601(5)	167.59
130	2.9020	3.6258(7)	142.97	2.6142	3.4591(7)	167.62
110	2.8890	3.6164(6)	143.35	2.6220	3.4665(7)	167.36

(vii) = 1-y,1+x-y,-0.667+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H19B···Se9^{v}	**N19···Se9^{v}**	**N19H19A···Se9^{v}**	**H19A···Se1^{iv}**	**N19···Se1^{iv}**	**N19H19A···Se1^{iv}**
373	2.6547	3.534(7)	165.74	2.8234	3.634(6)	155.66
363	2.6443	3.538(7)	163.68	2.8203	3.634(5)	154.16
353	2.6465	3.538(6)	163.20	2.8226	3.631(4)	153.14
343	2.6431	3.532(7)	165.30	2.8255	3.633(6)	154.95
333	2.6525	3.531(6)	164.28	2.8234	3.639(6)	154.54
323	2.6574	3.537(9)	159.40	2.8286	3.633(9)	150.50
313	2.6543	3.539(8)	163.98	2.8229	3.631(6)	153.20
303	2.6530	3.5232(5)	162.64	2.8275	3.6303(5)	156.06
293	2.6524	3.532(5)	162.37	2.8275	3.6230(8)	150.90
290	2.6510	3.5330(9)	160.78	2.8264	3.6221(8)	154.61
270	2.6462	3.5235(9)	161.82	2.8222	3.6199(6)	154.98
250	2.6442	3.5214(6)	161.81	2.8182	3.6162(6)	155.06
230	2.6434	3.5015(6)	162.01	2.8132	3.6088(6)	154.55
210	2.6414	3.4983(6)	161.71	2.8173	3.6016(6)	154.31
190	2.6474	3.4967(6)	162.37	2.8108	3.6067(6)	154.63
170	2.6502	3.4940(5)	163.71	2.7964	3.5970(5)	155.56
150	2.6486	3.4840(5)	164.20	2.7910	3.5921(5)	155.66
130	2.6453	3.4814(6)	164.43	2.7798	3.5818(6)	155.85
110	2.6415	3.4775(6)	164.37	2.7788	3.5789(6)	155.45

(iv) = y-x,1-x,-0.333+z; (v) = 1-y,1+x-y,0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H29A···Se1^{iv}	**N29···Se9^{iv}**	**N29H20A···Se9^{iv}**	**H29B···Se9^{v}**	**N29···Se9^{v}**	**N29H29B···Se9^{v}**
373	2.7722	3.595(8)	160.79	2.6568	3.523(9)	165.80
363	2.7833	3.601(8)	159.44	2.6520	3.528(9)	164.44
353	2.7716	3.590(8)	159.58	2.6538	3.521(7)	164.76
343	2.7902	3.602(8)	157.98	2.6530	3.515(8)	163.10
333	2.7685	3.584(8)	158.87	2.6511	3.516(8)	164.07
323	2.7774	3.591(2)	154.15	2.6529	3.514(3)	159.90
313	2.7827	3.590(9)	156.89	2.6550	3.514(8)	162.29
303	2.7888	3.6035(6)	158.68	2.6580	3.5016(5)	167.13
293	2.8079	3.599(2)	153.65	2.6598	3.501(2)	160.09
290	2.7965	3.5903(9)	156.24	2.6552	3.4964(9)	166.19
270	2.7720	3.5828(6)	157.75	2.6517	3.4953(6)	167.10
250	2.7725	3.5818(6)	157.40	2.6461	3.4891(6)	166.87
230	2.7690	3.5787(7)	157.50	2.6429	3.4861(6)	166.94
210	2.7659	3.5743(7)	157.20	2.6445	3.4870(6)	166.69
190	2.7690	3.5756(6)	156.82	2.6302	3.4727(6)	166.69
170	2.7692	3.5745(5)	156.52	2.6209	3.4623(5)	166.27
150	2.7601	3.5673(5)	156.93	2.6251	3.4673(5)	166.54
130	2.7658	3.5707(7)	156.44	2.6103	3.4529(7)	166.67
110	2.7706	3.5732(7)	155.97	2.6057	3.4475(6)	166.40

