

Appendix A

Supporting Information for

Effect of chelate ring and rigidity on Se...N interactions: A Computational Study

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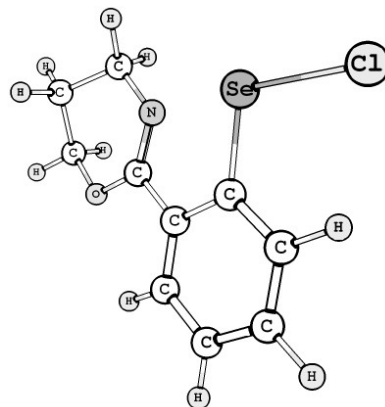
Table S1: Optimized geometries of compounds **1a-e**, **2a-e** and **3a-e** page 2 - 14

Figure S1: Molecular plots of compounds **1a-e**, **2a-e** and **3a-e** page 15 - 22

Table S1. Cartesian coordinates of the optimized geometries of **1a-e**, **2a-e** and **3a-e** (**a** = Cl, **b** = Br, **c** = I, **d** = SPh, **e** = CH₂Ph, Ph: Phenyl) computed at B3LYP/6-31G(d)/LanL2DZ level of theory. The LanL2DZ basis function is used for **c** = I compounds only.

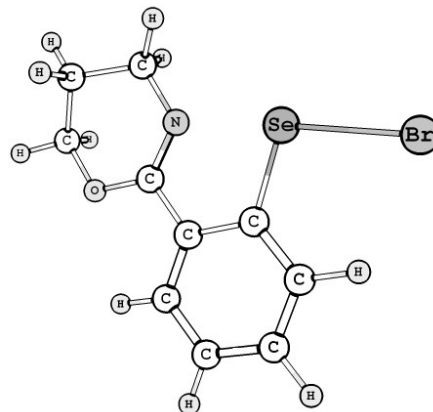
Optimized geometry of Se complex **1a**

7	1.259115000	-0.828745000	-0.097573000
6	1.510637000	0.438602000	-0.055779000
8	2.735095000	0.998885000	-0.033996000
6	3.854235000	0.103639000	-0.227478000
6	3.614714000	-1.233974000	0.461706000
6	2.308758000	-1.837315000	-0.065691000
1	4.715566000	0.636592000	0.179291000
1	3.997993000	-0.026900000	-1.307402000
1	3.546593000	-1.078042000	1.544533000
1	4.459212000	-1.905676000	0.273287000
1	1.967458000	-2.664153000	0.566263000
1	2.445776000	-2.241471000	-1.077501000
6	-0.678486000	3.498010000	0.049125000
6	-1.933597000	2.872712000	0.057685000
6	-2.052295000	1.486465000	0.029220000
6	-0.902806000	0.689089000	-0.005690000
6	0.362608000	1.321594000	-0.015677000
6	0.469161000	2.721321000	0.011078000
1	-0.605286000	4.581200000	0.070555000
1	-2.836321000	3.477174000	0.086512000
1	-3.029376000	1.019158000	0.036493000
34	-0.907723000	-1.228881000	-0.046284000
1	1.454416000	3.175927000	0.000599000
17	-3.250916000	-1.514269000	0.042648000



Optimized geometry of Se complex **1b**

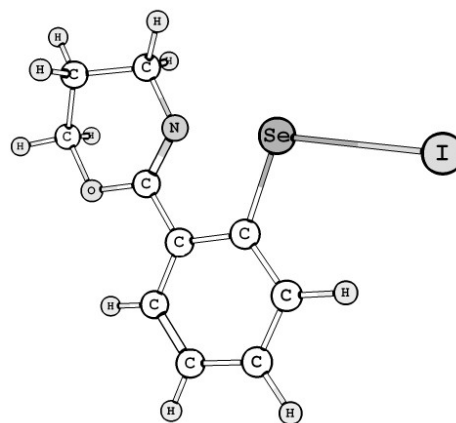
7	1.512468000	-0.974717000	-0.104270000
6	2.011093000	0.215179000	-0.055737000
8	3.323484000	0.521753000	-0.025429000
6	4.243609000	-0.577441000	-0.214028000
6	3.737204000	-1.842594000	0.467699000
6	2.340985000	-2.170628000	-0.071550000
1	5.190643000	-0.227294000	0.200912000
1	4.367582000	-0.731430000	-1.293385000
1	3.693348000	-1.679203000	1.550705000
1	4.432305000	-2.668723000	0.282404000
1	1.837525000	-2.916575000	0.552840000
1	2.402834000	-2.589384000	-1.084902000



6	0.500986000	3.661359000	0.049673000
6	-0.856469000	3.312246000	0.054797000
6	-1.260712000	1.980950000	0.023545000
6	-0.304686000	0.959798000	-0.011341000
6	1.065145000	1.314227000	-0.017023000
6	1.460387000	2.660990000	0.012735000
1	0.799682000	4.705106000	0.073221000
1	-1.613969000	4.091053000	0.083047000
1	-2.314265000	1.727794000	0.029019000
34	-0.715333000	-0.917114000	-0.057153000
1	2.518907000	2.899434000	0.005482000
35	-3.194105000	-0.738983000	0.029845000

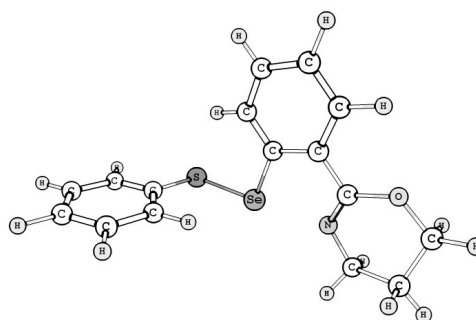
Optimized geometry of Se complex **1c**

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6	4.684689000	-0.926993000	-0.195916000
6	4.016195000	-2.132663000	0.480058000
6	2.591264000	-2.319268000	-0.086177000
1	5.642496000	-0.665211000	0.257525000
1	4.820905000	-1.090844000	-1.272326000
1	3.968871000	-1.967626000	1.563303000
1	4.618629000	-3.031757000	0.303484000
1	2.014331000	-3.024515000	0.521473000
1	2.624489000	-2.718437000	-1.109230000
6	1.277721000	3.710710000	0.052382000
6	-0.116704000	3.475708000	0.055218000
6	-0.636509000	2.170758000	0.021721000
6	0.240829000	1.069797000	-0.013108000
6	1.645717000	1.309908000	-0.016924000
6	2.160048000	2.626544000	0.015326000
1	1.659692000	4.727437000	0.078156000
1	-0.806383000	4.315683000	0.083542000
1	-1.710186000	2.012669000	0.024833000
34	-0.314910000	-0.814372000	-0.060223000
1	3.236384000	2.770480000	0.010305000
53	-3.197216000	-0.443295000	0.020045000



