Supporting Information

Reversible Olefin Addition to Extended Lattices of a Nickel/Selenium Framework

Dušan N. Sredojević[1,2,*], Salvador Moncho[1], Rajesh Kumar Raju[1], Milivoj R. Belić[1], Edward N. Brothers[1,*]

[1]*Science Program, Texas A&M University at Qatar, Texas A&M Engineering Building, Education City, Doha, Qatar*

[2]*Institute of Nuclear Sciences, Vinča, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia*

*Corresponding Authors E-mail: dusan.sredojevic@qatar.tamu.edu; ed.brothers@qatar.tamu.edu

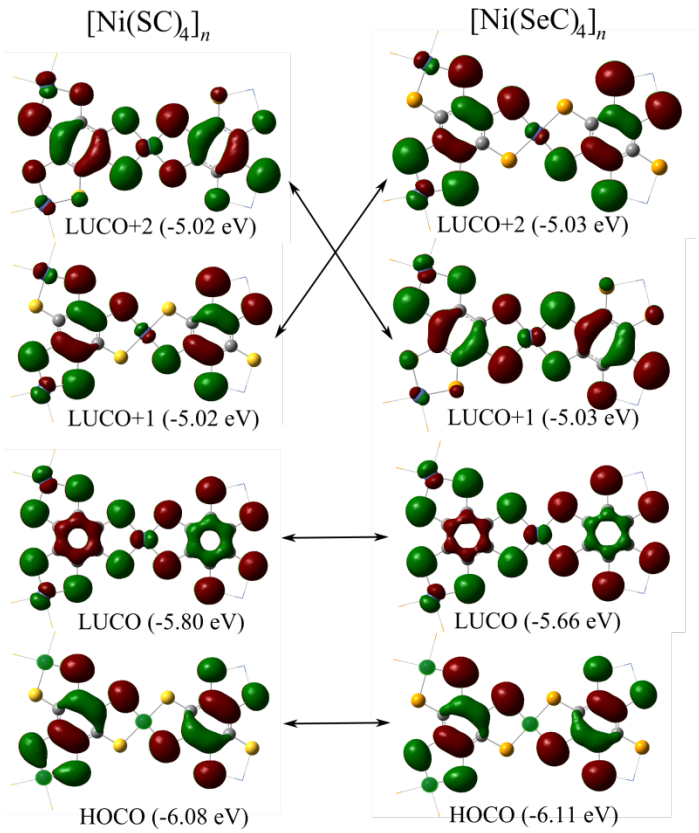

Figure S1. MO analysis of **1**$_{S}$ and **1**$_{Se}$. Note that LUCO+1 and LUCO+2 are degenerate orbitals and the difference in its relative order is due to small numerical differences. The Gaussview software has been used to obtain the relevant crystal orbitals by generating the cube files internally from the formatted checkpoint

files. Ni, S, Se and C atoms are presented as green, yellow, orange-brown and gray spheres, respectively. The negative parts of the wave-functions are presented as green, while positive parts are dark-red.

