Supporting Information

The Prodigious Hydrogen Bonds with Sulfur and Selenium in Molecular Assemblies, Structural Biology and Functional Materials

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The rise of S/SeCHBs: Milestones and Methods

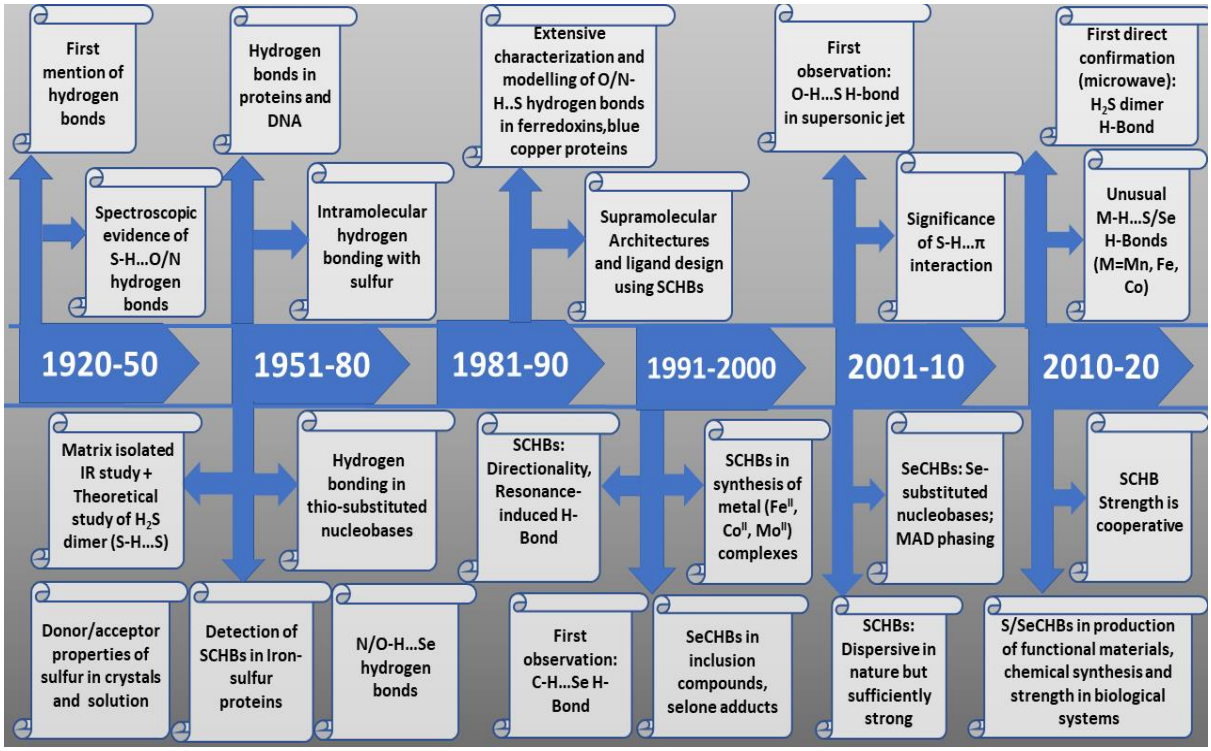


Figure S1: Schematic timeline of evolution of significant events relating to sulfur/selenium centered H-bonds (S/SeCHBs)[1–67]*, ranging from explorations on the unique nature and occurrence of these H-bonds*[3,21–26,68–71] *to their applicability in engineered natural systems as well as materials.(see main text for references)*

The significant milestones enunciated above have been achieved through an arsenal of techniques perfected over the years by the researchers working in this arena. It is interesting to have an idea of the methods and the model complexes that were employed to answer the *critica quaestiones* pertaining to the nature of various kinds of S/SeCHBs, as detailed in Fig S2 and Table S1.