Optimized geometry of Se complex **1d**

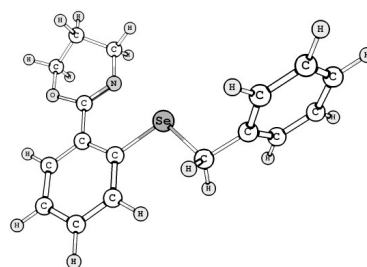
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6	-5.394306000	-0.296107000	0.769029000
6	-4.877816000	-0.535346000	2.044448000
6	-3.501744000	-0.703326000	2.203141000
6	-2.643880000	-0.633201000	1.104536000
1	-4.954490000	-0.035323000	-1.323960000



1	-6.464320000	-0.164230000	0.628910000
1	-5.540810000	-0.590053000	2.903511000
1	-3.085391000	-0.890756000	3.189967000
1	-1.574647000	-0.773387000	1.227570000
7	2.311099000	-1.079963000	-0.251461000
6	2.725467000	0.040252000	0.210605000
8	3.920714000	0.273300000	0.811629000
6	4.872412000	-0.809359000	0.775854000
6	4.178807000	-2.152092000	0.967763000
6	3.096436000	-2.296806000	-0.106950000
1	5.587878000	-0.587257000	1.570596000
1	5.396959000	-0.771340000	-0.187923000
1	3.726325000	-2.185178000	1.965956000
1	4.910861000	-2.965286000	0.906738000
1	2.408121000	-3.115569000	0.131999000
1	3.547158000	-2.541497000	-1.078881000
6	1.441646000	3.578762000	0.447176000
6	0.158274000	3.418765000	-0.081750000
6	-0.283356000	2.169478000	-0.512203000
6	0.547763000	1.050339000	-0.422460000
6	1.847458000	1.210661000	0.110959000
6	2.279861000	2.475411000	0.539982000
1	1.783287000	4.553968000	0.781509000
1	-0.509057000	4.272903000	-0.161762000
1	-1.280960000	2.062677000	-0.923146000
34	-0.021602000	-0.718438000	-0.999155000
1	3.281258000	2.573964000	0.944155000

Optimized geometry of Se complex **1e**

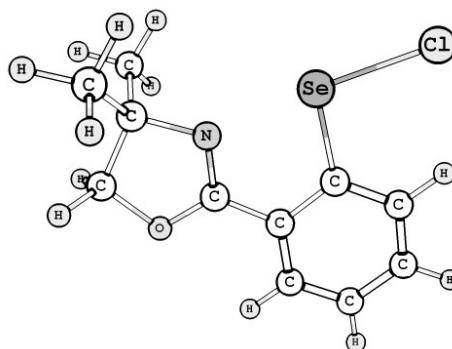
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6	-3.986482000	0.159173000	-1.120551000
6	-5.108678000	-0.669373000	-1.112214000
6	-5.557410000	-1.230141000	0.084998000
6	-4.872310000	-0.960791000	1.271932000
6	-3.750091000	-0.133405000	1.260720000
1	-3.637640000	0.591210000	-2.055742000
1	-5.633227000	-0.876344000	-2.041511000
1	-6.433239000	-1.873526000	0.093166000
1	-5.212410000	-1.395951000	2.208201000
1	-3.213417000	0.068281000	2.184923000
7	1.671249000	-1.442327000	-0.250925000
6	2.599891000	-0.586047000	-0.065252000
8	3.930792000	-0.853862000	0.102312000
6	4.338314000	-2.211234000	-0.140055000
6	3.309987000	-3.192498000	0.406893000
6	1.956457000	-2.869518000	-0.233652000
1	5.314000000	-2.309616000	0.342033000
1	4.469671000	-2.346204000	-1.222486000
1	3.249435000	-3.080132000	1.496068000



1	3.618655000	-4.222710000	0.194507000
1	1.138038000	-3.367756000	0.299322000
1	1.922794000	-3.242892000	-1.267293000
6	3.068453000	3.152182000	0.140079000
6	1.745553000	3.594077000	0.107826000
6	0.698982000	2.679437000	0.021403000
6	0.933805000	1.296736000	-0.031772000
6	2.280803000	0.851819000	-0.002984000
6	3.324216000	1.787898000	0.082681000
1	3.889042000	3.860697000	0.205379000
1	1.520977000	4.657016000	0.147528000
1	-0.313451000	3.062050000	-0.004661000
34	-0.522532000	0.044409000	-0.137652000
1	4.344034000	1.421714000	0.102020000
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1	-1.958385000	1.871552000	0.985840000

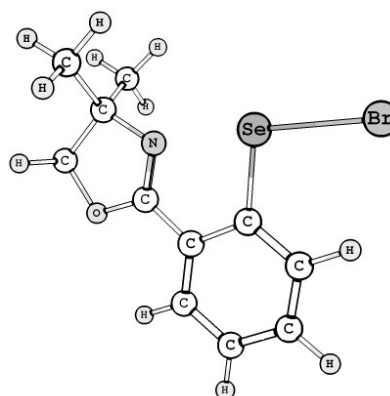
Optimized geometry of Se complex **2a**

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7	-1.332239000	-0.164025000	-0.039302000
6	1.259033000	0.513522000	-0.006507000
6	2.611348000	0.872456000	0.000641000
1	3.373456000	0.103017000	0.001664000
6	2.972786000	2.217299000	0.007834000
1	4.028233000	2.476283000	0.014106000
6	2.008887000	3.235305000	0.007272000
1	2.311989000	4.277871000	0.013022000
6	0.664201000	2.897545000	-0.001396000
1	-0.108487000	3.660218000	-0.002844000
6	0.288949000	1.545583000	-0.008484000
6	-1.079186000	1.098817000	-0.018340000
6	-3.316805000	1.091326000	-0.078963000
1	-3.813757000	1.308504000	-1.029177000
1	-3.976183000	1.364335000	0.748431000
6	-2.790422000	-0.381382000	0.006033000
6	-3.163166000	-1.056433000	1.334558000
1	-2.668191000	-2.028795000	1.418194000
1	-4.246294000	-1.213338000	1.397985000
1	-2.849744000	-0.442427000	2.185339000
6	-3.235157000	-1.228104000	-1.192830000
1	-2.772671000	-2.219161000	-1.151223000
1	-2.940676000	-0.755203000	-2.135219000
1	-4.323648000	-1.357832000	-1.192122000