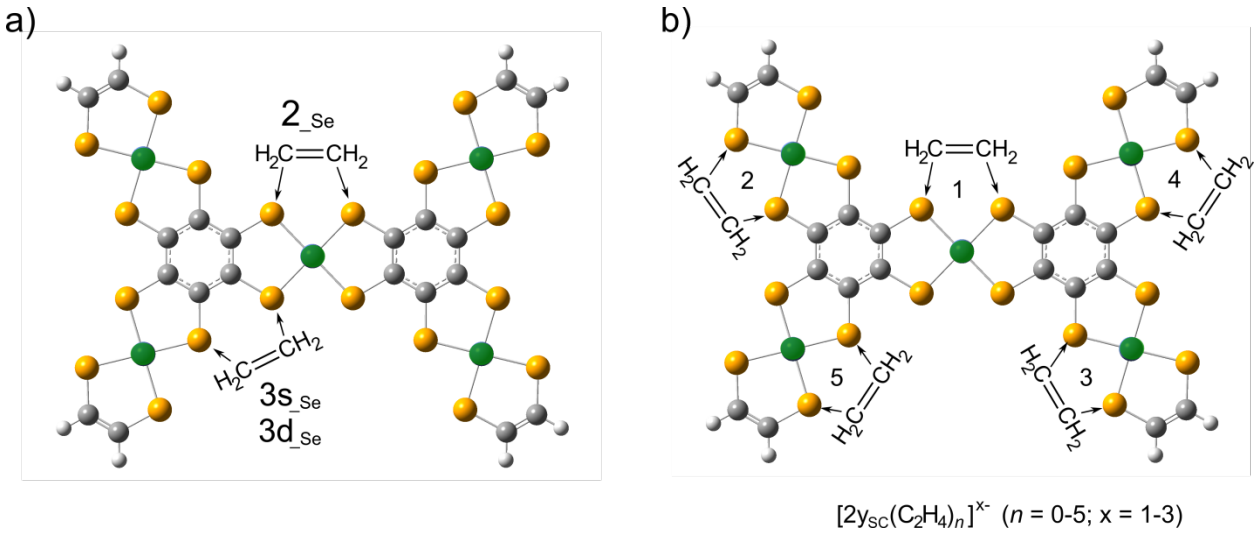

Figure S2. Model systems used in calculations for estimating **a)** the entropy effect of ethylene adsorption and **b)** the olefin dissociation ability of **1**$_{\_Se}$.

$[2y_{SC}(C_2H_4)_4]^{2-} \rightarrow [2y_{SC}(C_2H_4)_3]^{2-} + C_2H_4 \quad \Delta H = +4.9$ kcal/mol (6)

$[2y_{SC}(C_2H_4)_4]^{-} \rightarrow [2y_{SC}(C_2H_4)_3]^{-} + C_2H_4 \quad \Delta H = +6.4$ kcal/mol (7)

$[2y_{SC}(C_2H_4)_3]^{2-} \rightarrow [2y_{SC}(C_2H_4)_2]^{2-} + C_2H_4 \quad \Delta H = -2.8$ kcal/mol (8)

$[2y_{SC}(C_2H_4)_3]^{-} \rightarrow [2y_{SC}(C_2H_4)_2]^{-} + C_2H_4 \quad \Delta H = +5.2$ kcal/mol (9)

$[2y_{SC}(C_2H_4)_2]^{2-} \rightarrow [2y_{SC}(C_2H_4)]^{2-} + C_2H_4 \quad \Delta H = +1.1$ kcal/mol (10)

$[2y_{SC}(C_2H_4)_2]^{-} \rightarrow [2y_{SC}(C_2H_4)]^{-} + C_2H_4 \quad \Delta H = +6.7$ kcal/mol (11)

$[2y_{SC}(C_2H_4)]^{2-} \rightarrow [2y_{SC}]^{2-} + C_2H_4 \quad \Delta H = +2.7$ kcal/mol (12)

$[2y_{SC}(C_2H_4)]^{-} \rightarrow [2y_{SC}]^{-} + C_2H_4 \quad \Delta H = +7.2$ kcal/mol (13)

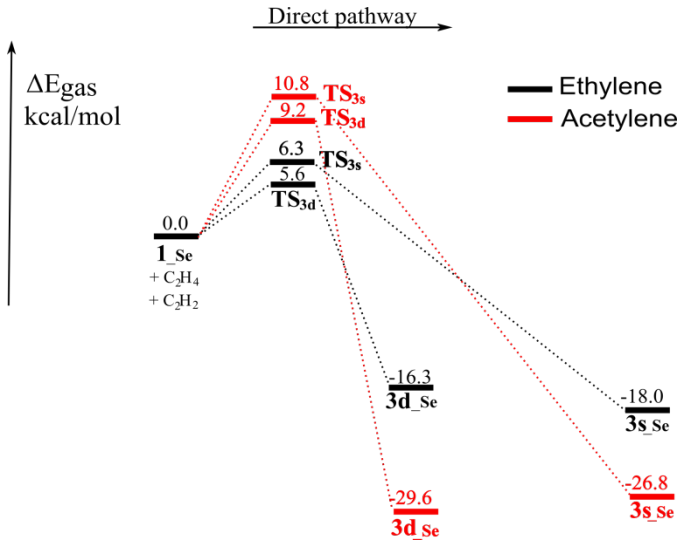

Figure S3. Energy profiles for the reaction of **1**$_{Se}$ with ethylene and acetylene via the direct pathways, calculated at the HSE06/DZ level.

