

Supplementary Material

On the Stability of 2-Aminoselenophene-3-carboxylates: Potential Dual-Acting Selenium-Containing Allosteric Enhancers of Adenosine A₁A Receptor Binding

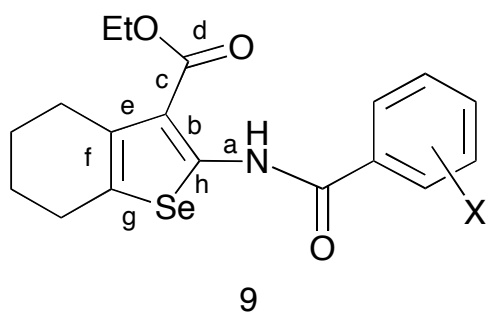
Peter J. Scammells,^{*a} Kylee M. Aumann,^{b,c} Jonathan M. White^{b,c} and Carl H. Schiesser^{*,b,c}

^a *Department of Medicinal Chemistry, Victorian College of Pharmacy, Monash University, 381 Royal Parade, Parkville VIC 3052*

^b *School of Chemistry, The University of Melbourne, Victoria 3010, Australia*

^c *Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Victoria 3010, Australia*

B3LYP/6-311G** optimised geometries of **9**, BHandHLYP/6-311G** and BHandHLYP/cc-pVDZ optimised geometries of **12** – **18** as Gaussian Archive Entries. Tables of key bond lengths and Mulliken populations for **9** (Tables S1 and S2). (19 pages).

Structural Data for Selenophene-3-carboxylates (**9**).

X	σ_x	Bond a (Å)	Bond b (Å)	Bond c (Å)	Bond d (Å)	Bond e (Å)	Bond f (Å)	Bond g (Å)	Bond h (Å)
<i>p</i> -NMe ₂	-0.83	1.370	1.393	1.464	1.229	1.459	1.360	1.903	1.880
H	0.00	1.374 (1.392)	1.392 (1.373)	1.466 (1.467)	1.228 (1.224)	1.456 (1.455)	1.360 (1.349)	1.901 (1.876)	1.879 (1.857)
<i>m</i> -OMe	0.12	1.373	1.392	1.466	1.229	1.456	1.360	1.901	1.878
<i>p</i> -Cl	0.23	1.375	1.391	1.467	1.229	1.458	1.360	1.901	1.878
<i>m</i> -Cl	0.37	1.375	1.393	1.467	1.235	1.457	1.365	1.891	1.864
<i>p</i> -NO ₂	0.78	1.376 (1.378)	1.391 (1.375)	1.468 (1.450)	1.229 (1.219)	1.457 (1.450)	1.361 (1.349)	1.900 (1.875)	1.877 (1.852)

Table S1 – B3LYP/6-311G** calculated bond lengths for ethyl 2-arylamido-4,5,6,7-tetrahydrobenzo[b]selenophene-3-carboxylates (**9**). (X-ray data in parentheses where available).

X	σ_x	Bond a (Å)	Bond b (Å)	Bond c (Å)	Bond d (Å)	Bond e (Å)	Bond f (Å)	Bond g (Å)	Bond h (Å)
<i>p</i> -NMe ₂	-0.83	0.375	0.483	0.370	0.541	0.432	0.579	0.256	0.345
H	0.00	0.344	0.484	0.362	0.540	0.432	0.576	0.259	0.344
<i>m</i> -OMe	0.12	0.371	0.481	0.361	0.539	0.430	0.576	0.259	0.371
<i>p</i> -Cl	0.23	0.367	0.485	0.362	0.538	0.432	0.576	0.261	0.344
<i>m</i> -Cl	0.37	0.366	0.486	0.360	0.538	0.432	0.575	0.261	0.344
<i>p</i> -NO ₂	0.78	0.365	0.486	0.359	0.536	0.432	0.573	0.263	0.344

Table S2 – Calculated Mulliken bond population data for ethyl 2-arylamido-4,5,6,7-tetrahydrobenzo[b]selenophene-3-carboxylates (**9**).

**Ethyl 2-[(4-nitrobenzoyl)amino]-4,5,6,7-tetrahydro-1-benzoselenophene-3-carboxylate
(9, X = *p*-NO₂)**

B3LYP/6-311G**

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Ethyl 2-[(4-chlorobenzoyl)amino]-4,5,6,7-tetrahydro-1-benzoselenophene-3-carboxylate (9, X = *p*-Cl)

B3LYP/6-311G**

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Ethyl 2-[(4-(dimethylamino)benzoyl)amino]-4,5,6,7-tetrahydro-1-benzoselenophene-3-carboxylate (9, X = *p*-NMe₂)

B3LYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FOpt\RB3LYP\6-311G(d,p)\C20H24N2O3Se1\KAUMANN\09-Feb-2005\1\#\B3LYP/6-311G** OPT=(GRAD,READFC) GUESS=CHECKPOINT FREQ=NORAMAN\p-Dimethylamino Benzoyl protected Selenophene\0,1\C\C,1,cc2\C,2,cc3,1,ccc3\C,3,cc4,2,ccc4,1,dih4,0\C,4,cc5,3,ccc5,2,dih5,0\C,1,cc6,2,ccc6,3,dih6,0\Se,4,sec7,3,secc7,2,dih7,0\C,7,cse8,4,csec8,3,dih8,0\C,5,cc9,4,ccc9,3,dih9,0\C,9,cc10,5,ccc10,4,dih10,0\O,10,oc11,9,oc11,5,dih11,0\O,10,oc12,9,oc12,5,dih12,0\C,11,co13,10,coc13,9,dih13,0\C,13,cc14,11,cco14,10,dih14,0\N,8,nc15,7,ncse15,4,dih15,0\C,15,cn16,8,cnc16,7,dih16,0\O,16,oc17,15,ocn17,8,dih17,0\C,16,cc18,15,ccn18,8,dih18,0\C,18,cc19,16,ccc19,15,dih19,0\C,19,cc20,18,ccc20,16,dih20,0\C,20,cc21,19,ccc21,18,dih21,0\C,21,cc22,20,ccc22,19,dih22,0\C,18,cc23,16,ccc23,15,dih23,0\N,21,nc24,20,ncc24,19,dih24,0\C,24,cn25,21,cnc25,20,dih25,0\C,24,cn26,21,cnc26,20,dih26,0\H,1,hc27,2,hcc27,3,dih27,0\H,1,hc28,2,hcc28,3,dih28,0\H,2,hc29,1,hcc29,6,dih29,0\H,2,hc30,1,hcc30,6,dih30,0\H,3,hc31,2,hcc31,1,dih31,0\H,3,hc32,2,hcc32,1,dih32,0\H,6,hc33,1,hcc33,2,dih33,0\H,6,hc34,1,hcc34,2,dih34,0\H,13,hc35,11,hco35,10,dih35,0\H,13,hc36,11,hco36,10,dih36,0\H,14,hc37,13,hcc37,11,dih37,0\H,14,hc38,13,hcc38,11,dih38,0\H,14,hc39,13,hcc39,11,dih39,0\H,15,hn40,8,hnc40,7,dih40,0\H,19,hc41,18,hcc41,16,dih41,0\H,20,hc42,19,hcc42,18,dih42,0\H,22,hc43,21,hcc43,20,dih43,0\H,23,hc44,18,hcc44,16,dih44,0\H,25,hc45,24,hcn45,21,dih45,0\H,25,hc46,24,hcn46,21,dih46,0\H,25,hc47,24,hcn47,21,dih47,0\H,26,hc48,24,hcn48,21,dih48,0\H,26,hc49,24,hcn49,21,dih49,0\H,26,hc50,24,hcn50,21,dih50,0\cc2=1.53060811\cc3=1.53572781\ccc3=110.28609077\cc4=1.50462617\ccc4=110.68050012\dih4=314.54273299\cc5=1.35969534\ccc5=126.25024706\dih5=15.74443672\cc6=1.53616942\ccc6=111.99053791\dih6=61.75010207\sec7=1.90302572\secc7=120.9458269\dih7=195.45908933\cse8=1.87961552\csec8=86.28873041\dih8=180.01642665\cc9=1.45928601\ccc9=114.4767678\dih9=180.52281707\cc10=1.46413081\ccc10=127.48875054\dih10=177.2263985\oc11=1.34907752\oc11=114.56493429\dih11=356.01975475\oc12=1.22868997\oc12=124.75702874\dih12=176.60026\co13=1.44706678\coc13=116.26105871\dih13=180.3629305\cc14=1.51524087\cco14=107.51211024\dih14=180.68355536\nc15=1.37075365\ncse15=122.35914354\dih15=179.91152659\cn16=1.38224955\cnc16=124.93413364\dih16=0.99450248\oc17=1.2266616\ocn17=120.58183022\dih17=358.41348491\cc18=1.48219475\ccn18=116.49503806\dih18=178.72826536\cc19=1.40140334\ccc19=117.67172529\dih19=172.01600258\cc20=1.38189638\ccc20=121.69591277\dih20=180.02295816\cc21=1.41603069\ccc21=120.90865221\dih21=-0.49413795\cc22=1.41530262\ccc22=117.23176399\dih22=360.1378605\cc23=1.40199373\ccc23=124.64212978\dih23=351.27915839\nc24=1.3758908\ncc24=121.40965173\dih24=180.42269501\cn25=1.45387636\cnc25=120.22476281\dih25=183.68130283\cn26=1.45405356\cnc26=120.19883358\dih26=-2.75227923\hc27=1.09695172\hcc27=108.85998675\dih27=300.78959493\hc28=1.09436724\hcc28=110.55423265\dih28=183.9887582\hc29=1.09635523\hcc29=109.41094385\dih29=301.42279284\hc30=1.09423264\hcc30=110.82249466\dih30=183.68105909\hc31=1.09558621\hcc31=110.13198472\dih31=192.11842315\hc32=1.09857644\hcc32=109.51929449\dih32=75.92316558\hc33=1.09104988\hcc33=109.72274633\dih33=193.16064625\hc34=1.09657626\hcc34=110.04899042\dih34=77.70319247\hc35=1.0924182\hco35=108.77015543\dih35=59.22488394\hc36=1.09235117\hco36=108.83

585506\dih36=302.26926891\hc37=1.0932628\hcc37=109.7027457\dih37=180.1767221\hc38=1.09212034\hcc38=111.03120159\dih38=60.53884693\hc39=1.09215103\hcc39=111.01423896\dih39=299.82775216\hn40=1.01914199\hnc40=112.89457756\dih40=183.20317465\hc41=1.08299513\hcc41=118.08301316\dih41=-0.18989539\hc42=1.08087337\hcc42=118.73694214\dih42=179.42668116\hc43=1.08072052\hcc43=120.3582005\dih43=180.36440814\hc44=1.08453726\hcc44=121.15406686\dih44=359.13302453\hc45=1.08856382\hcn45=109.11142198\dih45=180.16376084\hc46=1.09757675\hcn46=112.12664153\dih46=60.49191421\hc47=1.09582219\hcn47=111.59441069\dih47=299.13895244\hc48=1.08857244\hcn48=109.10308165\dih48=178.32569501\hc49=1.09543973\hcn49=111.49319254\dih49=59.43980191\hc50=1.09772437\hcn50=112.22764768\dih50=298.07398825\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-3513.6338071\RMSD=5.777e-09\RMSF=4.609e-05\Dipole=0.6794268,-1.284212,-1.2447803\PG=C01 [X(C20H24N2O3Se1)]\@