Optimized geometry of Se complex **2b**

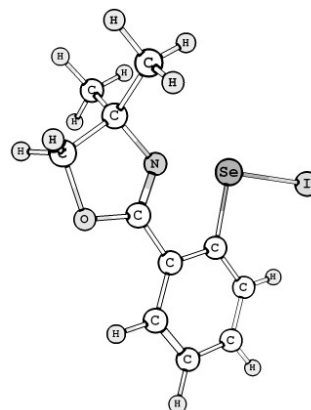
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35	3.078578000	-1.206960000	0.009519000



8	-3.053509000	1.279653000	0.010706000
7	-1.615566000	-0.451336000	-0.035276000
6	0.623252000	1.058461000	-0.007989000
6	1.772593000	1.855806000	-0.002540000
1	2.750345000	1.389073000	-0.002501000
6	1.658556000	3.243706000	0.004381000
1	2.564431000	3.844113000	0.008976000
6	0.407117000	3.874162000	0.005628000
1	0.337712000	4.957685000	0.010861000
6	-0.742925000	3.099113000	-0.000293000
1	-1.728409000	3.554580000	0.000217000
6	-0.639503000	1.699952000	-0.007271000
6	-1.784240000	0.824056000	-0.013563000
6	-3.902578000	0.098891000	-0.050257000
1	-4.590944000	0.141139000	0.797582000
6	-2.926886000	-1.125343000	0.004690000
6	-3.054714000	-1.912138000	1.317583000
1	-2.271992000	-2.674371000	1.380556000
1	-2.951073000	-1.247985000	2.182007000
1	-4.028946000	-2.411470000	1.376593000
6	-3.079727000	-2.046838000	-1.212026000
1	-2.314634000	-2.829179000	-1.193924000
1	-4.064217000	-2.529125000	-1.211490000
1	-2.967801000	-1.484088000	-2.144415000
1	-4.470987000	0.147790000	-0.983797000

Optimized geometry of Se complex **2c**

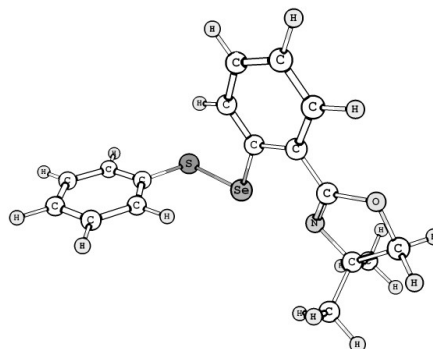
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1	-1.461385000	4.362428000	0.000102000
6	0.683964000	4.039676000	-0.000079000
1	0.927409000	5.098303000	-0.000136000
6	1.701899000	3.080854000	-0.000052000
1	2.750203000	3.366510000	-0.000088000
6	1.364587000	1.708422000	0.000056000
6	0.002636000	1.279341000	0.000047000
34	-0.313212000	-0.671894000	0.000157000
53	-3.194157000	-0.681188000	-0.000073000
6	-1.010214000	2.257902000	0.000127000
1	-2.055223000	1.965742000	0.000205000
8	3.708457000	0.846376000	-0.000212000
6	2.341346000	0.646927000	0.000013000
7	1.944291000	-0.597732000	0.000088000
6	3.111105000	-1.538429000	-0.000037000
6	3.085753000	-2.407922000	-1.274090000
1	2.187588000	-3.034900000	-1.291292000
1	3.083090000	-1.784680000	-2.175949000
1	3.964489000	-3.065130000	-1.304207000
6	4.323332000	-0.525444000	-0.000420000
1	4.941166000	-0.596396000	0.898017000
1	4.940606000	-0.596381000	-0.899253000



6	3.086299000	-2.407618000	1.274325000
1	3.084170000	-1.784060000	2.175961000
1	2.188024000	-3.034419000	1.292134000
1	3.964938000	-3.064965000	1.304208000

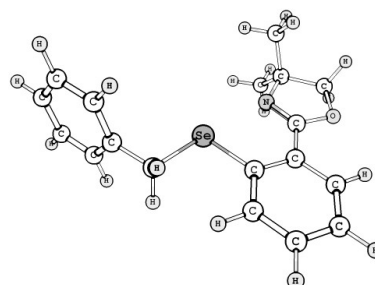
Optimized geometry of Se complex **2d**

34	-0.096074000	-0.583279000	-0.922767000
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8	3.763872000	0.768727000	0.877811000
7	2.361981000	-0.736669000	-0.063620000
6	-3.263971000	-0.533367000	-0.230366000
6	-4.646004000	-0.501691000	-0.464757000
1	-5.022079000	-0.377791000	-1.477205000
6	-5.537040000	-0.630110000	0.599930000
1	-6.606528000	-0.604992000	0.406949000
6	-5.062459000	-0.789856000	1.903692000
1	-5.758552000	-0.888593000	2.732003000
6	-3.686289000	-0.821770000	2.131769000
1	-3.303376000	-0.946404000	3.141620000
6	-2.785745000	-0.694384000	1.073080000
1	-1.715033000	-0.728828000	1.248226000
6	4.539441000	-0.454002000	0.829896000
1	4.897407000	-0.665300000	1.841375000
1	5.397608000	-0.283061000	0.171532000
6	3.555915000	-1.536203000	0.277898000
6	3.175987000	-2.571020000	1.348068000
1	2.797628000	-2.077752000	2.249909000
1	4.044565000	-3.180858000	1.625079000
1	2.392427000	-3.235540000	0.971009000
6	4.099112000	-2.223951000	-0.980887000
1	3.352828000	-2.911791000	-1.390485000
1	5.005883000	-2.796197000	-0.750366000
1	4.341077000	-1.486434000	-1.753277000
6	2.563843000	0.470419000	0.309798000
6	1.579498000	1.535790000	0.166319000
6	1.890579000	2.843678000	0.570507000
1	2.873980000	3.039322000	0.984615000
6	0.957194000	3.864078000	0.442750000
1	1.203975000	4.873494000	0.758081000
6	-0.299447000	3.574959000	-0.094772000
1	-1.040951000	4.362410000	-0.201077000
6	-0.621068000	2.280765000	-0.500152000
1	-1.600000000	2.077424000	-0.919633000
6	0.306944000	1.244455000	-0.377724000