(iv) = y-x,1-x,-0.333+z; (v) = 1-y,1+x-y,0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	N16···H27A^{i}	**N16···N27^{i}**	**N23···H18A**	**N23···N18**	**N19···H14A**	**N19···N14**
373	2.6200	3.380(3)	2.9300	3.570(4)	2.8200	3.400(3)
363	2.6500	3.400(4)	2.9300	3.570(5)	2.7600	3.360(4)
353	2.6600	3.410(3)	3.0300	3.590(6)	2.7800	3.350(3)
343	2.6400	3.410(5)	2.9000	3.560(3)	2.8400	3.400(5)
333	2.6100	3.390(3)	2.9700	3.580(4)	2.8900	3.400(4)
323	2.6000	3.390(6)	2.9000	3.560(3)	2.8400	3.320(6)
313	2.6200	3.400(4)	2.9500	3.570(5)	2.8200	3.380(3)
303	2.5830	3.3650(9)	2.8610	3.479(2)	2.9600	3.4840(8)
293	2.6200	3.400(6)	2.8000	3.490(6)	2.9300	3.430(4)
290	2.5750	3.362(2)	2.7670	3.480(2)	2.9590	3.488(1)
270	2.5700	3.351(1)	2.7780	3.496(2)	2.9800	3.4980(9)
250	2.5600	3.343(1)	2.7740	3.493(6)	2.9760	3.5030(9)
230	2.5570	3.340(2)	2.7740	3.492(2)	2.9460	3.4800(9)
210	2.5470	3.332(1)	2.7670	3.487(3)	2.9680	3.491(1)
190	2.5590	3.3460(9)	2.7740	3.498(6)	2.9580	3.4820(9)
170	2.5520	3.3430(8)	2.7740	3.493(2)	2.9560	3.4720(7)
150	2.5490	3.338(2)	2.7700	3.489(2)	2.9430	3.4620(7)
130	2.5380	3.327(1)	2.7730	3.491(6)	2.9420	3.454(1)
110	2.5490	3.338(1)	2.7730	3.492(5)	2.9470	3.452(2)

(i) = 1-x+y,1-x,-0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H11B···Se1^{ii}	**N11···Se1^{ii}**	**N11H11B···Se1^{i}**	**H11A···Se2^{i}**	**N11···Se2^{i}**	**N11H11A···Se2^{i}**
393	2.7907	3.6324(6)	166.49	3.1212	3.7945(6)	135.70
383	2.7811	3.6221(6)	166.20	3.1209	3.7952(6)	135.82

(i) = 1-y,1+x-y,0.333+z; (ii) = -y,x-y,0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H22B···Se2^{i}	**N22···Se2^{i}**	**N22H22B···Se2^{i}**	**H22A···Se1^{ii}**	**N22···Se1^{ii}**	**N22H22A···Se1^{ii}**
393	2.7765	3.5795(6)	156.04	2.9142	3.6987(6)	152.55
383	2.7620	3.5679(6)	156.64	2.9253	3.7026(6)	151.27

(i) = 1-y,1+x-y,0.333+z; (ii) = -y,x-y,0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H21B···Se2^{i}	**N21···Se2^{i}**	**N21H21B···Se2^{i}**	**H21A···Se1^{ii}**	**N21···Se1^{ii}**	**N21H21A···Se1^{ii}**
393	2.6764	3.5135(6)	164.79	2.9969	3.7678(4)	150.25
383	2.6789	3.5127(6)	163.70	3.0143	3.7732(3)	148.31

(i) = 1-y,1+x-y,0.333+z

Table S2 Continued. The distances of NH···Se and NH···N in selenourea phases α and γ.

	H21A···N11	**N21···N11**	**H11B···N22^{i}**	**N11···N22^{i}**	**H22A···N22^{ii}**	**N22···N22^{ii}**
393	2.9800	3.501(2)	3.1790	3.620(3)	3.0030	3.521(3)
383	2.9710	3.500(1)	3.1730	3.619(5)	3.0000	3.517(5)