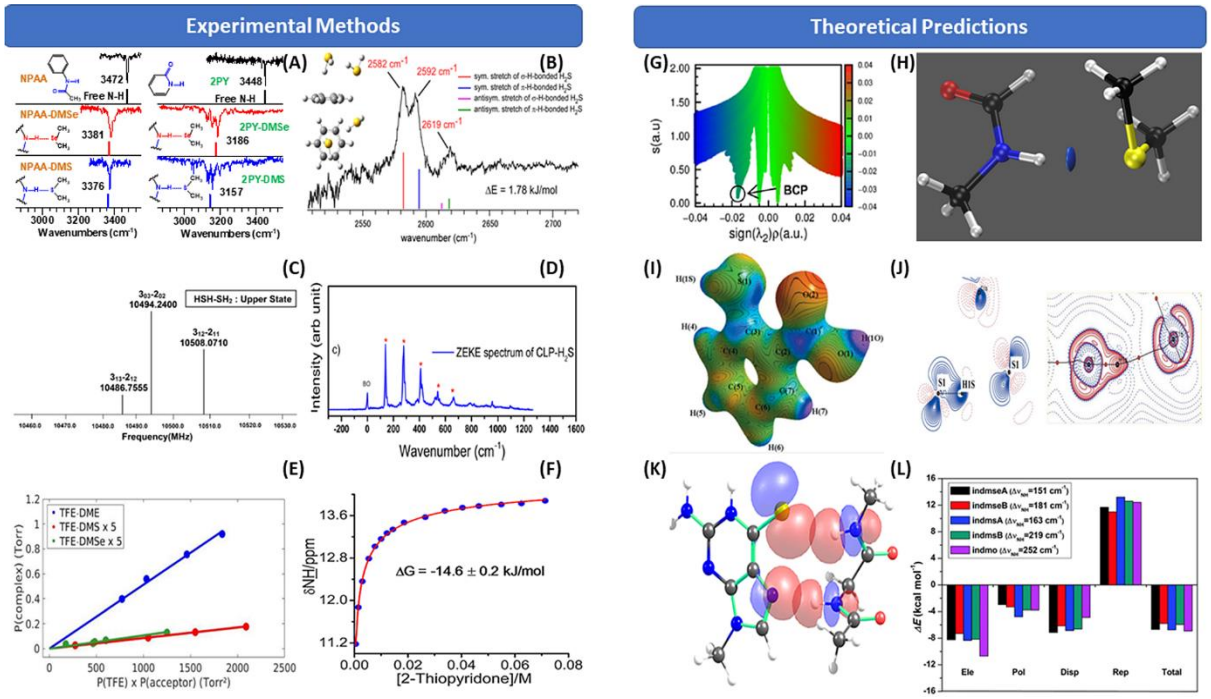


Figure S2: Graphical Representation of the communion of various methodologies adopted for detection and prediction of H-bonds with sulfur and selenium: (A) Gas phase resonant ion-dip infrared (RIDIR) spectra of N-phenylacetamide (NPAA) and pyridone (2PY) and their complexes with dimethyl sulphide (DMS) and dimethylselenide (DMSe) to probe N-H···S and N-H···Se H-bond , respectively. Reproduced with permission from ref.[56] *Copyright (2017) American Chemical Society. (B) Benzene-$(H_2S)_n$ clusters subjected to electronic (resonant two-photon ionization combined with mass spectrometry) and ionization depletion IR spectra for probing S-H···π interactions. Reproduced with permission from ref.*[72] *Copyright (2019) American Chemical Society., (C) Fourier Transform Microwave spectroscopy of H_2S dimer and several isotopomers for evidence of S-H···S hydrogen bonds by study of Ka = 1 transitions. Reproduced with permission from ref.*[59]*, Copyright (2018) Wiley Publishers., (D) High-Resolution Zero Kinetic-Energy Photoelectron-Spectroscopy (ZEKE-PE) spectra of p-chlorophenol-H_2S complex for determination of O-H···S H-bond dissociation energy. Adapted with permission from ref.*[70] *Copyright (2015) American Chemical Society. (E) Gibbs Energy determination at room level for -O-H•••O/S/Se H-bond formation in alcohol-dimethylselenide complex - The figure shows pressure of the complex versus the product of the donor and acceptor pressures, for complexes with TFE donor. Reproduced with permission from ref.*[62] *Copyright (2019) American Chemical Society. (F) Thioamide-N-H···S H-bonds in solution investigated through concentration dependent NMR spectroscopy. Reproduced with permission from ref.*[57] *Copyright (2017) American Chemical Society., (G) Electron density topology analysis through plot of reduced density gradient against*