Optimized geometry of Se complex **2e**

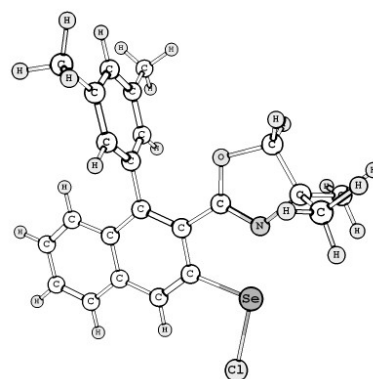
34	0.581203000	0.210166000	-0.040676000
6	2.200152000	1.392667000	-0.002327000
8	-3.911301000	-0.504413000	0.053423000



7	-1.766684000	-1.232705000	-0.042587000
6	3.382246000	0.467103000	0.012514000
6	3.858938000	-0.059594000	1.221326000
1	3.378022000	0.228721000	2.153198000
6	4.938662000	-0.941715000	1.236963000
1	5.302068000	-1.332988000	2.183670000
6	5.551159000	-1.321601000	0.040724000
1	6.393928000	-2.007592000	0.052169000
6	5.073409000	-0.816473000	-1.170016000
1	5.542031000	-1.109511000	-2.105920000
6	3.993577000	0.066402000	-1.183192000
1	3.620983000	0.454753000	-2.128313000
6	-4.035276000	-1.943627000	0.021094000
1	-4.616375000	-2.214409000	-0.866655000
1	-4.582233000	-2.257412000	0.915899000
6	-2.565523000	-2.473106000	-0.021558000
6	-2.280093000	-3.284384000	-1.293241000
1	-2.524696000	-2.702360000	-2.188253000
1	-2.872061000	-4.207884000	-1.307486000
1	-1.219878000	-3.551470000	-1.342058000
6	-2.207224000	-3.283044000	1.233242000
1	-1.144259000	-3.543444000	1.224836000
1	-2.792449000	-4.209791000	1.279006000
1	-2.406590000	-2.702211000	2.140220000
6	-2.569442000	-0.239601000	0.004184000
6	-2.171985000	1.168538000	0.010455000
6	-3.171802000	2.154357000	0.036231000
1	-4.208075000	1.835622000	0.052355000
6	-2.850015000	3.505526000	0.040809000
1	-3.634773000	4.255855000	0.060564000
6	-1.505770000	3.879524000	0.018503000
1	-1.230074000	4.931065000	0.020277000
6	-0.502463000	2.913464000	-0.007093000
1	0.527788000	3.246294000	-0.024935000
6	-0.803964000	1.543128000	-0.010428000
1	2.195886000	2.028106000	-0.890732000
1	2.159525000	2.011857000	0.896732000

Optimized geometry of Se complex **3a**

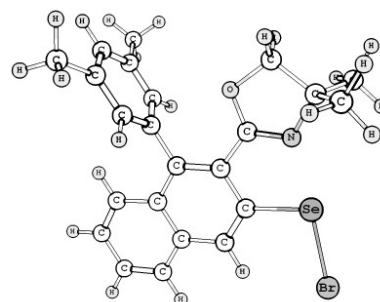
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6	0.964058000	2.247677000	-0.002955000
6	-0.285223000	2.953652000	-0.007417000
6	-0.275497000	4.376779000	-0.000839000
6	0.955308000	0.821782000	-0.009077000
6	2.261343000	0.087564000	-0.009251000
6	2.877673000	-0.257936000	-1.218848000
6	4.109706000	-0.918186000	-1.235993000
6	4.757738000	-1.318593000	-2.541796000



1	4.613156000	-2.387721000	-2.746921000
1	4.335321000	-0.763465000	-3.385430000
1	5.838531000	-1.138083000	-2.525555000
6	4.723321000	-1.219227000	-0.013114000
6	4.136495000	-0.877685000	1.209162000
6	4.832549000	-1.179201000	2.516813000
1	5.539490000	-2.008897000	2.412831000
1	5.399896000	-0.310024000	2.875575000
1	4.114960000	-1.441405000	3.301942000
6	2.898782000	-0.222323000	1.195958000
6	-0.270990000	0.150788000	-0.018513000
6	-1.520868000	0.865375000	-0.023347000
34	-3.155715000	-0.174485000	-0.039994000
17	-4.659237000	1.640806000	0.020914000
6	-1.505956000	2.240431000	-0.019073000
8	0.567942000	-2.186188000	0.044728000
6	-0.433701000	-1.289858000	-0.022067000
7	-1.628632000	-1.773431000	-0.071033000
6	-1.589861000	-3.241420000	0.037845000
6	-0.054084000	-3.496655000	-0.076396000
6	-2.152217000	-3.656940000	1.406746000
1	0.901443000	6.160422000	0.013043000
1	3.075837000	4.939335000	0.016814000
1	3.120801000	2.479389000	0.006496000
1	-1.227927000	4.900236000	-0.003409000
1	2.386679000	-0.009077000	-2.156673000
1	5.685227000	-1.729694000	-0.014449000
1	2.424373000	0.051668000	2.135459000
1	-2.438495000	2.792633000	-0.022318000
1	0.346528000	-4.127094000	0.720386000
1	0.232760000	-3.908746000	-1.049142000
1	-2.139110000	-4.747674000	1.515489000
1	-3.184349000	-3.309596000	1.513791000
1	-1.562509000	-3.218745000	2.218879000
6	-2.380434000	-3.882498000	-1.108152000
1	-3.435685000	-3.598260000	-1.047788000
1	-1.995764000	-3.554738000	-2.079179000
1	-2.317088000	-4.975634000	-1.057734000