(i) = -y,x-y,0.333+z; (ii) = -x,-x+y,0.333-z

S2. Figures

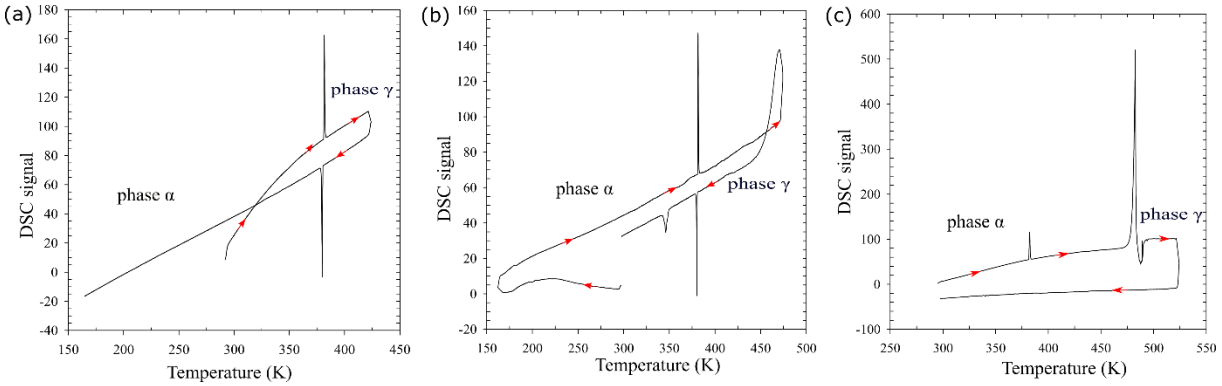

Figure S1 Differential scanning calorimetry (DSC) signal for selenourea at ambient pressure: (a) the heating and cooling runs below 425 K; (b) the sample heated up to the onset of melting and cooled down through the γ-α transition – a small exothermal signal about 340 K is associated with a product of the partial decomposition of $SeC(NH_2)_2$ at the m.p.; (c) the heating run through the α-γ transition, the sample melting at 473 K and fully decomposing just above the melting point as marked by the exothermic depression and absence of the freezing and γ-α endothermal signals on cooling.