the sign of the second eigenvalue of the electron-density Hessian matrix for the $Fe(CO)_4H_2$···DMS dimer to study Fe-H···S H-bond. Reproduced with permission from ref.[73] *Copyright (2019) American Chemical Society. (H) N-H···S H-bonds in NMFA-DMS complexes as revealed by colored isosurfaces of the reduced electron density gradient (3D-NCI-plot), following the NCI-plot topological analysis of the electron density at the MP2/aug-cc-pVDZ. Reproduced with permission from ref.*[51] *Copyright (2015) American Chemical Society. (I) Electrostatic potential plot drawn at an isosurface of 0.074 a.u. for S-H···S H-bond in 2-mercaptobenzoic acid and its (J) 2D deformation density and Laplacian plot of the interaction region. Reproduced with permission from ref.*[74] *Copyright (2017) International Union of Crystallography. (K) The plots of donor-acceptor interacting natural bond orbitals (NBO) i.e. overlap of p-type sulfur/oxygen/nitrogen lone pair and N-H σ* for the amide-N-H···S=C H-bond complex of 6-thioguanosine monophosphate (6-thio-GMP) and NUDT15 (PDB-5LPG). Reproduced with permission from ref.*[57] *Copyright (2017) American Chemical Society. (L) Contribution of different components of interaction energy (Electrostatics, polarisation, dispersion, repulsion) in various complexes of indole conformers, as obtained from SAPT analysis. Adapted with permission from ref.*[75] *Copyright (2017) Royal Society of Chemistry.*

Probing the Nature and Strength of S/SeCHBs

It has been established that the strength of conventional hydrogen bonds (with nitrogen/oxygen as donor and acceptor) varies between 4-15 kcal/mol (16.74 kJ/mol-62.76 kJ/mol). These depend on the type of model systems studied. From various studies[17,18,23,24,51,56,57,73,76–78], it has been proved that the strength of S/SeCHBs and conventional H-bonds in similar systems are comparable.

Table S1: Model Systems and Methodologies

(The absolute values of various energies (corrected for BSSE and/or ZPE, wherever applicable) have been indicated within parenthesis. The given range of values are considered from calculations from different levels of theory/conformations/environment/intra or inter-H-bonding modes. Wherever possible, the corrected energy values (e.g BSSE, ZPE) have been given)

Interaction	Systems Studied	Methods
N-H···S	Dimethylamine-dimethylsulfide[47], (3-methyl)Indole-Me_2S[23] (18.11-19.08 kJ/mol), N-methylformamide (NMFA)/N-	FTIRS, AIM, NBO, EDA, R2PI, FDIRS, NBO, Normal Coordinate Analysis

	phenylacetamide (NPAA)- Me_2S[51] (30-40 kJ/mol) Zinc enzyme model complex[33]	
O-H···S	*para*-cresol·Me_2S/MeSH/EtSh[77] (17.07-19.66 kJ/mol) , thiomalondialdehyde and thioacetylacetone derivatives[79] (40.0-42.1 kJ/mol), Alcohol-ethylene sulphide complex[80] (20.2-27.2 kJ/mol)	R2PI, FDIRS, AIM, EDA (KR, NVS, NEDA), NBO, Ab-initio, Gas phase FTIR
C-H···S	Complexes of 1,2,4,5-tetracyanobenzene with various sulfur containing solvents[81] (5.73-27.82 kJ/mol) CH_4 /C_2H_4 /C_2H_2···SH_2[82] 2,3-thienyl- and phenyl- or 2,3-dithienyl-substituted propenoic acid aggregates[83] (9.6-9.8 kJ/mol)	LIF, FDIR spectroscopy, Ab-initio Ab-initio, DFT, AIM IR spectroscopy, Ab-initio
S-H···O	H_2S-MeOH dimer[21] (6.65-14.06 kJ/mol), H_2S-Et_2O/Bu_2O/1,4-dioxane complex[71] (0.5 kJ/mol -17.70 kJ/mol), thiomalondialdehyde and thioacetylacetone derivatives[79] (20.3-25.4 kJ/mol) 3-mercaptopropionic acid[26]	Ab-initio, vibrational energy analysis IR Predissociation and VUV spectroscopy Microwave spectroscopy, AIM, NBO
S-H···N	Thiolimin tautomers of thioaminoacrolein[42] (16.08 kJ/mol-27.19 kJ/mol), H_2S: ammonia/aliphatic amines complex[43](7.37- 15.72 kJ/mol)	High-level ab-initio, NBO, AIM
S-H···S	Ethane-1,2-dithiol[84], 2 and 3-mercaptobenzoic acid[74] (9.1, 6.9 kJ/mol) Substituted (Z)-N-(Thionitrosomethylene)-thiohydroxylamine Systems (23.64 kJ/mol-31.35 kJ/mol) C_2H_4···H_2S and C_6H_5CCH···H_2S[45,85]	Electron Diffraction, X-ray diffraction, Multipole modelling, DFT DFT, NBO, AIM Microwave spectroscopy
S-H···π	[Benzene]-H_2S clusters[72]	IR, Electronic Spectroscopy