Optimized geometry of Se complex **3b**

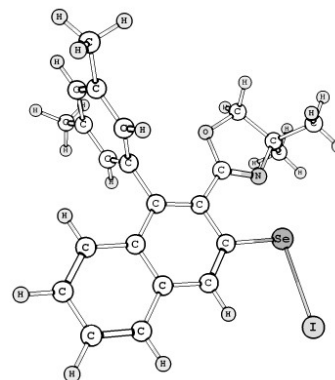
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6	1.852774000	4.574316000	0.023778000
6	2.081736000	3.218629000	0.014548000
6	0.997518000	2.292727000	0.003593000
6	-0.341010000	2.808072000	-0.001372000
6	-0.540784000	4.216935000	0.008600000
6	1.196716000	0.880487000	-0.004889000
6	2.596808000	0.346177000	-0.011663000
6	3.247746000	0.090886000	-1.222231000
6	4.562987000	-0.390414000	-1.246415000



6	5.244585000	-0.695002000	-2.560972000
1	4.912130000	-1.659151000	-2.968353000
1	5.019406000	0.067113000	-3.315419000
1	6.332148000	-0.746089000	-2.446228000
6	5.218333000	-0.600515000	-0.029645000
6	4.595364000	-0.341920000	1.198566000
6	5.341085000	-0.546260000	2.497611000
1	5.949474000	-1.457416000	2.471712000
1	6.022690000	0.290196000	2.701758000
1	4.654100000	-0.622123000	3.346539000
6	3.280620000	0.131961000	1.192294000
6	0.082420000	0.036250000	-0.015500000
6	-1.259102000	0.560496000	-0.024549000
34	-2.729791000	-0.707362000	-0.049251000
35	-4.607754000	0.913247000	0.004930000
6	-1.443430000	1.923053000	-0.017988000
8	1.270265000	-2.140991000	0.072032000
6	0.139642000	-1.414271000	-0.013238000
7	-0.963294000	-2.078149000	-0.070504000
6	-0.694997000	-3.520917000	0.049124000
6	0.864332000	-3.534572000	-0.029654000
6	-1.216632000	-4.016050000	1.407677000
1	0.361898000	6.154094000	0.028964000
1	2.691604000	5.264871000	0.032702000
1	3.097054000	2.838338000	0.015769000
1	-1.559960000	4.594341000	0.005558000
1	2.721047000	0.266097000	-2.157622000
1	6.242239000	-0.971055000	-0.036596000
1	2.777119000	0.336974000	2.134037000
1	-2.446282000	2.335161000	-0.022752000
1	1.340240000	-4.077677000	0.789946000
1	1.235235000	-3.917353000	-0.985791000
1	-1.032635000	-5.090409000	1.524645000
1	-2.293248000	-3.837541000	1.487835000
1	-0.724248000	-3.486741000	2.230319000
6	-1.348943000	-4.283034000	-1.109155000
1	-2.437041000	-4.170438000	-1.072647000
1	-1.000195000	-3.901352000	-2.074055000
1	-1.113598000	-5.352046000	-1.050379000

Optimized geometry of Se complex **3c**

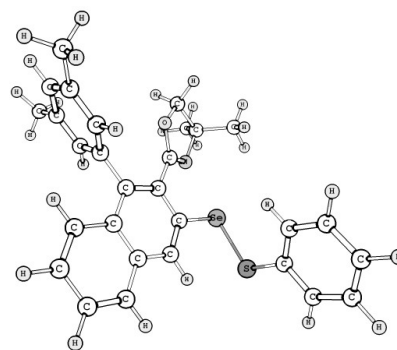
6	0.554004000	5.083281000	0.006208000
6	1.924166000	4.675565000	0.008501000
6	2.256705000	3.329333000	0.007842000
6	1.237241000	2.318964000	0.004567000
6	-0.144492000	2.735182000	0.003085000
6	-0.455602000	4.133087000	0.003797000
6	1.550781000	0.919076000	0.003702000
6	2.990569000	0.487208000	0.005158000
6	3.684925000	0.328843000	-1.212707000



6	5.040883000	-0.051707000	-1.228278000
6	5.779689000	-0.247717000	-2.540785000
1	5.869099000	-1.315384000	-2.788310000
1	5.257357000	0.240089000	-3.371741000
1	6.796984000	0.160967000	-2.493675000
6	5.698284000	-0.260119000	0.005221000
6	5.029065000	-0.100515000	1.235007000
6	5.744963000	-0.341399000	2.552866000
1	6.829841000	-0.411247000	2.413513000
1	5.547452000	0.466010000	3.269671000
1	5.409312000	-1.278496000	3.019509000
6	3.669753000	0.281091000	1.219852000
6	0.495574000	-0.011969000	0.000865000
6	-0.891874000	0.412738000	0.000384000
34	-2.273740000	-1.009602000	-0.003784000
53	-4.665069000	0.645807000	0.003070000
6	-1.187787000	1.764535000	0.001436000
8	1.842424000	-2.148890000	-0.008635000
6	0.649723000	-1.456161000	-0.005184000
7	-0.425333000	-2.202985000	-0.009132000
6	-0.092123000	-3.661003000	-0.012436000
6	1.483096000	-3.607347000	-0.026683000
6	-0.637426000	-4.329545000	1.267215000
1	0.308798000	6.142435000	0.006668000
1	2.706830000	5.429909000	0.010922000
1	3.298705000	3.026358000	0.009978000
1	-1.500140000	4.434861000	0.002493000
1	3.162870000	0.502555000	-2.151562000
1	6.749440000	-0.546790000	0.004971000
1	3.138702000	0.417231000	2.160283000
1	-2.218839000	2.105241000	0.000849000
1	1.937968000	-4.055215000	0.860103000
1	1.919775000	-4.028351000	-0.935717000
1	-0.352089000	-5.389188000	1.292812000
1	-1.730759000	-4.267790000	1.296671000
1	-0.244761000	-3.839212000	2.165621000
6	-0.660132000	-4.331385000	-1.280769000
1	-1.754219000	-4.276348000	-1.287269000
1	-0.289282000	-3.837863000	-2.186582000
1	-0.369214000	-5.389314000	-1.313437000

Optimized geometry of Se complex **3d**

6	-0.527077000	3.969568000	-1.260254000
6	-0.169029000	2.622099000	-0.983033000
6	1.156889000	2.327808000	-0.528858000
6	2.079573000	3.404785000	-0.397044000
6	1.702833000	4.698871000	-0.676187000
6	0.385417000	4.987000000	-1.107945000
6	1.508726000	0.968775000	-0.247693000
6	0.559478000	-0.039750000	-0.426234000