Ethyl 2-[benzoylamino]-4,5,6,7-tetrahydro-1-benzoselenophene-3-carboxylate (9, X = H)

B3LYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\Fopt\RB3LYP\6-311G(d,p)\C18H19N1O3Se1\KAUMANN\05-Feb-2005\1\#\B3LYP/6-311G** OPT=(GRAD,READFC) GUESS=CHECKPOINT FREQ=NORAMAN\Benzoyl protected Selenophene\0,1\C\C,1,cc2\C,2,cc3,1,ccc3\C,3,cc4,2,ccc4,1,dih4,0\C,4,cc5,3,ccc5,2,dih5,0\C,1,cc6,2,ccc6,3,dih6,0\Se,4,sec7,3,secc7,2,dih7,0\C,7,cse8,4,csec8,3,dih8,0\C,5,cc9,4,ccc9,3,dih9,0\C,9,cc10,5,ccc10,4,dih10,0\O,10,oc11,9,occ11,5,dih11,0\O,10,oc12,9,occ12,5,dih12,0\C,11,co13,10,coc13,9,dih13,0\C,13,cc14,11,cco14,10,dih14,0\N,8,nc15,7,ncse15,4,dih15,0\C,15,cn16,8,cnc16,7,dih16,0\O,16,oc17,15,ocn17,8,dih17,0\C,16,cc18,15,ccn18,8,dih18,0\C,18,cc19,16,ccc19,15,dih19,0\C,19,cc20,18,ccc20,16,dih20,0\C,20,cc21,19,ccc21,18,dih21,0\C,21,cc22,20,ccc22,19,dih22,0\C,18,cc23,16,ccc23,15,dih23,0\H,1,hc24,2,hcc24,3,dih24,0\H,1,hc25,2,hcc25,3,dih25,0\H,2,hc26,1,hcc26,6,dih26,0\H,2,hc27,1,hcc27,6,dih27,0\H,3,hc28,2,hcc28,1,dih28,0\H,3,hc29,2,hcc29,1,dih29,0\H,6,hc30,1,hcc30,2,dih30,0\H,6,hc31,1,hcc31,2,dih31,0\H,13,hc32,11,hco32,10,dih32,0\H,13,hc33,11,hco33,10,dih33,0\H,14,hc34,13,hcc34,11,dih34,0\H,14,hc35,13,hcc35,11,dih35,0\H,14,hc36,13,hcc36,11,dih36,0\H,15,hn37,8,hnc37,7,dih37,0\H,19,hc38,18,hcc38,16,dih38,0\H,20,hc39,19,hcc39,18,dih39,0\H,21,hc40,20,hcc40,19,dih40,0\H,22,hc41,21,hcc41,20,dih41,0\H,23,hc42,18,hcc42,16,dih42,0\cc2=1.53111446\cc3=1.53554006\ccc3=110.10155904\cc4=1.50469287\cc4=110.53785145\dih4=313.77442462\cc5=1.36048612\ccc5=126.16549933\dih5=16.05226801\cc6=1.53634787\ccc6=111.8172307\dih6=62.29731731\sec7=1.90138878\secc7=121.0435907\dih7=196.10640746\cse8=1.87864866\csec8=86.28269091\dih8=179.53056511\cc9=1.4579446\ccc9=114.44806923\dih9=181.00359967\cc10=1.46627422\ccc10=127.44481007\dih10=176.86113531\oc11=1.34670939\occ11=114.56274357\dih11=356.35293823\oc12=1.22843899\occ12=124.59116262\dih12=176.97123916\co13=1.44873883\coc13=116.27346523\dih13=180.53082639\cc14=1.51501808\cco14=107.54039509\dih14=179.19836672\nc15=1.37412911\ncse15=122.51647107\dih15=180.31775461\cn16=1.37615752\cnc16=124.94976297\dih16=1.03603575\oc17=1.22399389\ocn17=121.33720894\dih17=357.51264913\cc18=1.49547225\ccn18=116.19420306\dih18=177.7840467\cc19=1.39964798\ccc19=117.1761377\dih19=165.80753157\cc20=1.3895701\cc20=120.38162792\dih20=179.4316607\cc21=1.3944616\ccc21=120.05681787\dih21=359.45828829\cc22=1.39339348\ccc22=119.89964908\dih22=-0.1353372\cc23=1.40078392\ccc23=123.48807156\dih23=344.22901473\hc24=1.09680728\hcc24=108.88781805\dih24=301.34241515\hc25=1.09421607\hcc25=110.63985179\dih25=184.43732839\hc26=1.09619716\hcc26=109.50342769\dih26=301.93996758\hc27=1.09408547\hcc27=110.84649291\dih27=184.07375308\hc28=1.0

9539499\hcc28=110.16881254\dih28=191.43415993\hc29=1.09836937\hcc29=109.52688618\dih29=75.12718511\hc30=1.09117251\hcc30=109.78636091\dih30=193.29385518\hc31=1.09638767\hcc31=110.04695697\dih31=77.8198517\hc32=1.09215437\hco32=108.69783969\dih32=57.71964488\hc33=1.09226707\hco33=108.74331962\dih33=300.79922993\hc34=1.09318888\hcc34=109.63608724\dih34=180.28764504\hc35=1.09211133\hcc35=111.11093815\dih35=60.67218915\hc36=1.09206746\hcc36=110.98670047\dih36=299.86686319\hn37=1.02047709\hc37=112.86617981\dih37=183.37943628\hc38=1.08266177\hcc38=118.32045897\dih38=-0.42163643\hc39=1.08399332\hcc39=119.84413562\dih39=179.5939103\hc40=1.08420454\hcc40=120.10670304\dih40=180.18326559\hc41=1.08385874\hcc41=120.15278808\dih41=180.74208691\hc42=1.08405381\hcc42=121.07438752\dih42=-0.442628\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-3379.6287394\RMSD=9.926e-09\RMSF=3.487e-05\Dipole=-0.5678076,-0.4259618,-0.97445\PG=C01 [X(C18H19N1O3Se1)]\@

Ethyl 2-[3-chlorobenzoylamino]-4,5,6,7-tetrahydro-1-benzoselenophene-3-carboxylate (9, X = *m*-Cl)

B3LYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET17\Freq\RB3LYP\6-311G(d,p)\C18H18ClN1O3Se1\KAUMANN\09-Feb-2005\1\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RB3LYP/6-311G(D,P) FREQ\m-Chloro Benzoyl protected Selenophene\0,1\C\C,1,cc2\C,2,cc3,1,ccc3\C,3,cc4,2,ccc4,1,dih4,0\C,4,cc5,3,ccc5,2,dih5,0\C,1,cc6,2,ccc6,3,dih6,0\Se,4,sec7,3,secc7,2,dih7,0\C,7,cse8,4,csec8,3,dih8,0\C,5,cc9,4,ccc9,3,dih9,0\C,9,cc10,5,ccc10,4,dih10,0\O,10,oc11,9,occ11,5,dih11,0\O,10,oc12,9,occ12,5,dih12,0\C,11,co13,10,co13,9,dih13,0\C,13,cc14,11,cco14,10,dih14,0\N,8,nc15,7,ncse15,4,dih15,0\C,15,cn16,8,cnc16,7,dih16,0\O,16,oc17,15,ocn17,8,dih17,0\C,16,cc18,15,ccn18,8,dih18,0\C,18,cc19,16,ccc19,15,dih19,0\C,19,cc20,18,ccc20,16,dih20,0\C,20,cc21,19,ccc21,18,dih21,0\C,21,cc22,20,ccc22,19,dih22,0\C,18,cc23,16,ccc23,15,dih23,0\Cl,22,clc24,21,clcc24,20,dih24,0\H,1,hc25,2,hcc25,3,dih25,0\H,1,hc26,2,hcc26,3,dih26,0\H,2,hc27,1,hcc27,6,dih27,0\H,2,hc28,1,hcc28,6,dih28,0\H,3,hc29,2,hcc29,1,dih29,0\H,3,hc30,2,hcc30,1,dih30,0\H,6,hc31,1,hcc31,2,dih31,0\H,6,hc32,1,hcc32,2,dih32,0\H,13,hc33,11,hco33,10,dih33,0\H,13,hc34,11,hco34,10,dih34,0\H,14,hc35,13,hcc35,11,dih35,0\H,14,hc36,13,hcc36,11,dih36,0\H,14,hc37,13,hcc37,11,dih37,0\H,15,hn38,8,hnc38,7,dih38,0\H,19,hc39,18,hcc39,16,dih39,0\H,20,hc40,19,hcc40,18,dih40,0\H,21,hc41,20,hcc41,19,dih41,0\H,23,hc42,18,hcc42,16,dih42,0\cc2=1.53072415\cc3=1.5357636\ccc3=110.22300237\cc4=1.50479845\ccc4=110.58522857\dih4=314.23090716\cc5=1.36093488\ccc5=126.22807178\dih5=15.75839941\cc6=1.53620225\ccc6=111.8542382\dih6=62.12027443\sec7=1.90047742\secc7=120.96434908\dih7=195.78939799\cse8=1.87785318\csec8=86.2656315\dih8=179.63343816\cc9=1.45745754\ccc9=114.41838267\dih9=180.87373049\cc10=1.46758468\ccc10=127.5295667\dih10=177.2191624\oc11=1.34480967\occ11=114.62254164\dih11=356.21672582\oc12=1.22852662\occ12=124.44437982\dih12=176.77271698\co13=1.44991656\coc13=116.32812791\dih13=180.41481596\cc14=1.51476767\cco14=107.48629813\dih14=180.36348018\nc15=1.37566168\ncse15=122.63095566\dih15=180.11608821\cn16=1.37319694\cnc16=124.94169664\dih16=1.00572648\oc17=1.22360059\ocn17=121.69365742\dih17=357.90436184\cc18=1.49850538\ccn18=116.278837\dih18=178.3069897\cc19=1.39848398\ccc19=117.13103625\dih19=165.83553319\cc20=1.38929016\ccc20=120.19596986\dih20=179.62489806\cc21=1.39327761\ccc21=120.50483822\dih21=359.44320151\cc22=1.39095024\ccc22=118.86574875\dih22=-0.10141912\cc23=1.40006421\ccc23=123.15900943\dih23=344.42591233\clc24=1.75933024\clcc24=119.30400608\dih24=180.71912638\hc25=1.09679513\h