	Indole/3-methyl-indole- H_2S[76] (20.46 kJ/mol-21.63 kJ/mol) Cysteine SH-aromatic interactions (8.34-15.5[86])	FDIRS, R2PI, EDA PDB analysis, Ab-initio calculations
N-H···Se	Amine adducts of chiral selones[30], 2-pyridone/NPAA/NMFA- Me_2Se complex[56] (29.5-50.4 kJ/mol)	^1H-^{77}Se HMQC NMR, IR/UV double resonance spectroscopy, NBO, NCI
O-H···Se	p-substituted phenol-SeH_2 complexes[52,87] (4-15 kJ/mol (neutral), 32-57 kJ/mol (charged)) peri-substituted naphthalenes[88], selenosalicylaldehyde[89], Hydrated 6-selenoguanine tautomers[48] (28.62-47.28 kJ/mol) Alcohol-dimethylselenide complex[62], 2-(Methylseleno)ethanol[35]	NBO, NRT, QTAIM, DFT (B3LYP/6-311+G*), NICS, PDI, ATI, FTIR Spectroscopy
C-H···Se	Q_3CH···SeH_2 complex (Q =Cl, F, H)[60] (3.97-10.58 kJ/mol), Aldols of chiral N-acyl selones[34] Diselenocin[15]	NBO, AIM, Normal Mode analysis, ^1H-^{77}Se HMQC NMR and XRD, Solid Phase IR, ^1H NMR
Se-H···N	p-substituted pyridine-SeH_2 complexes[63](10-15 kJ/mol), 3-imino-propeneselenol[46] (39.35- 41.03 kJ/mol)	NBO, NRT, AIM
Se-H···O	Selenoacetic acid[90], Tautomer of hydrated 6-selenoguanine[48] (29.20-32.17 kJ/mol), 2-selenoformyl-3-thioxo-propionaldehyde[91] (5.71-11.77 kJ/mol)	FTIR, Raman, UV spectra, ^1H-^{77}Se NMR, Ab-initio, vibrational energy analysis, AIM, NBO
S-H···Se Se-H···S Se-H···Se	Selenal tautomer of 3-mercapto propeneselenal[92] (31.45-46.37 kJ/mol) Thial tautomer of 3-mercapto propeneselenal[92] (31.69-45.87 kJ/mol) Selenophenol[53] (3.2 kJ/mol)	TD-DFT, AIM, NBO

(FDIRS- fluorescence dip infrared spectroscopy, FTIR- Fourier Transform IR spectroscopy, R2PI - resonant two-photon ionization, LIF-Laser Induced Fluorescence, DFT- Density

Functional Analysis, AIM – Atoms-in-molecules theoretical calculations, NBO-Natural Bond Orbital Analysis, EDA- Energy Decomposition Analysis, NICS- Nucleus Independent Chemical Shifts, PDI- para delocalization index, NRT- Natural Resonance Theory)

Drug-Biomolecule Interactions

Table S2 : Interactions between approved sulfur-containing drugs with biomolecules

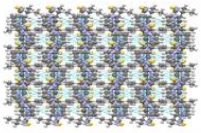
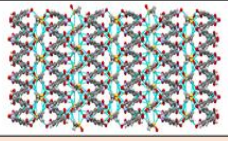
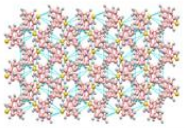
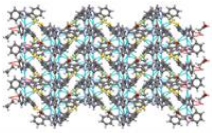
PDB ID	Drug	Biomolecule	Donor ··· Acceptor
1I2W	Cefoxitin	Beta-Lactamase from Bacillus Licheniformis BS3	CB_{ALA} ··· $S1_{1Q1}$ (Chain A, B)
1IYP	Cephalothin	Toho-1 Beta-Lactamase	CB_{PRO} ··· $S19_{CEP}$ (Chain A) CB_{ASN} ··· $S19_{CEP}$
2C5W	Cefotaxime	Penicillin-Binding Protein 1A(PBP-1A) (Acyl-Enzyme Complex) from Streptococcus Pneumoniae	CB_{TRP} ··· $S1_{CEF}$ (Chain A)
3VSL		Penicillin-Binding Protein 3 (PBP3) from Methicillin-resistant Staphylococcus aureus (MRSA)	CD_{PRO} ··· $S2_{CEF}$ (Chain A)
2ZQA		beta-lacta Toho-1 E166A/R274N/R276N triple mutant	CB_{PRO} ··· $S2_{CEF}$ (Chain A)
5NZY		(E-coli)	CB_{ASN} ··· S_{SO4}
5ZQD		DNA cross-link repair protein 1A	CG_{PRO} ··· $S1_{CE3}$ (Chain A)
		Penicillin-Binding Protein D2 from Listeria monocytogenes	$CE2_{PHE}$ ··· $S2_{CEF}$ (Chain A, B, C, E, G)
3Q1F	Piperacillin	CTX-M-9 S70G	CB_{LEU} ··· SAI_{YPP} (Chain B)
6I1G		TP domain from Chlamydia trachomatis Penicillin-Binding Protein 3	CB_{ASP} ··· S_{JPP} (Chain A)