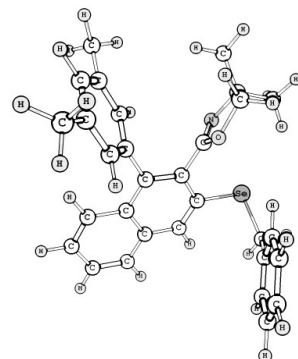


6	-0.759390000	0.266106000	-0.905490000
6	-1.097004000	1.569491000	-1.168931000
6	2.912521000	0.659441000	0.172537000
6	4.673269000	0.702308000	1.855669000
6	3.357781000	0.964304000	1.466525000
6	5.548824000	0.137068000	0.917860000
6	3.808475000	0.097014000	-0.741317000
6	5.135436000	-0.173094000	-0.380257000
6	5.143998000	1.005848000	3.259767000
6	6.089450000	-0.795738000	-1.374285000
6	0.833188000	-1.454242000	-0.138782000
6	1.770019000	-3.242214000	0.820907000
8	1.706255000	-1.795292000	0.842821000
6	0.558840000	-3.671663000	-0.057060000
7	0.200683000	-2.402663000	-0.725542000
6	0.934789000	-4.734696000	-1.093261000
6	-0.641226000	-4.123215000	0.792700000
34	-2.042264000	-1.191549000	-1.157256000
16	-3.971743000	-0.042196000	-1.347170000
6	-4.511998000	0.281891000	0.343449000
6	-4.283825000	0.194003000	2.748156000
6	-3.788757000	-0.099063000	1.476912000
6	-5.496962000	0.866352000	2.901567000
6	-5.731512000	0.957404000	0.492460000
6	-6.218095000	1.245217000	1.767110000
1	-1.538751000	4.177839000	-1.599028000
1	3.092037000	3.193834000	-0.072629000
1	2.422019000	5.506174000	-0.568002000
1	0.100084000	6.013120000	-1.323722000
1	-2.094978000	1.811749000	-1.520329000
1	2.663161000	1.404479000	2.177688000
1	6.579775000	-0.060542000	1.207590000
1	3.469910000	-0.123279000	-1.751354000
1	6.124062000	1.496975000	3.257307000
1	4.440392000	1.658885000	3.785712000
1	5.246230000	0.087380000	3.852713000
1	5.977708000	-0.351888000	-2.369997000
1	5.908034000	-1.873595000	-1.480886000
1	7.131273000	-0.668746000	-1.062872000
1	1.722083000	-3.594497000	1.854030000
1	2.731866000	-3.530629000	0.381290000
1	1.248296000	-5.663468000	-0.601452000
1	1.754547000	-4.384992000	-1.729548000
1	0.078299000	-4.959711000	-1.736505000
1	-1.527938000	-4.243124000	0.163251000
1	-0.872752000	-3.379720000	1.562725000
1	-0.430701000	-5.080157000	1.285199000
1	-3.712419000	-0.106802000	3.622883000
1	-2.850509000	-0.629403000	1.350775000
1	-5.877039000	1.093640000	3.893709000
1	-6.297311000	1.256489000	-0.386309000