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\dih26=184.25009693\hc27=1.09618689\hcc27=109.44913873\dih27=301.80140
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283\hcc29=110.18616624\dih29=191.86605361\hc30=1.09832535\hcc30=109.56
548693\dih30=75.54948436\hc31=1.09103161\hcc31=109.77925846\dih31=193.
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211348\hco33=108.64489836\dih33=58.89352258\hc34=1.09203176\hco34=108.
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80.37035327\hc36=1.09208761\hcc36=111.07911306\dih36=60.76093569\hc37=
1.09207444\hcc37=111.00741779\dih37=299.9698808\hn38=1.02145386\hnc38=
112.55970118\dih38=183.65584156\hc39=1.08208114\hcc39=118.38681865\dih
39=-0.2433598\hc40=1.08368205\hcc40=120.0379582\dih40=179.57287543\hc4
1=1.08231925\hcc41=121.10940245\dih41=180.21204433\hc42=1.08251298\hcc
42=122.02081335\dih42=-0.54747992\\Version=x86-Linux-G03RevB.04\State=
1-A\HF=-3839.2491642\RMSD=7.546e-09\RMSF=1.782e-05\Dipole=-0.6426339,0
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29,0.1470491,-0.0395649,-0.0004563,-0.0380056,0.0522946,0.1693262,-0.0
549131,-0.0451921,0.0674348,0.0998239,-0.0220254,0.0267596,-0.0482834,
0.039134,0.0451622,0.0408635,-0.0541826,-0.0024791,0.2186197,-0.015051
1,-0.1484782,0.068243,0.1613731,-0.122945,-0.0096535,0.0559854,-0.1973
77,-0.0500033,0.0423531,-0.1285329,0.1181095,-0.1374771,-0.0106978,-0.
0582244,-0.042124,0.1913126,-0.1314474,0.0750714,0.2735528,-0.1168666,
0.0394946,0.1611109,0.0156261,-0.0055804,-0.0058483,0.1622876,-0.04233
59,-0.021799,-0.0225406,0.0805007,0.4640864,-0.1883993,0.0336833,-0.11
50381,0.0989396,-0.1824574,0.1249085,-0.2336754,-0.0826526,0.8835295,-
0.2677745,0.4312914,-0.622491,0.4504583,0.1366124,-0.0545025,0.4237649
,0.535785,-0.3983093,-0.0808426,-0.4042331,-0.2232512,-0.1877325,-0.36
33117,-0.6151434,-0.2202745,-0.9451249,1.6546286,-0.1712522,0.7280329,
-0.0520362,0.8341065,0.7745318,0.8539566,0.6136303,1.8671606,-1.295655
3,-0.110466,-0.9489427,-0.0967497,-0.4634443,-0.3920522,-0.8666229,-0.
3653166,-1.3968535,-0.8985725,0.3055967,0.0298574,0.2426247,-0.7049975
, -0.3818656,-0.0754269,-0.2914641,-0.8299703,0.463964,0.0974484,0.2382
697,0.2423504,0.4333396,0.3504588,0.4235348,0.2283544,0.9477078,-0.012
7501,0.0043242,-0.0672905,-0.002306,0.0906506,-0.0110685,-0.0790225,-0
.0069009,0.026825,-1.9297564,0.8256736,-0.4072524,0.7990212,-0.7235985
,0.0052156,-0.5024266,0.0629185,-0.5830136,2.044873,-1.0332678,0.24374
15,-0.5334756,0.864409,0.3484748,0.9526598,-0.1266394,0.9996411,-0.966
1828,0.4022316,-0.0507536,0.0906175,-0.6078457,-0.3274286,-0.492723,-0
.0386096,-0.8249552,-0.1699854,0.194216,0.1093014,0.1582983,-0.1536829
, -0.042988,0.1307338,-0.0591402,-0.0380099,-0.0965069,-0.044071,-0.054
7718,0.08044,-0.0640445,0.0578837,0.0971149,-0.016223,-0.0347503,0.150
2868,-0.031102,0.1047182,-0.0053406,-0.0858952,0.032953,0.1176039,0.02
094,-0.0434595,-0.0592792,-0.0530323,-0.0576014,-0.007874,-0.1501807,-
0.0753758,-0.0095586,-0.1055565,-0.1497184,-0.0944814,0.1744862,0.1522
811,-0.0387906,0.6743066,0.6477554,-0.0121106,0.7563826,0.5489827,-0.0
687439,0.0368698,-0.0000551,0.0487937,-0.2309091,-0.1319737,-0.056012,
-0.0881585,-0.1492179,-0.0695663,-0.0900004,-0.0832793,0.0362775,-0.49
68277,-0.3621093,0.0263062,-0.4318461,-0.4127741,0.0123431,-0.1128258,
0.0558784,-0.0372568,-0.1227636,0.0494036,0.0413028,0.0259059,-0.00914
7,-0.1923334,0.0778002,-0.0872417,0.0317481,0.0353173,-0.0024863,-0.08
68236,0.0127458,0.0013659,-0.0233162,-0.0584429,0.0196858,-0.1285445,-
0.0707173,0.0824255,0.0040641,0.0498225,-0.0033088,-0.074439,0.1254999
,0.0556696,0.1459368,-0.1079891,-0.0951461,0.0418863,-0.0695938,-0.000
4293,0.0037768,0.0404068,-0.0176158,0.0251054,0.0372559,0.0488675,0.02
40068,-0.0244254,-0.1553146,-0.048199,-0.0203518,0.0306386,0.0133217,-
0.1961758,-0.0543043,0.044428,0.0037346,0.0377686,-0.0107348,0.0199423
,0.0285003,0.0205007,0.0670701,0.0460193,-0.0186503,0.0227082,-0.11975

91,-0.1130553,-0.0528635,-0.0595249,-0.0645889,-0.0822909,0.0046789,-0.0206534,0.0383897,0.0510229,0.0243788,0.030073,-0.0214368,-0.0231415,-0.1109502,-0.0338111,-0.072943,0.0472591,-0.0624728,-0.0692519,-0.0264041,0.0759658,-0.0826718,0.0111834,-0.019008,-0.0188855,-0.0196232,-0.0897294,0.0364135,0.00469,-0.030475,-0.0203619,0.0092249,-0.1154673,-0.0607089,-0.0954852,-0.0868257,0.0287204,-0.0085751,-0.0181247,0.0442694,-0.1135191,0.0715809,0.0078955,0.0374914,0.0833959,-0.0500944,-0.0205872,0.0520747,-0.0036076,0.0616558,0.0575822,0.1184207,0.0434835,-0.0109088,0.3396155,0.0088727,0.1138028,0.0378962,0.2200302,0.0307878,0.186248,-0.0189078,0.3729847,0.1579684,-0.0246223,0.0018287,-0.0242991,0.0722373,-0.0585238,-0.0327268,-0.0480373,0.0682077,-0.0638967,0.0219758,-0.0741707,0.0126426,0.0821897,-0.0372389,-0.0810077,-0.0340896,0.0622327,0.0332743,0.064654,0.0099503,0.07228,0.0513674,-0.04279,0.0135385,-0.0456965,0.1016957,0.0282306,-0.003338,-0.0446829,-0.0351792,0.1334928,-0.0142718,-0.0537074,-0.0085241,0.0882995\Polar=321.8494459,-86.1221624,242.8681463,39.0163114,69.964092,238.9305532\PG=C01 [X(C18H18C11N1O3Se1)]\@

Ethyl 2-[3-methoxybenzoylamino]-4,5,6,7-tetrahydro-1-benzoselenophene-3-carboxylate (9, X = *m*-OMe)

B3LYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET20\FOpt\RB3LYP\6-311G(d,p)\C19H21N1O4Se1\KAUMANN\07-Feb-2005\1\#\B3LYP/6-311G** OPT=(GRAD,READFC) GUESS=CHECK GEOM=CHECKPOINT FREQ=NORAMAN\m-Methoxy Benzoyl protected Selenophene\0,1\C\C,1,cc2\C,2,cc3,1,ccc3\C,3,cc4,2,ccc4,1,dih4,0\C,4,cc5,3,ccc5,2,dih5,0\C,1,cc6,2,ccc6,3,dih6,0\Se,4,sec7,3,secc7,2,dih7,0\C,7,cse8,4,csec8,3,dih8,0\C,5,cc9,4,ccc9,3,dih9,0\C,9,cc10,5,ccc10,4,dih10,0\O,10,oc11,9,occ11,5,dih11,0\O,10,oc12,9,occ12,5,dih12,0\C,11,co13,10,coc13,9,dih13,0\C,13,cc14,11,cco14,10,dih14,0\N,8,nc15,7,ncse15,4,dih15,0\C,15,cn16,8,cnc16,7,dih16,0\O,16,oc17,15,ocn17,8,dih17,0\C,16,cc18,15,ccn18,8,dih18,0\C,18,cc19,16,ccc19,15,dih19,0\C,19,cc20,18,ccc20,16,dih20,0\C,20,cc21,19,ccc21,18,dih21,0\C,21,cc22,20,ccc22,19,dih22,0\C,18,cc23,16,ccc23,15,dih23,0\O,22,oc24,21,occ24,20,dih24,0\C,24,co25,22,coc25,21,dih25,0\H,1,hc26,2,hcc26,3,dih26,0\H,1,hc27,2,hcc27,3,dih27,0\H,2,hc28,1,hcc28,6,dih28,0\H,2,hc29,1,hcc29,6,dih29,0\H,3,hc30,2,hcc30,1,dih30,0\H,3,hc31,2,hcc31,1,dih31,0\H,6,hc32,1,hcc32,2,dih32,0\H,6,hc33,1,hcc33,2,dih33,0\H,13,hc34,11,hco34,10,dih34,0\H,13,hc35,11,hco35,10,dih35,0\H,14,hc36,13,hcc36,11,dih36,0\H,14,hc37,13,hcc37,11,dih37,0\H,14,hc38,13,hcc38,11,dih38,0\H,15,hc39,8,hnc39,7,dih39,0\H,19,hc40,18,hcc40,16,dih40,0\H,20,hc41,19,hcc41,18,dih41,0\H,21,hc42,20,hc42,19,dih42,0\H,23,hc43,18,hcc43,16,dih43,0\H,25,hc44,24,hco44,22,dih44,0\H,25,hc45,24,hco45,22,dih45,0\H,25,hc46,24,hco46,22,dih46,0\cc2=1.53073022\cc3=1.53581601\ccc3=110.18734097\cc4=1.50481273\ccc4=110.62814596\dih4=314.3669575\cc5=1.36037899\ccc5=126.24622398\dih5=15.54406917\cc6=1.53609592\ccc6=111.84918474\dih6=62.1452991\sec7=1.90188562\secc7=120.93119658\dih7=195.46482218\cse8=1.87818297\csec8=86.25237047\dih8=179.66332362\cc9=1.45850149\ccc9=114.43629117\dih9=180.89238885\cc10=1.46560099\ccc10=127.50941827\dih10=176.92411929\oc11=1.34665415\oc11=114.54784455\dih11=356.58436626\oc12=1.2294683\occ12=124.66591269\dih12=177.15712468\co13=1.44809741\coc13=116.42689896\dih13=180.27750089\cc14=1.51509162\cco14=107.48303134\dih14=180.63792559\nc15=1.37287523\ncse15=122.48938601\dih15=179.98630782\cn16=1.37801889\cnc16=125.11644375\dih16=1.01905819\oc17=1.22339317\ocn17=121.29867478\dih17=357.85265645\cc18=1.49550717\ccn18=115.92149712\dih18=178.50384178\cc19=1.39430909\ccc19=117.37920658\dih19=162.79468517\cc20=1.39359568\ccc20=1