4DKI 5TX9 5TXI 6G88	Ceftobiprole	PBP2A from Methicillin-resistant Staphylococcus aureus (MRSA) S. aureus penicillin binding protein 4 (PBP4) mutant (E183A, F241R) wild-type S. aureus penicillin binding protein 4 (PBP4) Enterococcus Faecium D63r Penicillin-Binding protein 5 (PBP5fm)	CB_{GLN} ··· SBE_{RB6} (Chain B) CB_{SER} ··· SAS_{RB6} (Chain A & B) CB_{SER} ··· SAS_{RB6} (Chain A & B) CG_{GLN} ··· SBE_{RB6} (Chain A, B & C) $CE2_{TYR}$ ··· SBE_{RB6} (Chain B)
4JF4 4N91	Meropenem	OXA-23 β-lactamase β-lactamase PenP_E166S	CB_{SER} ··· $S14_{MER}$ (Chain A & B) CB_{ALA} ··· SAK_{DWZ} (Chain B)
4ML1	Oxacillin	Class D β-lactamase OXA-1 K70D	$CZ2_{TRP}$ ··· SAR_{1S6} (Chain D)
4R1G	Cloxacillin	peptidoglycan glycosyltransferase from Atopobium parvulum	CB_{TYR} ··· $S1_{CFU}$ (Chain A & B)
4RA7 5TY2	Nafcillin	peptidoglycan glycosyltransferase from Atopobium parvulum S. aureus penicillin binding protein 4 (PBP4) mutant (E183A, F241R)	CB_{TYR} ··· $S1_{NXU}$ } Chain A CB_{SER} ··· SAS_{NFF}
5CGX 6PT5	Cefoxitin	Fox-4 cephamycinase mutant Y150F Class D Beta-lactamase OXA-48	$CE2_{PHE}$ ··· $S1_{1S7}$ } Chain A $CZ2_{TRP}$ ··· $S1_{1S7}$
5TB8, 5TBC	Lamivudine (Triphosphate)	Human DNA Polymerase Beta	CA_{PHE} ··· $S3'_{1RZ}$ (Chain A)
6G3V	Famotidine	Human carbonic anhydrase I	$CE1_{HIS}$ ··· S_{F09} (Chain B)
6I1F	Amoxicillin	TP domain from Chlamydia trachomatis Penicillin-Binding Protein 3	CB_{ASP} ··· $S4_{AXL}$ (Chain A & B)
6MKF	Imipenem	penicillin binding protein 5 (PBP5) from Enterococcus faecium	CG_{GLU} ··· S_{SO4} (Chain A)
6P54	Ceftriaxone	transpeptidase domain of PBP2 from Neisseria gonorrhoeae	CA_{GLY} ··· $S2_{CEF}$ (Chain B)

6UN1	Temocillin	Pseudomonas aeruginosa PBP3	$CE2_{TYR}$ ··· $S1_{TJ7}$ (Chain A)
4ACS	Azathioprine	Glutathione transferase (GST) A2-2	$SG2_{GSH}$ ··· $O(H)_{TYR}$