1 -7.165104000 1.768709000 1.871486000

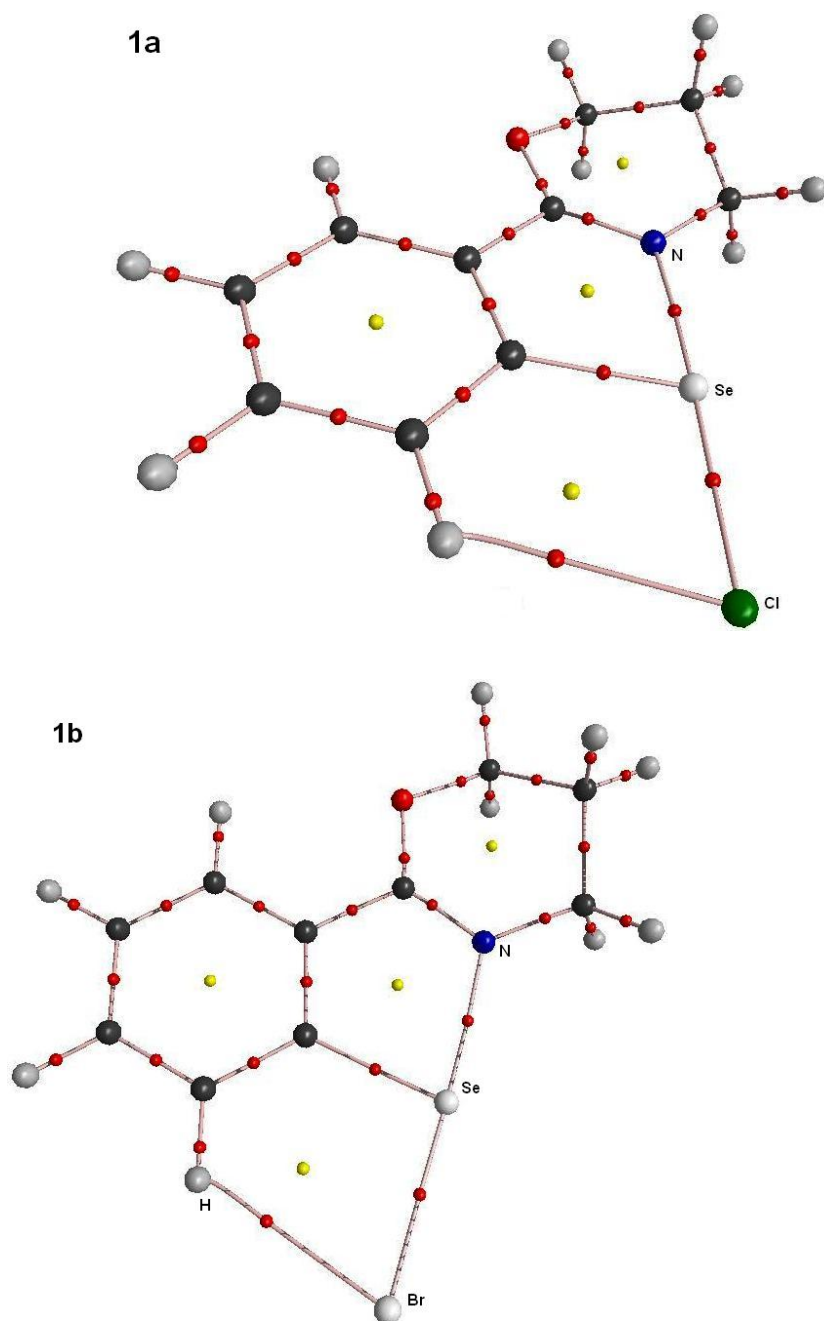
Optimized geometry of Se complex **3e**

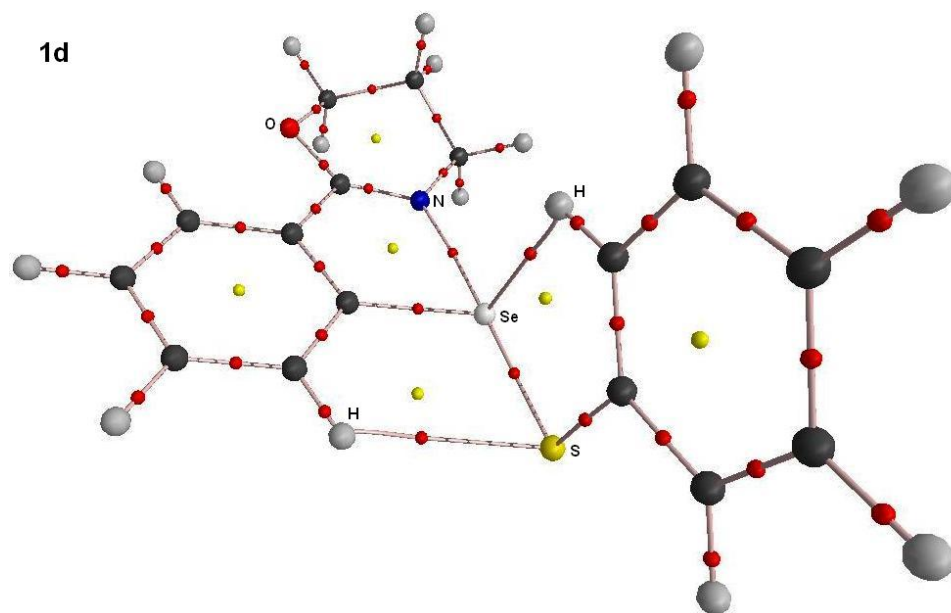
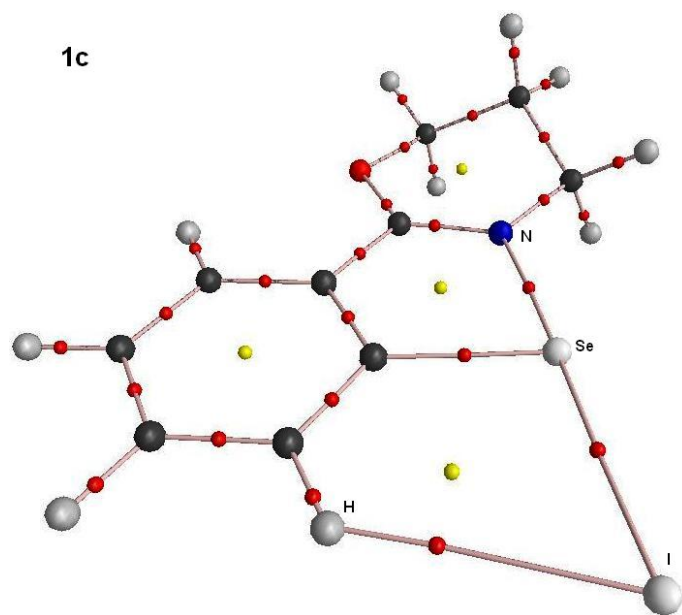
6	-1.229928000	3.800040000	-1.867744000
6	-0.788363000	2.512635000	-1.458262000
6	0.524721000	2.365140000	-0.902766000
6	1.347072000	3.521933000	-0.804977000
6	0.890162000	4.755643000	-1.212547000
6	-0.412823000	4.899571000	-1.745541000
6	0.967574000	1.061294000	-0.499596000
6	0.122178000	-0.028207000	-0.663513000
6	-1.186848000	0.128475000	-1.206343000
6	-1.614445000	1.371284000	-1.608451000
6	2.335426000	0.869139000	0.074089000
6	3.934874000	1.211185000	1.882808000
6	2.662584000	1.391863000	1.334254000
6	4.888955000	0.502573000	1.139828000
6	3.306683000	0.158214000	-0.640095000
6	4.594481000	-0.027562000	-0.119515000
6	4.270275000	1.741852000	3.258100000
6	5.647082000	-0.758862000	-0.921533000
6	0.551122000	-1.394229000	-0.263813000
6	1.087001000	-2.998970000	1.199850000
8	0.618467000	-1.634931000	1.078237000
6	1.061327000	-3.554488000	-0.257238000
7	0.802663000	-2.344293000	-1.074477000
6	2.399748000	-4.181610000	-0.660841000
6	-0.100593000	-4.536525000	-0.478333000
34	-2.312120000	-1.426094000	-1.366057000
6	-4.002569000	-0.699867000	-0.616628000
6	-3.914802000	-0.143670000	0.786055000
6	-3.044353000	-0.193898000	3.051359000
6	-3.048347000	-0.681989000	1.745773000
6	-3.899023000	0.847903000	3.418334000
6	-4.757791000	0.911397000	1.158890000
6	-4.754207000	1.402496000	2.465501000
1	-2.229797000	3.897576000	-2.283898000
1	2.350552000	3.421335000	-0.407005000
1	1.536600000	5.625177000	-1.129676000
1	-0.762334000	5.878430000	-2.062677000
1	-2.600164000	1.498718000	-2.046699000
1	1.905918000	1.932916000	1.897019000
1	5.885644000	0.360429000	1.555018000
1	3.054145000	-0.253202000	-1.613702000
1	5.274384000	2.180441000	3.285188000
1	3.557210000	2.509208000	3.576025000
1	4.247738000	0.942026000	4.010208000
1	6.117267000	-0.094961000	-1.659226000
1	5.216253000	-1.600084000	-1.475826000
1	6.443483000	-1.147718000	-0.278352000