19.52811121\dih20=180.32786731\cc21=1.38702324\ccc21=120.65903204\dih21=359.53610944\cc22=1.40144524\ccc22=120.02187207\dih22=-0.24974604\cc23=1.40401147\ccc23=122.38232035\dih23=342.00730996\oc24=1.36115298\oc24=115.80334632\dih24=180.58926878\co25=1.42286639\coc25=118.54818241\dih25=180.00577965\hc26=1.09681337\hcc26=108.90921437\dih26=301.18077199\hc27=1.09418914\hcc27=110.5917249\dih27=184.28479239\hc28=1.09621159\hcc28=109.44226488\dih28=301.83825126\hc29=1.09406226\hcc29=110.87515427\dih29=183.99736347\hc30=1.09545167\hcc30=110.17084147\dih30=191.99590127\hc31=1.0983746\hcc31=109.55218742\dih31=75.71986735\hc32=1.09106044\hcc32=109.74884725\dih32=192.92026629\hc33=1.0965101\hcc33=109.9998384\dih33=77.42589322\hc34=1.09236437\hco34=108.71412332\dih34=59.2278688\hc35=1.09218711\hco35=108.77998439\dih35=302.23509665\hc36=1.09316605\hcc36=109.68711079\dih36=180.38933224\hc37=1.09203437\hcc37=111.03904334\dih37=60.75615706\hc38=1.09204204\hcc38=110.98097412\dih38=300.03481029\hn39=1.02000414\hnc39=112.8606758\dih39=184.2191268\hc40=1.0817926\hcc40=118.84695314\dih40=0.24884317\hc41=1.08398265\hcc41=119.85902264\dih41=179.52625175\hc42=1.08321411\hcc42=121.66457154\dih42=180.11173181\hc43=1.0811693\hcc43=120.47512614\dih43=358.14462473\hc44=1.08852408\hco44=105.71486937\dih44=178.47587294\hc45=1.09520643\hco45=111.61912595\dih45=59.58865355\hc46=1.09559044\hco46=111.41810439\dih46=297.05923899\Version=x86-Linux-G03RevB.04\State=1-A\HF=-3494.1824564\RMSD=6.864e-09\RMSF=1.134e-05\Dipole=-1.0503237,-0.4110604,-1.1892549\PG=C01 [X(C19H21N1O4Se1)]\@

2-Amino-3-carboxy-1H-selenophenium (12a)

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET23\FOpt\RBHandHLYP\6-311G(d,p)\C5H6N1O2Se1(1+)\KAUMANN\30-Aug-2005\1\#\BHANDHLYP/6-311G** OPT=(GRAD,READFC) GUESS=CHECK GEOM=CHECKPOINT FREQ=NORAMAN\Selenophene Protonated at Selenium\1,1\Se\C,1,R1\N,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\H,3,R4,2,A3,1,D2,0\C,2,R5,3,A4,4,D3,0\C,6,R6,2,A5,3,D4,0\O,7,R7,6,A6,2,D5,0\O,7,R8,6,A7,2,D6,0\H,9,R9,7,A8,6,D7,0\C,6,R10,2,A9,1,D8,0\H,11,R11,6,A10,2,D9,0\C,11,R12,6,A11,2,D10,0\H,13,R13,11,A12,6,D11,0\H,1,R14,2,A13,3,D12,0\R1=1.95341288\R2=1.32079396\R3=0.99902893\R4=1.01104245\R5=1.35899514\R6=1.4678016\R7=1.1985973\R8=1.31937437\R9=0.95893177\R10=1.44304583\R11=1.07665339\R12=1.33165279\R13=1.07031035\R14=1.46980588\A1=120.60175836\A2=123.38921106\A3=115.68245724\A4=131.02667884\A5=119.00896992\A6=122.74460983\A7=112.76989352\A8=109.23688692\A9=115.89385299\A10=120.13155733\A11=118.76008332\A12=131.5279354\A13=93.49424589\D1=15.57800421\D2=181.21300948\D3=193.21211072\D4=3.33246961\D5=-2.38904556\D6=177.7047138\D7=-180.19585919\D8=0.19877212\D9=182.46403107\D10=1.63311354\D11=184.39846372\D12=77.71217234\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.4204283\RMSD=5.252e-09\RMSF=9.313e-06\Dipole=0.6747999,-0.211661,-1.4187492\PG=C01 [X(C5H6N1O2Se1)]\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET9\FOpt\RBHandHLYP\CC-pVDZ\C5H6N1O2Se1(1+)\KAUMANN\30-Aug-2005\1\#\BHANDHLYP/CC-pVDZ OPT=(GRAD,READFC) GUESS=CHECK GEOM=CHECKPOINT FREQ=NORAMAN\Selenophene Protonated at Selenium\1,1\Se\C,1,R1\N,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\H,3,R4,2,A3,1,D2,0\C,2,R5,3,A4,4,D3,0\C,6,R6,2,A5,3,D4,0\O,7,R7,6,A6,2,D5,0\O,7,R8,6,A7,2,D6,0\H,9,R9,7,A8,6,D7,0\C,6,R10,2,A9,1,D8,0\H,11,R11,6,A10,2,D9,0\C,11,R12,6,A11,2,D10,0\H,13,R13,11,A12,6,D11,0\H,1,R14,2,A13,3,D12,0\R1=1.95506746\R2=1.32229703\R3=1.00386364\R4=1.01764358\R5=1.36448607\R6=

1.46908453\R7=1.20417551\R8=1.3208777\R9=0.96441584\R10=1.44417747\R11=1.0844003\R12=1.33810996\R13=1.07936675\R14=1.47595285\A1=121.00166378\A2=123.279806\A3=114.76279678\A4=130.59800006\A5=118.8742574\A6=122.78528202\A7=112.82747874\A8=108.62318255\A9=115.77880992\A10=120.20807248\A11=118.75495824\A12=131.34305085\A13=93.53057161\D1=16.45971796\D2=180.48641345\D3=194.08379782\D4=3.47306047\D5=-2.18186684\D6=177.88946222\D7=-180.14958842\D8=0.40159949\D9=182.39124921\D10=1.53403848\D11=184.53400631\D12=77.18697571\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.3578819\RMSD=4.806e-09\RMSF=1.329e-05\Dipole=0.6890458,-0.2244959,-1.3595395\PG=C01 [X(C5H6N1O2Se1)]\@

3-Carboxy-2-imino-2,5-dihydro-1H-selenophenium (12b)

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET3\FOpt\RBHandHLYP\6-311G(d,p)\C5H6N1O2Se1(1+)\KAUMANN\23-Aug-2005\1\#\BHANDHLYP/6-311G** OPT=(GRAD,READFC) GUESS=(CHECK,READ) GEOM=CHECKPOINT OPTCYC=200 FREQ=NORAMAN\\Broken Protonated Selenophene (Tautomer)\\1,1\C\C,1,cc2\Se,2,sec3,1,secc3\C,3,cse4,2,csec4,1,dih4,0\C,1,cc5,2,ccc5,3,dih5,0\N,4,nc6,3,ncse6,2,dih6,0\C,5,cc7,1,ccc7,2,dih7,0\O,7,oc8,5,occ8,1,dih8,0\O,7,oc9,5,occ9,1,dih9,0\H,1,hc10,2,hcc10,3,dih10,0\H,2,hc11,1,hcc11,5,dih11,0\H,2,hc12,1,hcc12,5,dih12,0\H,3,hse13,2,hsec13,1,dih13,0\H,6,hn14,4,hnc14,3,dih14,0\H,8,ho15,7,hoc15,5,dih15,0\\cc2=1.49341555\sec3=1.96191298\secc3=106.20911715\cse4=2.03612269\csec4=88.54437171\dih4=360.52047428\cc5=1.32574982\ccc5=120.72973739\dih5=-0.57298729\nc6=1.22250085\ncse6=116.94271851\dih6=179.20969534\cc7=1.49114556\ccc7=124.59483601\dih7=180.70764219\oc8=1.31676102\occ8=112.18226594\dih8=359.8181685\oc9=1.19026395\cc9=122.38071949\dih9=179.87207514\hc10=1.07704946\hcc10=117.89942653\dih10=180.28104897\hc11=1.08309154\hcc11=112.99415671\dih11=239.60601855\hc12=1.08410958\hcc12=112.19411775\dih12=116.39808775\hse13=1.46386563\hsec13=96.72331218\dih13=266.46802105\hn14=1.01840732\hnc14=112.93137959\dih14=179.61820558\ho15=0.9595243\hoc15=109.44324446\dih15=179.97926599\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.4186782\RMSD=3.116e-09e1)\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET20\FOpt\RBHandHLYP\CC-pVDZ\C5H6N1O2Se1(1+)\KAUMANN\23-Aug-2005\1\#\BHANDHLYP/CC-pVDZ OPT=(GRAD,READFC) GUESS=(CHECK,READ) GEOM=CHECKPOINT OPTCYC=200 FREQ=NORAMAN\\Broken Protonated Selenophene (Tautomer)\\1,1\C\C,1,cc2\Se,2,sec3,1,secc3\C,3,cse4,2,csec4,1,dih4,0\C,1,cc5,2,ccc5,3,dih5,0\N,4,nc6,3,ncse6,2,dih6,0\C,5,cc7,1,ccc7,2,dih7,0\O,7,oc8,5,occ8,1,dih8,0\O,7,oc9,5,occ9,1,dih9,0\H,1,hc10,2,hcc10,3,dih10,0\H,2,hc11,1,hcc11,5,dih11,0\H,2,hc12,1,hcc12,5,dih12,0\H,3,hse13,2,hsec13,1,dih13,0\H,6,hn14,4,hnc14,3,dih14,0\H,8,ho15,7,hoc15,5,dih15,0\\cc2=1.49444617\sec3=1.96227992\secc3=106.34792855\cse4=2.03605085\csec4=88.5767804\dih4=360.79067055\cc5=1.33122639\ccc5=120.5552845\dih5=-0.83578408\nc6=1.22911235\ncse6=117.14010666\dih6=178.92407662\cc7=1.49194513\ccc7=124.70108123\dih7=180.81129543\oc8=1.31843338\occ8=112.23293016\dih8=359.69345618\oc9=1.19564116\occ9=122.40323286\dih9=179.74288966\hc10=1.08483813\hcc10=118.05796892\dih10=180.07543251\hc11=1.0918004\hcc11=113.1873424\dih11=239.06808937\hc12=1.09299062\hcc12=112.24046648\dih12=116.05662696\hse13=1.4696337\hsec13=96.87149618\dih13=266.65375604\hn14=1.02585499\hnc14=111.48080391\dih14=179.62403338\ho15=0.96508033\hoc15=108.81284546\dih15=179.96527469\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.3570336\RMSD=8.768e