More examples of S/SeCHBs in crystal structures and their applications

Sulfur and selenium centered H-bonds have been exploited in crystal engineering for design of three-dimensional stacked, channel, interpenetrated and tubular architectures.[31,36,49,54,55,61,64,93] Some examples from the Cambridge Structural Database corresponding to several kinds of S/SeCHBs have been presented in Fig S3. This also includes attractive features like host-guest formations[16,94], layered packing features[28] and finite chain of cooperative/anti-cooperative H-bonds in co-crystals.[37] These can be particularly useful when such assembling of molecular units can be manipulated with an intention of targeting specific functionalities. For example, Thomas et al.[53] observed participation of S-H···S and Se-H···Se H-bonds in crystal structure organization (as seen in Fig S3(G) could lead to the formation of intriguing organic alloys of thiophenol and selenophenol. Another study shows the importance of the C-H···S H-bonds in the intersheet stability in crystals of Bis(ethylenedithio)tetrathiafulvalene (BDET-TTF)[29]; usually employed in the doping of superconducting materials as well as in development of organic light emitting diodes. Several S/SeCHBs are known to confer stability to metal complexes that are not only significant from their synthetic utility but also for optical/thermal properties.[58] This is illustrated by how complexes of iridium and rhodium with 2-aminoethanethiolate are known to yield dimeric structures bridged by triple S-H···S H-bonds. One of these H-bonds is converted to a covalent S-S disulphide bond on controlled oxidation, a feature that is being actively explored for creation of such coordination spheres in future.[65] It was also reported in a resonance Raman spectroscopic study of a synthesized dioxomolybdenum(VI) complex that the Mo^{VI}=O bond with the oxo groups could be stabilised by the *trans* effect of the two N-H···S H-bonded thiolate ligands.[95]As seen in thiolate complexes, nickel complexes with xanthate ions or ligands, like the complex (Et_4N)[N-(carbamoylmethyl)ethylxanthate)], often exhibit the presence of N-H···S as well as C-H···S H-bonds. This trait of sulfur in xanthates to act as H-bond acceptor, can be exploited to induce formation of its metal complexes.[39] Another excellent example of the usage of a combined N-H···S and C-H···S H-bonded interaction network was noted from a recent study by Ushakov et al.[96] on layered nanocrystals of MoS_2. The interlinking of the layers through the afore-mentioned H-bonds formed by alkyldiammonium ions was responsible for stability of these sheets.

(A) N-H···S	(B) O-H···S	(C) S-H···S	(D) C-H···S
			
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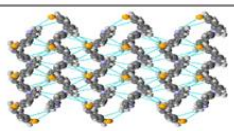	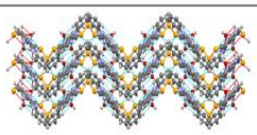	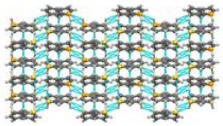	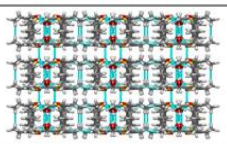
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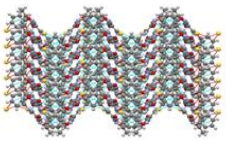	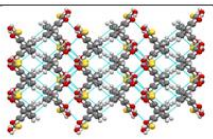	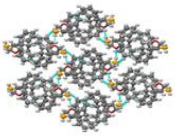	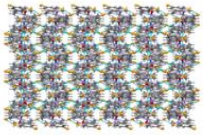
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Figure S3: Various types of supramolecular architectures like connected helices, stacked sheets, columns, host-guest structures, zig-zag/wavy ribbons, etc are sustained by different types of S/SeCHBs in crystal structures of (A) 5,5-dimethyldecahydro-3H-1,2,4-benzotriazepine-3-thione[97]*, (B) 4-nitrobenzoic acid dimethyl sulfoxide solvate*[66]*, (C) 1-(Hydrogen sulfido)-tetra-μH-nido-decaborane*[44]*, (D) bis(2-(1H-Benzimidazol-2-yl)phenyl)disulphide acetone solvate*[41]*, (E) 10H-phenoselenazine*[67]*, (F) 2,3-Dimethyl-4-(phenylseleno)phenol*[38]*, (G) organic alloy of benzenethiol and benzeneselenol*[53]*, (H) (selanyldicyclohex-1-ene-2,1-diyl)dimethanol*[98]*, (I) Ethyl (E)-3-anilino-2-cyano-3-mercaptoacrylate*[99]*, (J) 2-Hydroxythiobenzoic acid*[100]*, (K) 17-Oxapentacyclo[6.6.5.0^{2,7}.0^{9,14}.0^{15,19}]nonadeca-2,4,6,9,11,13-hexaene-1-selenol*[101]*, (L) trans-bis(2-(3-(Dimethylamino)propyliminomethyl)-4,6-dihydroselenophenolato-N,N',O)-zinc(ii)*[102]

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