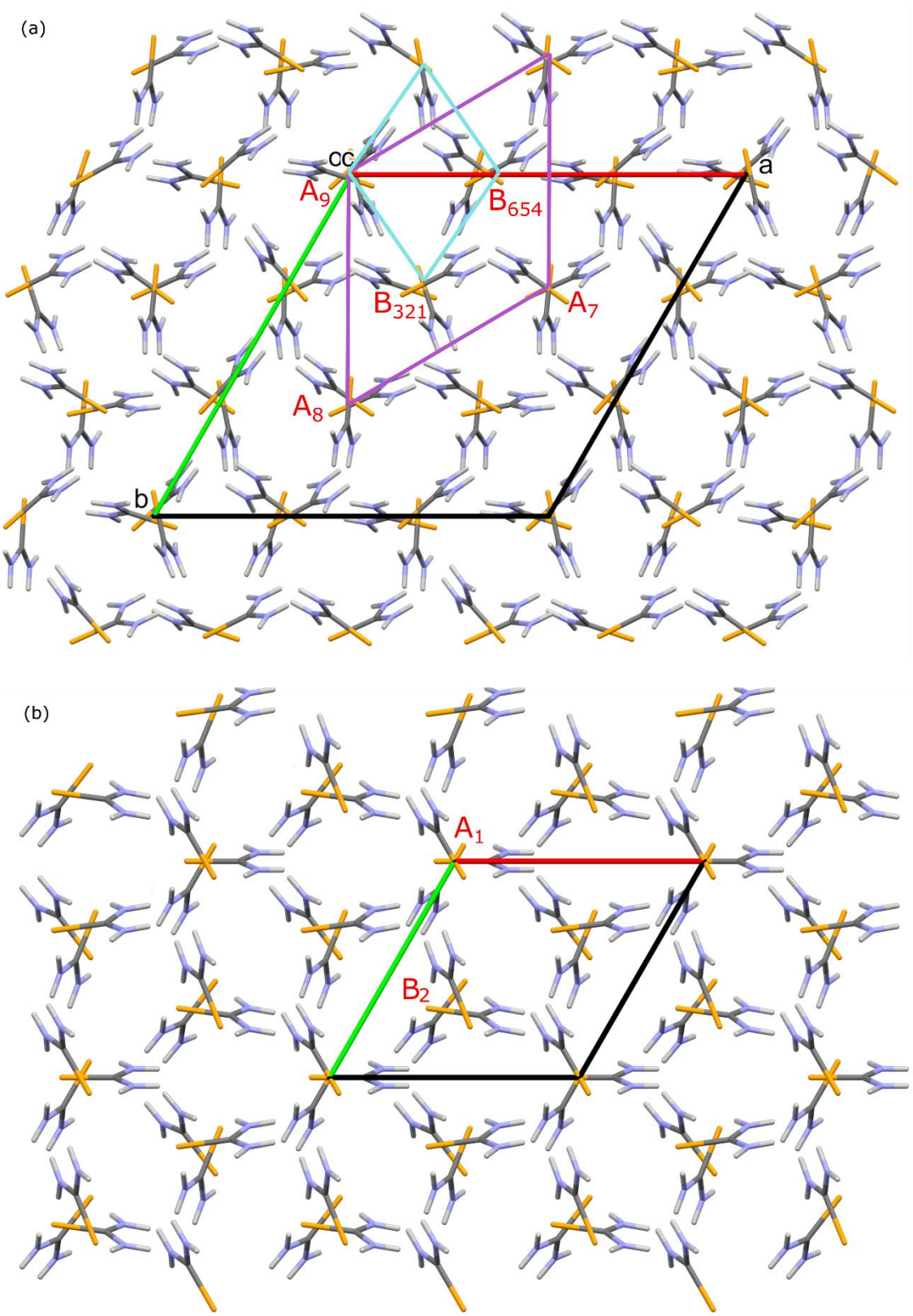

Figure S2 Crystal structure of selenourea phase (a) α and (b) γ projected down [z]. Note their orientation difference of 30° about [z] (*cf*. Figure 4 in the main article). Labels of helices (capital letters A-B in phase α and γ) and molecules (numbers 1-9 in phase α and γ) in phase α are indicated.

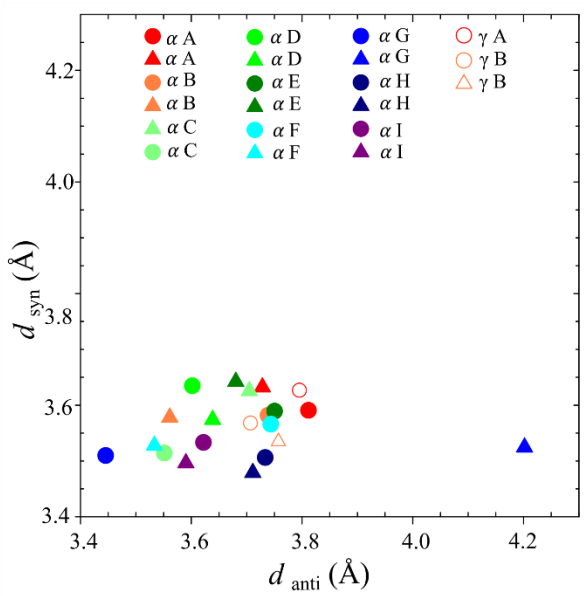

Figure S3 Correlation between the distances of intermolecular contacts of H-atoms in the *anti* and *syn* positions. Capital letters A-I for phase α and A-B for phase γ label the independent molecules. The contacts of H atoms at nitrogen atom N1 are indicates as circles and those at N2 as triangles.

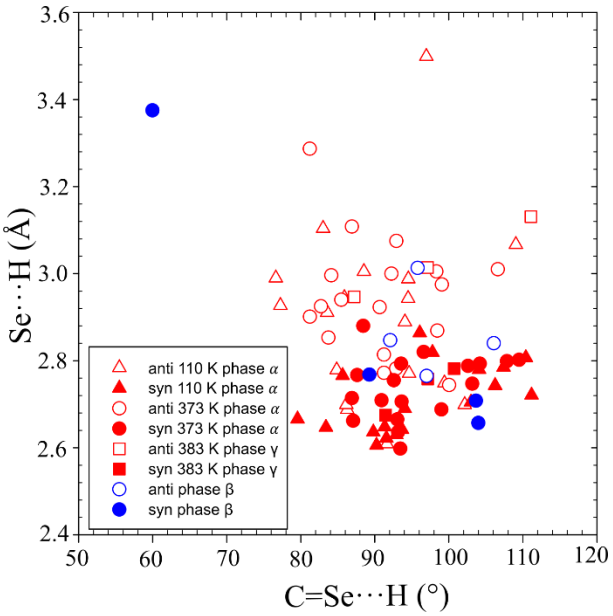

Figure S4 The distribution of Se···H distances in selenourea phases α and γ as a function of C=Se···H angles, plotted for the structures of phase α at 110 and 373 K, phase γ at 383 K (red symbols), as well as the high-pressure phase β at 0.21 GPa/296 K (blue symbols).