-09\RMSF=1.503e-05\Dipole=-1.5089081,-0.3956936,1.1325087\PG=C01 [X(C5H6N1O2Se1)]\@

3-Carboxy-2-imino-2,3-dihydro-1H-selenophenium (12c)

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET8\FOpt\RBHandHLYP\6-311G(d,p)\C5H6N1O2Se1(1+)\KAUMANN\30-Aug-2005\1\#\BHANDHLYP/6-311G** OPT=(GRAD,READFC) GUESS=CHECK GEOM=CHECKPOINT FREQ=NORAMAN\Selenophene Tautomer Protonated at Selenium\1,1\H\Se,1,R1\C,2,R2,1,A1\N,3,R3,2,A2,1,D1,0\H,4,R4,3,A3,2,D2,0\C,3,R5,2,A4,1,D3,0\H,6,R6,3,A5,2,D4,0\C,6,R7,3,A6,2,D5,0\O,8,R8,6,A7,3,D6,0\O,8,R9,6,A8,3,D7,0\H,10,R10,8,A9,6,D8,0\C,6,R11,3,A10,4,D9,0\H,12,R12,6,A11,3,D10,0\C,12,R13,6,A12,3,D11,0\H,14,R14,12,A13,6,D12,0\|R1=1.46896939\R2=2.0998278\R3=1.21253258\R4=1.00677916\R5=1.50905024\R6=1.08397746\R7=1.53368405\R8=1.17626834\R9=1.3324486\R10=0.95992568\R11=1.49643998\R12=1.07778176\R13=1.31778096\R14=1.07306858\A1=95.48114416\A2=126.35551442\A3=122.91252542\A4=104.85655112\A5=108.22141723\A6=110.31645252\A7=123.95073739\A8=109.88249742\A9=109.77931633\A10=109.74078619\A11=118.67146776\A12=120.59181256\A13=127.83425105\D1=-60.96817503\D2=-2.02554249\D3=118.54607502\D4=-147.11424247\D5=95.81638465\D6=140.03110651\D7=-41.87167055\D8=181.22461682\D9=154.89844407\D10=-164.41873537\D11=17.37509642\D12=-182.37181729\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.3950403\RMSD=5.427e-09\RMSF=1.791e-05\Dipole=-1.293281,-0.3191675,-1.3225639\PG=C01 [X(C5H6N1O2Se1)]\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET19\FOpt\RBHandHLYP\CC-pVDZ\C5H6N1O2Se1(1+)\KAUMANN\30-Aug-2005\1\#\BHANDHLYP/CC-PVDZ OPT=(GRAD,READFC) GUESS=CHECK GEOM=CHECKPOINT FREQ=NORAMAN\Selenophene Tautomer Protonated at Selenium\1,1\H\Se,1,R1\C,2,R2,1,A1\N,3,R3,2,A2,1,D1,0\H,4,R4,3,A3,2,D2,0\C,3,R5,2,A4,1,D3,0\H,6,R6,3,A5,2,D4,0\C,6,R7,3,A6,2,D5,0\O,8,R8,6,A7,3,D6,0\O,8,R9,6,A8,3,D7,0\H,10,R10,8,A9,6,D8,0\C,6,R11,3,A10,4,D9,0\H,12,R12,6,A11,3,D10,0\C,12,R13,6,A12,3,D11,0\H,14,R14,12,A13,6,D12,0\|R1=1.47514337\R2=2.09832149\R3=1.21914204\R4=1.01284866\R5=1.51092988\R6=1.09124583\R7=1.53379988\R8=1.18129813\R9=1.33419105\R10=0.96589214\R11=1.49779244\R12=1.08589889\R13=1.32423438\R14=1.08226279\A1=95.74406065\A2=126.54138244\A3=121.90654951\A4=104.76426117\A5=108.35569064\A6=110.14349475\A7=124.07409013\A8=109.78084713\A9=109.16075553\A10=109.51491497\A11=118.89111364\A12=120.43011639\A13=127.69550554\D1=-59.81312932\D2=-1.89020272\D3=119.84747051\D4=-148.47041833\D5=94.33273648\D6=140.31189874\D7=-41.52805688\D8=181.20096625\D9=153.81259386\D10=-163.76604077\D11=18.23059189\D12=-182.50758617\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.3323892\RMSD=7.231e-09\RMSF=2.146e-05\Dipole=-1.2197462,-0.2881856,-1.3449168\PG=C01 [X(C5H6N1O2Se1)]\@

3-(Dihydroxymethylene)-2-imino-2,3-dihydro-1H-selenophenium (12d)

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET17\FOpt\RBHandHLYP\6-311G(d,p)\C5H6N1O2Se1(1+)\KAUMANN\23-Aug-2005\1\#\BHANDHLYP/6-311G** OPT=(GRAD,READFC) GUESS=CHECK GEOM=CHECKPOINT FREQ=NORAMAN\Selenophene Tautomer Protonated at Selenium\1,1\H\Se,1,R1\C,2,R2,1,A1\N,3,R3,2,A2,1,D1,0\H,4,R4,3,A3,2,D2,0\C,3,R5,2,A4,1,D3,0\C,6,R6,3,A5,2,D4,0\O,7,R7,6,A6,3,D5,

```

0\H,8,R8,7,A7,6,D6,0\O,7,R9,6,A8,3,D7,0\H,10,R10,7,A9,6,D8,0\C,6,R11,3
,A10,4,D9,0\H,12,R12,6,A11,3,D10,0\C,12,R13,6,A12,3,D11,0\H,14,R14,12,
A13,6,D12,0\|R1=1.47016311\R2=2.04336576\R3=1.24447255\R4=1.00442148\R
5=1.42872252\R6=1.38416217\R7=1.28812824\R8=0.97965282\R9=1.29688126\R
10=0.9592518\R11=1.43302581\R12=1.07684574\R13=1.33236969\R14=1.070314
28\A1=93.2717559\A2=126.14385635\A3=121.18287945\A4=105.00447053\A5=11
8.36326883\A6=124.0095584\A7=110.83586478\A8=119.91100759\A9=111.17515
21\A10=116.74289839\A11=120.20569045\A12=119.44233755\A13=129.6656867\
D1=-80.40974524\D2=-1.97694439\D3=99.98212395\D4=178.66453506\D5=0.888
70263\D6=-0.21051234\D7=180.67703006\D8=180.14001516\D9=-179.22523008\
D10=177.47281477\D11=-1.80555121\D12=-182.88148156\|Version=x86-Linux-
G03RevB.04\State=1-A\HF=-2800.4093072\RMSD=5.255e-09\RMSF=2.468e-05\Di
pole=-0.2819653,-0.1464388,-0.3328685\PG=C01 [X(C5H6N1O2Se1)]\|@

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BHandHLYP/cc-pVDZ

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET14\FOpt\RBHandHLYP\CC-pVDZ\C5H6N1O
2Se1(1+)\KAUMANN\30-Aug-2005\1\|#BHANDHLYP/CC-PVDZ OPT=(GRAD,READFC) G
UESS=CHECK GEOM=CHECKPOINT FREQ=NORAMAN\|Selenophene Tautomer Protonat
ed at Selenium\|1,1\H\Se,1,R1\C,2,R2,1,A1\N,3,R3,2,A2,1,D1,0\H,4,R4,3,
A3,2,D2,0\C,3,R5,2,A4,1,D3,0\C,6,R6,3,A5,2,D4,0\O,7,R7,6,A6,3,D5,0\H,8
,R8,7,A7,6,D6,0\O,7,R9,6,A8,3,D7,0\H,10,R10,7,A9,6,D8,0\C,6,R11,3,A10,
4,D9,0\H,12,R12,6,A11,3,D10,0\C,12,R13,6,A12,3,D11,0\H,14,R14,12,A13,6
,D12,0\|R1=1.47671401\R2=2.03915523\R3=1.25148375\R4=1.00996778\R5=1.4
3107965\R6=1.38976281\R7=1.28909314\R8=0.98990796\R9=1.29861942\R10=0.
96467\R11=1.43438978\R12=1.08454939\R13=1.33891319\R14=1.07930031\A1=9
3.38028043\A2=126.41606067\A3=120.4372675\A4=105.15303919\A5=117.97380
311\A6=123.61466206\A7=109.84382436\A8=119.93028731\A9=110.62971739\A1
0=116.67097403\A11=120.34026022\A12=119.31679588\A13=129.55354104\D1=-
80.09031911\D2=-1.80650453\D3=100.40184981\D4=178.59322627\D5=0.847417
97\D6=-0.18133464\D7=180.66028168\D8=180.10770584\D9=-179.26119604\D10
=177.52492023\D11=-1.73519136\D12=-182.9475851\|Version=x86-Linux-G03R
evB.04\State=1-A\HF=-2800.3488834\RMSD=1.615e-09\RMSF=2.919e-05\Dipole
=-0.2244762,-0.1258937,-0.3443344\PG=C01 [X(C5H6N1O2Se1)]\|@

```

Transition state (13a)

BHandHLYP/6-311G**

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET3\FTS\RBHandHLYP\6-311G(d,p)\C5H6N
1O2Se1(1+)\KAUMANN\02-Sep-2005\1\|#BHANDHLYP/6-311G** OPT=(GRAD,TS,NOF
REEZE,NOEIGENTEST,READFC) GUESS=(CHECK,READ) GEOM=CHECKPOINT OPTCYC=20
0 FREQ=NORAMAN\|Broken Protonated Selenophene (Tautomer)\|1,1\C\C,1,cc
2\Se,2,sec3,1,secc3\C,3,cse4,2,csec4,1,dih4,0\C,1,cc5,2,ccc5,3,dih5,0\
N,4,nc6,3,ncse6,2,dih6,0\C,5,cc7,1,ccc7,2,dih7,0\O,7,oc8,5,occ8,1,dih8
,0\O,7,oc9,5,occ9,1,dih9,0\H,1,hc10,2,hcc10,3,dih10,0\H,2,hc11,1,hcc11
,5,dih11,0\H,2,hc12,1,hcc12,5,dih12,0\H,3,hse13,2,hsec13,1,dih13,0\H,6
,hn14,4,hnc14,3,dih14,0\H,8,ho15,7,hoc15,5,dih15,0\|cc2=1.48407207\sec
3=1.94473282\secc3=111.25804814\csec4=83.02332554\dih4=360.48023307\cc
5=1.32900919\ccc5=125.37529577\dih5=-0.60095148\nc6=1.15652186\ncse6=1
14.66103263\dih6=179.57655267\cc7=1.50202288\ccc7=123.79797236\dih7=18
0.58603821\oc8=1.31816266\occ8=111.40440165\dih8=359.84703415\oc9=1.18
634704\oc9=122.71111239\dih9=179.88414512\hc10=1.07835899\hcc10=116.9
2128163\dih10=180.04991349\hc11=1.08376803\hcc11=110.92792998\dih11=23
6.51452966\hc12=1.08553992\hcc12=109.91263581\dih12=118.27293628\hse13
=1.46066458\hsec13=95.74139463\dih13=270.3600591\hn14=1.00184615\hnc14

```