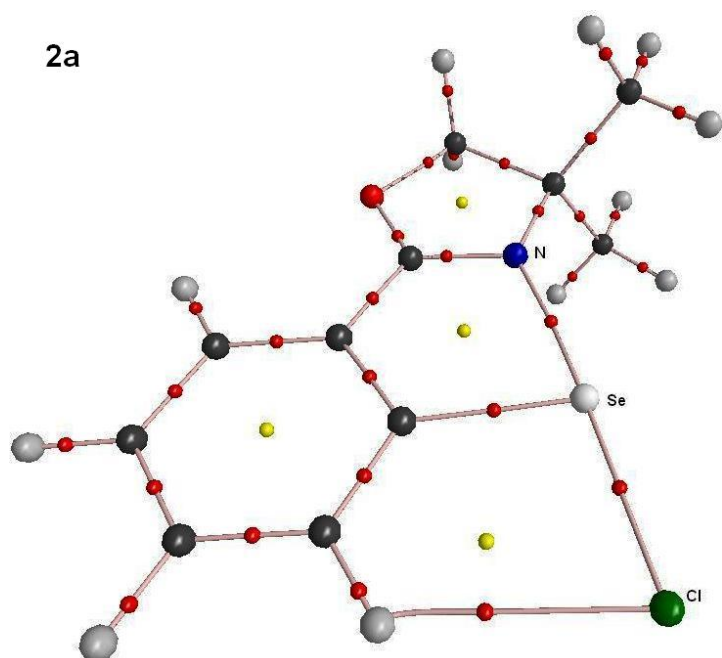
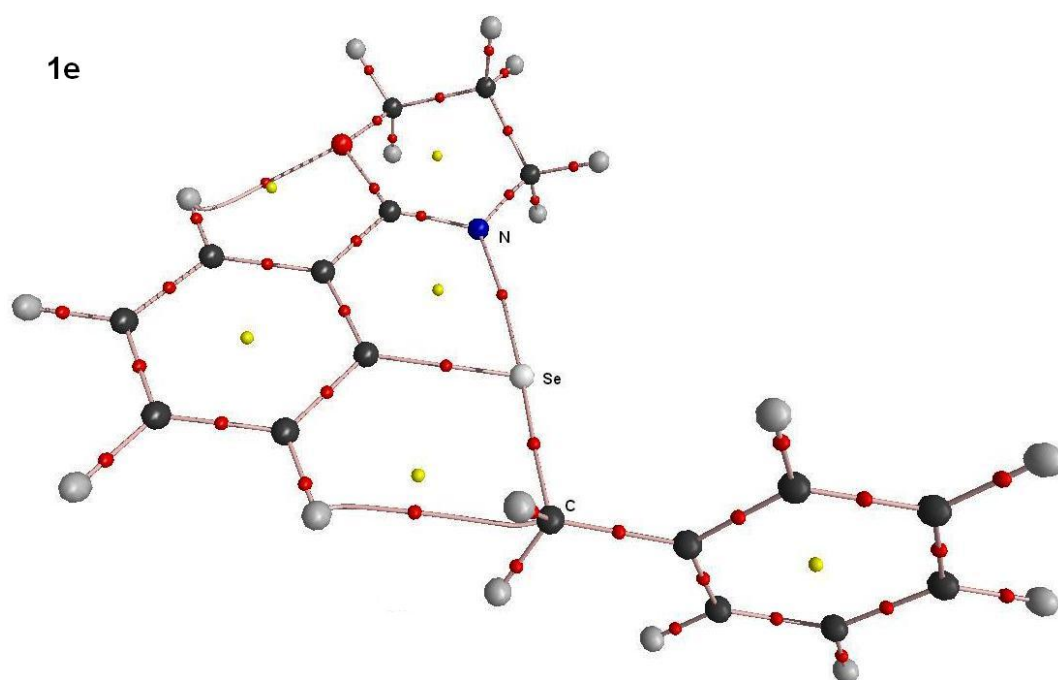


1	0.417289000	-3.526048000	1.885024000
1	2.095393000	-2.971957000	1.627850000
1	2.611791000	-5.074288000	-0.059210000
1	3.219502000	-3.468434000	-0.521214000
1	2.378346000	-4.474800000	-1.715288000
1	-0.133212000	-4.851853000	-1.526267000
1	-1.055023000	-4.054060000	-0.244603000
1	0.014897000	-5.428365000	0.150036000
1	-2.361322000	-0.621692000	3.780657000
1	-2.355296000	-1.461207000	1.445655000
1	-3.890746000	1.230997000	4.435379000
1	-5.428020000	1.348805000	0.421605000
1	-5.415453000	2.222057000	2.735188000
1	-4.426348000	0.028398000	-1.312016000
1	-4.646050000	-1.587724000	-0.650444000

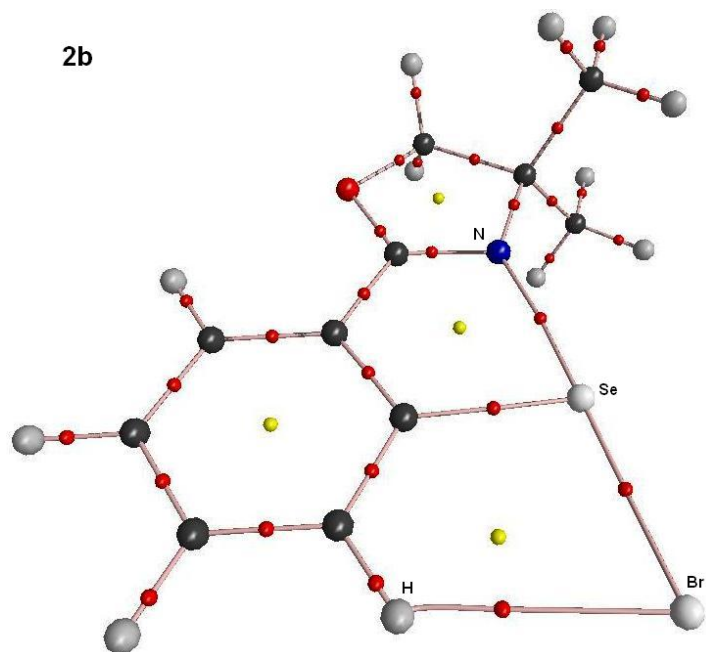
Figure S1: Molecular plots of the compounds **1a – 1e**, **2a – 2e** and **3a – 3e** obtained from AIM theory. The Bond Critical points (BCP) and Ring Critical Points (RCP) are shown in small spheres in Red and Yellow color respectively.







2b



2c