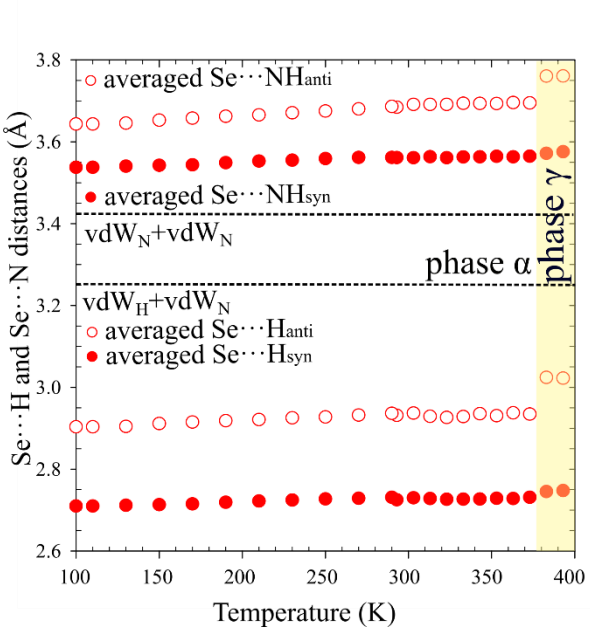

Figure S5 Averaged lengths of hydrogen bonds N-H_{syn}···Se and N-H_{anti}···Se in selenourea as a function of temperature.

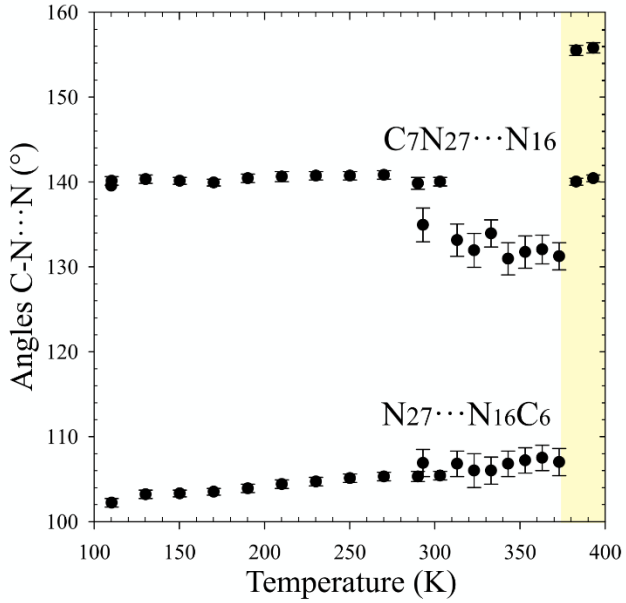

Figure S6 Angles C7N27···N16 and N27···N16C6 across hydrogen bond N27H27A···N16 in selenourea phase α (white background), and for the corresponding short contact in phase γ (yellow background).

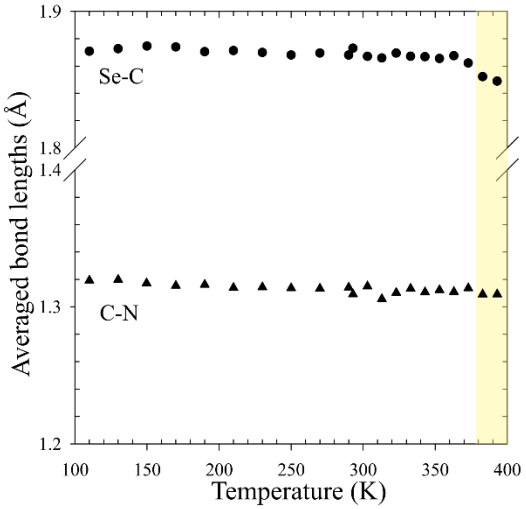

Figure S7 Averaged lengths of covalent bonds C-N (triangles) and C-Se (circles) in selenourea phases α and γ as a function of temperature. This plot illustrates the effect of thermally-induced molecular vibrations for the 'riding model' (Cruickshank, 1961), significantly shortening the averaged bond lengths in phase γ.