```
=149.75269773\dih14=179.91004611\ho15=0.95938416\hoc15=109.31815513\di
h15=179.96460712\cse4=2.53457791\\Version=x86-Linux-G03RevB.04\State=1
-A\HF=-2800.4070909\RMSD=5.118e-09\RMSF=2.981e-05\Dipole=-0.3485194,-
.281619,0.0772031\PG=C01 [X(C5H6N1O2Se1)]\@
```

BHandHLYP/cc-pVDZ

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET7\FTS\RBHandHLYP\CC-pVDZ\C5H6N1O2S
e1(1+)\KAUMANN\02-Sep-2005\1\#\BHANDHLYP\CC-PVDZ OPT=(GRAD,TS,NOFREEZE
,NOEIGENTEST,READFC) GUESS=(CHECK,READ) GEOM=CHECKPOINT OPTCYC=200 FRE
Q=NORAMAN\Broken Protonated Selenophene (Tautomer)\1,1\C\C,1,cc2\Se,
2,sec3,1,secc3\C,3,cse4,2,csec4,1,dih4,0\C,1,cc5,2,ccc5,3,dih5,0\N,4,n
c6,3,ncse6,2,dih6,0\C,5,cc7,1,ccc7,2,dih7,0\O,7,oc8,5,occ8,1,dih8,0\O,
7,oc9,5,occ9,1,dih9,0\H,1,hc10,2,hcc10,3,dih10,0\H,2,hc11,1,hcc11,5,di
h11,0\H,2,hc12,1,hcc12,5,dih12,0\H,3,hse13,2,hsec13,1,dih13,0\H,6,hn14
,4,hnc14,3,dih14,0\H,8,ho15,7,hoc15,5,dih15,0\cc2=1.48484821\sec3=1.9
4458178\secc3=111.73153714\csec4=82.68115485\dih4=360.84696403\cc5=1.3
3492783\ccc5=125.54230253\dih5=-1.00293977\nc6=1.16195075\ncse6=114.11
382482\dih6=179.25133478\cc7=1.50264652\ccc7=123.90859112\dih7=180.668
0706\oc8=1.31989395\occ8=111.46668244\dih8=359.77813987\oc9=1.1914366\
occ9=122.62013063\dih9=179.81682502\hc10=1.08616672\hcc10=117.03798657
\dih10=179.69535006\hc11=1.09241074\hcc11=110.88509732\dih11=235.51685
286\hc12=1.09438177\hcc12=109.71197051\dih12=117.94791855\hse13=1.4665
745\hsec13=95.72339566\dih13=270.88535101\hn14=1.0072746\hnc14=149.816
7049\dih14=179.73119377\ho15=0.96494525\hoc15=108.66764992\dih15=179.9
6533676\cse4=2.56794243\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-28
00.343672\RMSD=6.816e-09\RMSF=3.299e-05\Dipole=-0.2903685,-0.2841941,-
0.0222912\PG=C01 [X(C5H6N1O2Se1)]\@
```

Transition state (13b)

BHandHLYP/6-311G**

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET19\FTS\RBHandHLYP\6-311G(d,p)\C5H6
N1O2Se1(1+)\CARLHS\09-Jan-2007\1\#\BHANDHLYP\6-311G** OPT=(TS,GRAD,NOE
IGENTEST,READFC,NOFREEZE) GEOM=CHECKPOINT GUESS=READ\Selenophene Prot
onated at Selenium ring-opening TS\1,1\Se\C,1,R1\N,2,R2,1,A1\H,3,R3,2
,A2,1,D1,0\H,3,R4,2,A3,1,D2,0\C,2,R5,3,A4,4,D3,0\C,6,R6,2,A5,3,D4,0\O,
7,R7,6,A6,2,D5,0\O,7,R8,6,A7,2,D6,0\H,9,R9,7,A8,6,D7,0\C,6,R10,2,A9,1,
D8,0\H,11,R11,6,A10,2,D9,0\C,11,R12,6,A11,2,D10,0\H,13,R13,11,A12,6,D1
1,0\H,1,R14,2,A13,3,D12,0\R2=1.25251229\R3=1.01232614\R4=1.01025968\R
5=1.30551973\R6=1.52847135\R7=1.18375577\R8=1.31174522\R9=0.96025074\R
10=1.44613099\R11=1.07419562\R12=1.33344831\R13=1.07531073\R14=1.45939
634\A1=106.15195557\A2=121.39978311\A3=121.63005446\A4=160.48723317\A5
=110.67475243\A6=122.36319408\A7=110.80391126\A8=109.54896648\A9=128.3
8323847\A10=115.15942465\A11=124.98433358\A12=120.1891672\A13=135.2163
0753\D1=104.19264849\D2=283.09785508\D3=322.64521784\D4=-43.71587228\D
5=11.73771032\D6=191.28298797\D7=-179.48268493\D8=-2.37138076\D9=182.6
1366378\D10=7.28218832\D11=173.1060046\D12=108.86590955\R1=2.94811391\
\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.3931936\RMSD=9.234e-0
9\RMSF=2.078e-05\Dipole=0.8375333,-0.1756629,0.5493761\PG=C01 [X(C5H6N
1O2Se1)]\@
```

BHandHLYP/cc-pVDZ

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET18\FTS\RBHandHLYP\CC-pVDZ\C5H6N1O2
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```

Se1(1+)\CARLHS\09-Jan-2007\1\#\BHANDHLYP/CC-PVDZ OPT=(TS,GRAD,NOEIGENT
EST,READFC,NOFREEZE) GEOM=CHECKPOINT GUESS=READ\\Selenophene Protonate
d at Selenium ring-opening TS\\1,1\Se\C,1,R1\N,2,R2,1,A1\H,3,R3,2,A2,1
,D1,0\H,3,R4,2,A3,1,D2,0\C,2,R5,3,A4,4,D3,0\C,6,R6,2,A5,3,D4,0\O,7,R7,
6,A6,2,D5,0\O,7,R8,6,A7,2,D6,0\H,9,R9,7,A8,6,D7,0\C,6,R10,2,A9,1,D8,0\
H,11,R11,6,A10,2,D9,0\C,11,R12,6,A11,2,D10,0\H,13,R13,11,A12,6,D11,0\H
,1,R14,2,A13,3,D12,0\\R2=1.25751789\R3=1.01746761\R4=1.01530447\R5=1.3
1570479\R6=1.52586316\R7=1.18919075\R8=1.31450283\R9=0.96566678\R10=1.
44672424\R11=1.08171248\R12=1.34010405\R13=1.08423496\R14=1.46587026\A
1=106.48789078\A2=121.31913602\A3=121.61681492\A4=158.81975088\A5=110.
77634418\A6=122.30924333\A7=110.98244029\A8=108.86244029\A9=128.077461
13\A10=115.30316209\A11=124.72127026\A12=120.15752724\A13=135.35646291
\D1=104.23143097\D2=283.20689326\D3=325.56594634\D4=-46.09260531\D5=10
.51516866\D6=189.9316718\D7=-179.4520912\D8=-1.51564243\D9=181.7753784
1\D10=6.40007859\D11=172.85610472\D12=109.34073757\R1=2.92564596\\Vers
ion=x86-Linux-G03RevB.04\State=1-A\HF=-2800.3311658\RMSD=8.053e-09\RMS
F=1.794e-05\Dipole=0.8421869,-0.1639942,0.5121563\PG=C01 [X(C5H6N1O2Se
1)]\@

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Structure (14a)

BHandHLYP/6-311G**

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FOpt\RBHandHLYP\6-311G(d,p)\C5H6
N1O2Se1(1+)\CARLHS\09-Jan-2007\0\#\BHANDHLYP/6-311G** OPT=READFC GEOM=
CHECKPOINT GUESS=READ\\Selenophene Protonated at Selenium ring-opening
product\\1,1\Se,0.8022289757,-0.1440877793,-2.0394966366\C,0.80639819
28,-0.0986156123,0.9593706623\N,2.0162047798,-0.1053137394,1.276689072
9\H,2.481440597,0.7329964967,1.6026742613\H,2.5699096775,-0.9499622851
,1.2366772525\C,-0.4720925772,0.1559319839,0.9269742825\C,-1.064397953
6,0.0980082592,2.3353584572\O,-0.3867706302,0.0283927442,3.3035099548\
O,-2.3741061653,0.1446405945,2.2928625487\H,-2.7260475984,0.1142038183
,3.1858327775\C,-1.3188635561,0.3795495076,-0.2240350158\H,-2.33605759
68,0.6360408237,0.0068628298\C,-0.9574985478,0.2092857371,-1.496824191
2\H,-1.6920925258,0.3015919231,-2.2767600623\H,0.4393698294,-1.0479160
677,-3.1252701238\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.393
1959\RMSD=5.349e-09\RMSF=1.443e-05\Dipole=0.8630664,-0.1364328,0.59347
67\PG=C01 [X(C5H6N1O2Se1)]\@

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BHandHLYP/cc-pVDZ

```

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET13\FOpt\RBHandHLYP\CC-pVDZ\C5H6N1O
2Se1(1+)\CARLHS\09-Jan-2007\0\#\BHANDHLYP/CC-PVDZ OPT\\Selenophene Pro
tonated at Selenium ring-opening product\\1,1\Se,0.8082681728,-0.14934
19924,-2.0411949256\C,0.8064462792,-0.1036729851,0.9705406878\N,2.0235
193519,-0.0946281733,1.2750588515\H,2.4853004867,0.756357487,1.5896795
775\H,2.5881543395,-0.9386343478,1.2373539637\C,-0.4804791275,0.154115
6504,0.9318146458\C,-1.0754032346,0.099449006,2.3366337522\O,-0.396697
3241,-0.0081309879,3.3073028263\O,-2.3849426969,0.1959135399,2.2987415
953\H,-2.7269288975,0.1648461975,3.2013238521\C,-1.3223454518,0.370369
7766,-0.2252641239\H,-2.3486938268,0.625143475,0.0019329921\C,-0.95195
08497,0.2020340421,-1.5029808315\H,-1.6933207302,0.2937604973,-2.28897
80289\H,0.4452497629,-0.9974817109,-3.1789170017\\Version=x86-Linux-G0
3RevB.04\State=1-A\HF=-2800.3311772\RMSD=4.646e-09\RMSF=1.284e-05\Dipo
le=0.8895757,-0.0940415,0.5832636\PG=C01 [X(C5H6N1O2Se1)]\@

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Structure (14b)**BHandHLYP/6-311G****

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET6\POpt\RBHandHLYP\6-311G(d,p)\C5H5
N1O2Se1\KAUMANN\31-Aug-2005\1\#\BHANDHLYP/6-311G** OPT=(GRAD,READFC) G
UESS=CHECK GEOM=CHECKPOINT OPTCYC=200 FREQ=NORAMAN\Broken Selenophene
(Tautomer)\0,1\H\Se,1,R1\C,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\H,3,R7,2,A6,
1,D5,0\C,3,R4,2,A3,1,D2,0\H,6,R5,3,A4,2,D3,0\C,6,R6,3,A5,2,D4,0\C,8,R8
,6,A7,3,D6,0\O,9,R9,8,A8,6,D7,0\O,9,R10,8,A9,6,D8,0\H,11,R11,9,A10,8,D
9,0\C,8,R12,6,A11,3,D10,0\X,13,1.,8,90.,6,D11,0\N,13,R14,14,A13,9,D12,
0\|R1=1.45776218\R2=1.97609671\R3=1.07511153\R4=1.47698998\R5=1.078271
91\R6=1.34056031\R7=1.08249497\R8=1.48292713\R9=1.19504095\R10=1.32591
012\R11=0.95673548\R12=1.42912288\R14=1.140563\A1=93.89352573\A2=107.9
5187211\A3=109.52393547\A4=115.49061939\A5=128.10364475\A6=104.1274408
2\A7=123.24053383\A8=124.80316366\A9=112.08805107\A10=107.92954596\A11
=118.79150844\A13=89.48028773\D1=51.71362322\D2=-72.79244993\D3=281.93
964821\D4=101.46517605\D5=-190.54876022\D6=-1.71537112\D7=-9.78228143\
D8=-189.10603663\D9=-181.14259396\D10=-180.86058613\D11=-68.15278771\D
12=151.65039218\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.09540
2\RMSD=6.411e-09\RMSF=5.708e-06\Dipole=-0.0816419,1.1663729,0.1980232\
PG=C01 [X(C5H5N1O2Se1)]\@

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BHandHLYP/cc-pVDZ

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET7\POpt\RBHandHLYP\CC-pVDZ\C5H5N1O2
Se1\KAUMANN\31-Aug-2005\1\#\BHANDHLYP/CC-pVDZ OPT=(GRAD,READFC) GUESS=
CHECK GEOM=CHECKPOINT OPTCYC=200 FREQ=NORAMAN\Broken Selenophene (Tau
tomer)\0,1\H\Se,1,R1\C,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\H,3,R7,2,A6,1,D5,
0\C,3,R4,2,A3,1,D2,0\H,6,R5,3,A4,2,D3,0\C,6,R6,3,A5,2,D4,0\C,8,R8,6,A7
,3,D6,0\O,9,R9,8,A8,6,D7,0\O,9,R10,8,A9,6,D8,0\H,11,R11,9,A10,8,D9,0\C
,8,R12,6,A11,3,D10,0\X,13,1.,8,90.,6,D11,0\N,13,R14,14,A13,9,D12,0\|R1
=1.46439947\R2=1.97563721\R3=1.0838786\R4=1.47937556\R5=1.08616867\R6=
1.34593477\R7=1.09073549\R8=1.48367956\R9=1.20038306\R10=1.32755779\R1
1=0.96222633\R12=1.43434159\R14=1.14908431\A1=93.57565417\A2=107.88642
191\A3=109.6639984\A4=115.77910275\A5=127.8879033\A6=104.23471839\A7=1
23.2114371\A8=124.81632546\A9=112.15922717\A10=107.28069301\A11=118.88
533519\A13=89.49893023\D1=50.93946903\D2=-73.31020569\D3=280.34156589\
D4=99.78373307\D5=-191.2709707\D6=-1.95452633\D7=-9.30058004\D8=-188.5
5756385\D9=-181.08845538\D10=-180.97482772\D11=-68.20492785\D12=151.50
579675\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.0317708\RMSD=5
.866e-09\RMSF=7.020e-06\Dipole=-0.0991566,1.1268286,0.1623216\PG=C01 [
X(C5H5N1O2Se1)]\@

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Selenol (15)**BHandHLYP/6-311G****

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET14\POpt\RBHandHLYP\6-311G(d,p)\C5H
5N1O2Se1\KAUMANN\02-Sep-2005\1\#\BHANDHLYP/6-311G** OPT=GRAD FREQ=NORA
MAN\Broken Protonated Selenophene (Tautomer)\0,1\H\Se,1,R1\C,2,R2,1,
A1\H,3,R3,2,A2,1,D1,0\C,3,R4,2,A3,1,D2,0\H,5,R5,3,A4,2,D3,0\C,5,R6,3,A
5,2,D4,0\H,7,R7,5,A6,3,D5,0\C,7,R8,5,A7,3,D6,0\O,9,R9,7,A8,5,D7,0\O,9,
R10,7,A9,5,D8,0\H,11,R11,9,A10,7,D9,0\C,7,R12,5,A11,3,D10,0\X,13,1.,7,
90.,5,D11,0\N,13,R14,14,A13,9,D12,0\|R1=1.453531\R2=1.889823\R3=1.0772
67\R4=1.323979\R5=1.076676\R6=1.516197\R7=1.083771\R8=1.523968\R9=1.18

```


6107\R10=1.327867\R11=0.957495\R12=1.459647\R14=1.138449\A1=98.016\A2=109.237\A3=133.599\A4=117.008\A5=129.459\A6=107.56\A7=109.454\A8=123.122\A9=112.564\A10=108.261\A11=114.434\A13=88.668\D1=175.531\D2=-4.63\D3=178.545\D4=0.565\D5=195.536\D6=82.047\D7=87.89\D8=-89.743\D9=-183.223\D10=-45.989\D11=-75.044\D12=164.629\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.0774744\RMSD=6.945e-09\RMSF=2.013e-05\Dipole=0.339509,0.8229866,0.5475557\PG=C01 [X(C5H5N1O2Se1)]\\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET2\POpt\RBHandHLYP\CC-pVDZ\C5H5N1O2Se1\KAUMANN\02-Sep-2005\1\#\BHANDHLYP/CC-PVDZ OPT=(GRAD,READFC) GUESS=(CHECK,READ) GEOM=CHECKPOINT FREQ=NORAMAN\Broken Protonated Selenophene (Tautomer)\0,1\H\Se,1,R1\C,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\C,3,R4,2,A3,1,D2,0\H,5,R5,3,A4,2,D3,0\C,5,R6,3,A5,2,D4,0\H,7,R7,5,A6,3,D5,0\C,7,R8,5,A7,3,D6,0\O,9,R9,7,A8,5,D7,0\O,9,R10,7,A9,5,D8,0\H,11,R11,9,A10,7,D9,0\C,7,R12,5,A11,3,D10,0\X,13,1.,7,90.,5,D11,0\N,13,R14,14,A13,9,D12,0\\R1=1.46013486\R2=1.88994942\R3=1.08630296\R4=1.33039177\R5=1.08465821\R6=1.51730418\R7=1.09104625\R8=1.52416228\R9=1.19099613\R10=1.32996479\R11=0.96320183\R12=1.46460831\R14=1.14687502\A1=97.88593093\A2=109.37167023\A3=133.57055278\A4=116.93556879\A5=129.31029572\A6=107.64299313\A7=109.66394457\A8=123.21080901\A9=112.60217287\A10=107.59269789\A11=114.30854033\A13=89.05929165\D1=174.71675757\D2=-5.50932405\D3=178.42164932\D4=0.61192123\D5=195.04433147\D6=81.46188212\D7=87.53439405\D8=-90.21257666\D9=-183.06190401\D10=-46.40963343\D11=-68.40605197\D12=168.7000572\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-2800.0137718\RMSD=7.453e-09\RMSF=3.055e-05\Dipole=0.3008591,0.8182547,0.5020127\PG=C01 [X(C5H5N1O2Se1)]\\@

(E)-2-Cyano-2-butenic acid (16)

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET19\FOpt\RBHandHLYP\6-311G(d,p)\C5H5N1O2\KAUMANN\31-Aug-2005\1\#\BHANDHLYP/6-311G** OPT=(GRAD,READFC) GUESS=CHECK GEOM=CHECKPOINT OPTCYC=200 FREQ=NORAMAN\Neutral Intermediate (Tautomer)\0,1\H\C,1,R1\C,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\C,3,R4,2,A3,1,D2,0\C,5,R6,3,A5,2,D4,0\O,6,R7,5,A6,3,D5,0\O,6,R8,5,A7,3,D6,0\H,8,R9,6,A8,5,D7,0\C,5,R10,3,A9,2,D8,0\X,10,1.,5,90.,3,D9,0\N,10,R11,11,90.,5,D10,0\H,2,R12,3,A10,4,D11,0\H,2,R13,3,A11,4,D12,0\\R1=1.08753435\R2=1.4824182\R3=1.07713657\R4=1.33417459\R6=1.48266233\R7=1.18909222\R8=1.33558965\R9=0.95614046\R10=1.42948559\R11=1.14020373\R12=1.0875347\R13=1.08212208\A1=109.69855517\A2=117.16909223\A3=126.26902283\A5=122.68307114\A6=124.16076557\A7=112.67671189\A8=107.14609646\A9=121.60843455\A10=109.69041184\A11=112.61929931\D1=-58.39727831\D2=121.60159565\D4=179.99912442\D5=-179.99756681\D6=0.00224441\D7=180.00022105\D8=0.00057795\D9=-89.9920025\D10=182.11265864\D11=58.38415968\D12=-180.00801692\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-398.6043588\RMSD=7.241e-09\RMSF=2.829e-05\Dipole=0.2124685,-1.9313654,-1.186097\PG=C01 [X(C5H5N1O2)]\\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET7\FOpt\RBHandHLYP\CC-pVDZ\C5H5N1O2\KAUMANN\31-Aug-2005\1\#\BHANDHLYP/CC-PVDZ OPT=(GRAD,READFC) GUESS=CHECK GEOM=CHECKPOINT OPTCYC=200 FREQ=NORAMAN\Neutral Intermediate (Tautomer)\0,1\H\C,1,R1\C,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\C,3,R4,2,A3,1,D2,0\C,5,R6,3,A5,2,D4,0\O,6,R7,5,A6,3,D5,0\O,6,R8,5,A7,3,D6,0\H,8,R9,6,A8,5,D7,0\C,5,R10,3,A9,2,D8,0\X,10,1.,5,90.,3,D9,0\N,10,R11,11,90.,5,D10,0\H,2,R12,3,A10,4,D11,0\H,2,R13,3,A11,4,D12,0\\R1=1.08753435\R2=1.4824182\R3=1.07713657\R4=1.33417459\R6=1.48266233\R7=1.18909222\R8=1.33558965\R9=0.95614046\R10=1.42948559\R11=1.14020373\R12=1.0875347\R13=1.08212208\A1=109.69855517\A2=117.16909223\A3=126.26902283\A5=122.68307114\A6=124.16076557\A7=112.67671189\A8=107.14609646\A9=121.60843455\A10=109.69041184\A11=112.61929931\D1=-58.39727831\D2=121.60159565\D4=179.99912442\D5=-179.99756681\D6=0.00224441\D7=180.00022105\D8=0.00057795\D9=-89.9920025\D10=182.11265864\D11=58.38415968\D12=-180.00801692\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-398.6043588\RMSD=7.241e-09\RMSF=2.829e-05\Dipole=0.2124685,-1.9313654,-1.186097\PG=C01 [X(C5H5N1O2)]\\@

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omer)\0,1\H\C,1,R1\C,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\C,3,R4,2,A3,1,D2,0\C,5,R6,3,A5,2,D4,0\O,6,R7,5,A6,3,D5,0\O,6,R8,5,A7,3,D6,0\H,8,R9,6,A8,5,D7,0\C,5,R10,3,A9,2,D8,0\X,10,1.,5,90.,3,D9,0\N,10,R11,11,90.,5,D10,0\H,2,R12,3,A10,4,D11,0\H,2,R13,3,A11,4,D12,0\|R1=1.09528114|R2=1.48319204|R3=1.08491918|R4=1.33971807|R6=1.48354557|R7=1.19423033|R8=1.33672713|R9=0.96166807|R10=1.43474891|R11=1.14871473|R12=1.09528738|R13=1.08998706|A1=109.75118174|A2=117.33977328|A3=126.23003805|A5=122.70095144|A6=124.05869012|A7=112.7781824|A8=106.51536355|A9=121.64148478|A10=109.7341892|A11=112.56154968|D1=-58.32668429|D2=121.67312469|D4=179.9977276|D5=-179.99968423|D6=0.00041096|D7=179.99974904|D8=-0.00139945|D9=-89.99367962|D10=182.0716298|D11=58.32931301|D12=-180.0036394\|Version=x86-Linux-G03RevB.04|State=1-A|HF=-398.5281186|RMSD=5.330e-09|RMSF=3.222e-05|Dipole=0.2129623,-1.8851718,-1.1592641|PG=C01 [X(C5H5N1O2)]\|@

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Selenyl radical (17)

BHandHLYP/6-311G**

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET20\FOpt\UBHandHLYP\6-311G(d,p)\C5H4N1O2Se1(2)\KAUMANN\19-Aug-2005\1\|#BHANDHLYP/6-311G** OPT=GRAD FREQ=NORAMAN\Selenophene Dimer Cleaved (Se radical)\0,2\Se\C,1,R1\H,2,R2,1,A1\H,2,R3,1,A2,3,D1,0\C,2,R4,1,A3,3,D2,0\H,5,R5,2,A4,1,D3,0\C,5,R6,2,A5,1,D4,0\C,7,R7,5,A6,2,D5,0\O,8,R8,7,A7,5,D6,0\O,8,R9,7,A8,5,D7,0\H,10,R10,8,A9,7,D8,0\C,7,R11,5,A10,2,D9,0\X,12,1.,7,90.,5,D10,0\N,12,R12,13,90.,7,D11,0\|R1=1.96283333|R2=1.08631203|R3=1.08116727|R4=1.4771202|R5=1.07613403|R6=1.33564565|R7=1.48289863|R8=1.18881189|R9=1.33425574|R10=0.95624918|R11=1.42843578|R12=1.14031299|A1=104.15769626|A2=108.43345874|A3=110.78866966|A4=117.0579114|A5=125.45280471|A6=122.54967641|A7=124.04281661|A8=112.55583308|A9=107.3054421|A10=121.57783075|D1=-115.61216657|D2=119.30499889|D3=294.37219416|D4=113.01049671|D5=181.00042635|D6=179.97587019|D7=-0.14581078|D8=179.82230055|D9=0.89412413|D10=270.47072124|D11=182.40316901\|Version=x86-Linux-G03RevB.04|State=2-A|HF=-2799.4710414|S2=0.75407|S2-1=0.|S2A=0.750008|RMSD=6.843e-09|RMSF=1.778e-05|Dipole=1.6747936,1.1494226,-0.4956438|PG=C01 [X(C5H4N1O2Se1)]\|@

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BHandHLYP/cc-pVDZ

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET15\FOpt\UBHandHLYP\CC-pVDZ\C5H4N1O2Se1(2)\KAUMANN\20-Aug-2005\1\|#BHANDHLYP/CC-pVDZ OPT=(GRAD,READFC) GUESS=(CHECK,READ) GEOM=CHECKPOINT FREQ=NORAMAN\Selenophene Dimer Cleaved (Se radical)\0,2\Se\C,1,R1\H,2,R2,1,A1\H,2,R3,1,A2,3,D1,0\C,2,R4,1,A3,3,D2,0\H,5,R5,2,A4,1,D3,0\C,5,R6,2,A5,1,D4,0\C,7,R7,5,A6,2,D5,0\O,8,R8,7,A7,5,D6,0\O,8,R9,7,A8,5,D7,0\H,10,R10,8,A9,7,D8,0\C,7,R11,5,A10,2,D9,0\X,12,1.,7,90.,5,D10,0\N,12,R12,13,90.,7,D11,0\|R1=1.97499995|R2=1.09035473|R3=1.09006748|R4=1.48165256|R5=1.08445864|R6=1.34072116|R7=1.48474797|R8=1.19356514|R9=1.33549154|R10=0.96182713|R11=1.43324906|R12=1.14866374|A1=108.0417804|A2=107.27201804|A3=108.36523659|A4=117.40123653|A5=125.57040809|A6=122.49315547|A7=123.89554586|A8=112.64708737|A9=106.70842671|A10=121.66585675|D1=-119.19792866|D2=119.80452129|D3=289.04208308|D4=108.33935804|D5=180.4210146|D6=180.6684905|D7=0.60898349|D8=179.98722393|D9=0.86972599|D10=277.19200705|D11=182.27356554\|Version=x86-Linux-G03RevB.04|State=2-A|HF=-2799.4049284|S2=0.753961|S2-1=0.|S2A=0.750009|RMSD=4.888e-09|RMSF=6.847e-06|Dipole=1.6102823,1.1200827,-0.2884657|PG=C01 [X(C5H4N1O2Se1)]\|@

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3-Carboxy-3-cyano-2-butenyl radical (18)

BHandHLYP/6-311G**

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET8\FOpt\UBHandHLYP\6-311G(d,p)\C5H4
N1O2(2)\KAUMANN\03-Sep-2005\1\#\BHANDHLYP/6-311G** OPT=GRAD GUESS=CHEC
K GEOM=CHECKPOINT FREQ=NORAMAN\Carbon Radical (Tautomer)\0,2\H\C,1,R
1\C,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\C,3,R4,2,A3,1,D2,0\C,5,R6,3,A5,2,D4,0
\O,6,R7,5,A6,3,D5,0\O,6,R8,5,A7,3,D6,0\H,8,R9,6,A8,5,D7,0\C,5,R10,3,A9
,2,D8,0\X,10,1.,5,90.,3,D9,0\N,10,R11,11,90.,5,D10,0\H,2,R12,3,A10,4,D
11,0\|R1=1.07457479\R2=1.36041215\R3=1.07668553\R4=1.39962972\R6=1.474
70101\R7=1.19428553\R8=1.32838487\R9=0.95634165\R10=1.41070666\R11=1.1
4449682\R12=1.07631943\A1=120.59300188\A2=120.11455642\A3=124.8675182\
A5=118.67787256\A6=123.52804633\A7=112.75484235\A8=107.87930639\A9=121
.5518545\A10=121.63766441\D1=0.00001362\D2=179.99998628\D4=179.9999370
9\D5=0.00017056\D6=180.00016422\D7=180.00002251\D8=-0.00007358\D9=-90.
02938522\D10=182.04784997\D11=180.00002023\|Version=x86-Linux-G03RevB.
04\State=2-A\HF=-397.9682536\S2=0.821028\S2-1=0.\S2A=0.752333\RMSD=8.9
24e-09\RMSF=1.351e-04\Dipole=0.4838744,-0.0000151,-0.7702175\PG=C01 [X
(C5H4N1O2)]\@
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BHandHLYP/cc-pVDZ

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET3\FOpt\UBHandHLYP\CC-pVDZ\C5H4N1O2
(2)\KAUMANN\03-Sep-2005\1\#\BHANDHLYP/CC-PVDZ OPT=(GRAD,READFC) GUESS=
(CHECK,READ) GEOM=CHECKPOINT FREQ=NORAMAN\Carbon Radical (Tautomer)\0,2\H\C,1,R1\C,2,R2,1,A1\H,3,R3,2,A2,1,D1,0\C,3,R4,2,A3,1,D2,0\C,5,R6,3,A5,2,D4,0\O,6,R7,5,A6,3,D5,0\O,6,R8,5,A7,3,D6,0\H,8,R9,6,A8,5,D7,0\C,5,R10,3,A9,2,D8,0\X,10,1.,5,90.,3,D9,0\N,10,R11,11,90.,5,D10,0\H,2,R12,3,A10,4,D11,0\|R1=1.08293653\R2=1.36489943\R3=1.08424168\R4=1.40356541\R6=1.47621741\R7=1.19909962\R8=1.3299388\R9=0.96192646\R10=1.41595984\R11=1.15317458\R12=1.0846301\A1=120.56642742\A2=120.2573834\A3=124.87983551\A5=118.68202445\A6=123.49780839\A7=112.7936845\A8=107.29594398\A9=121.6053598\A10=121.47114121\D1=0.0000154\D2=179.99998804\D4=179.99992375\D5=0.00013098\D6=180.00012217\D7=180.00001996\D8=-0.00004461\D9=-90.02960585\D10=181.98811587\D11=180.00002114\|Version=x86-Linux-G03RevB.04\State=2-A\HF=-397.8944555\S2=0.824336\S2-1=0.\S2A=0.75263\RMSD=5.786e-09\RMSF=1.212e-05\Dipole=0.4738085,-0.0000136,-0.7182237\PG=C01 [X(C5H4N1O2)]\@
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