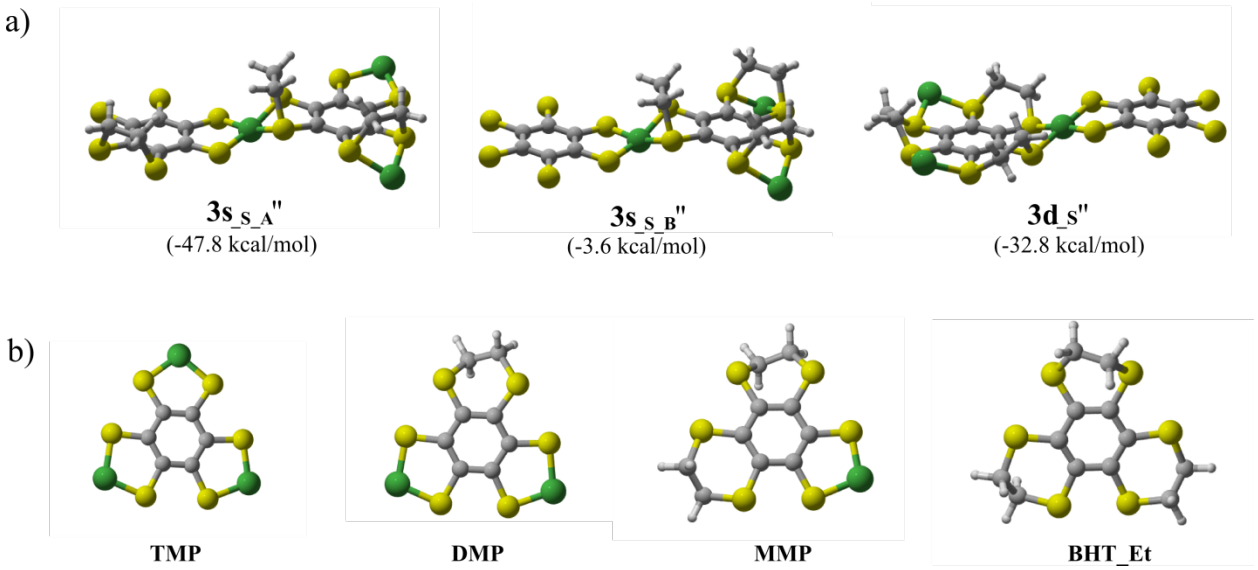

Figure S4. (a) Optimized geometries of triple ethylene-coordinated intraligand products of **1**$_{S}$. The relative stabilities with respect to the reactants (**1**$_{S}$ + 3 ethylene) are given in brackets. (b) Plausible decomposition species.

Table S1. Absolute and relative energies of various metal decomposition species calculated at HSE06/DZ level.

1_S		
Species	Energy (Hartree)	Relative energy (kcal/mol)
^{3}MMP	-4280.78600188	0.0
^{1}MMP	-4280.76436630	13.6
^{5}DMP	-5710.22571716	0.0
^{3}DMP	-5710.21406289	7.3
^{1}DMP	-5710.18002784	28.7
^{7}TMP	-7139.66637524	0.0
^{5}TMP	-7139.64282514	14.8
^{3}TMP	-7139.62774875	24.2
^{1}TMP	-7139.58191245	53.0

1_Se		
Species	Energy (Hartree)	Relative energy (kcal/mol)
^{3}MMP	-16298.8701241	0.0
^{1}MMP	-16298.8521303	11.3
^{5}DMP	-17728.3225449	0.0
^{3}DMP	-17728.3131757	5.9
^{1}DMP	-17728.2825288	25.1
^{7}TMP	-19157.7720339	0.0
^{5}TMP	-19157.7529023	12.0
^{3}TMP	-19157.7374522	21.7
^{1}TMP	-19157.6877113	52.9

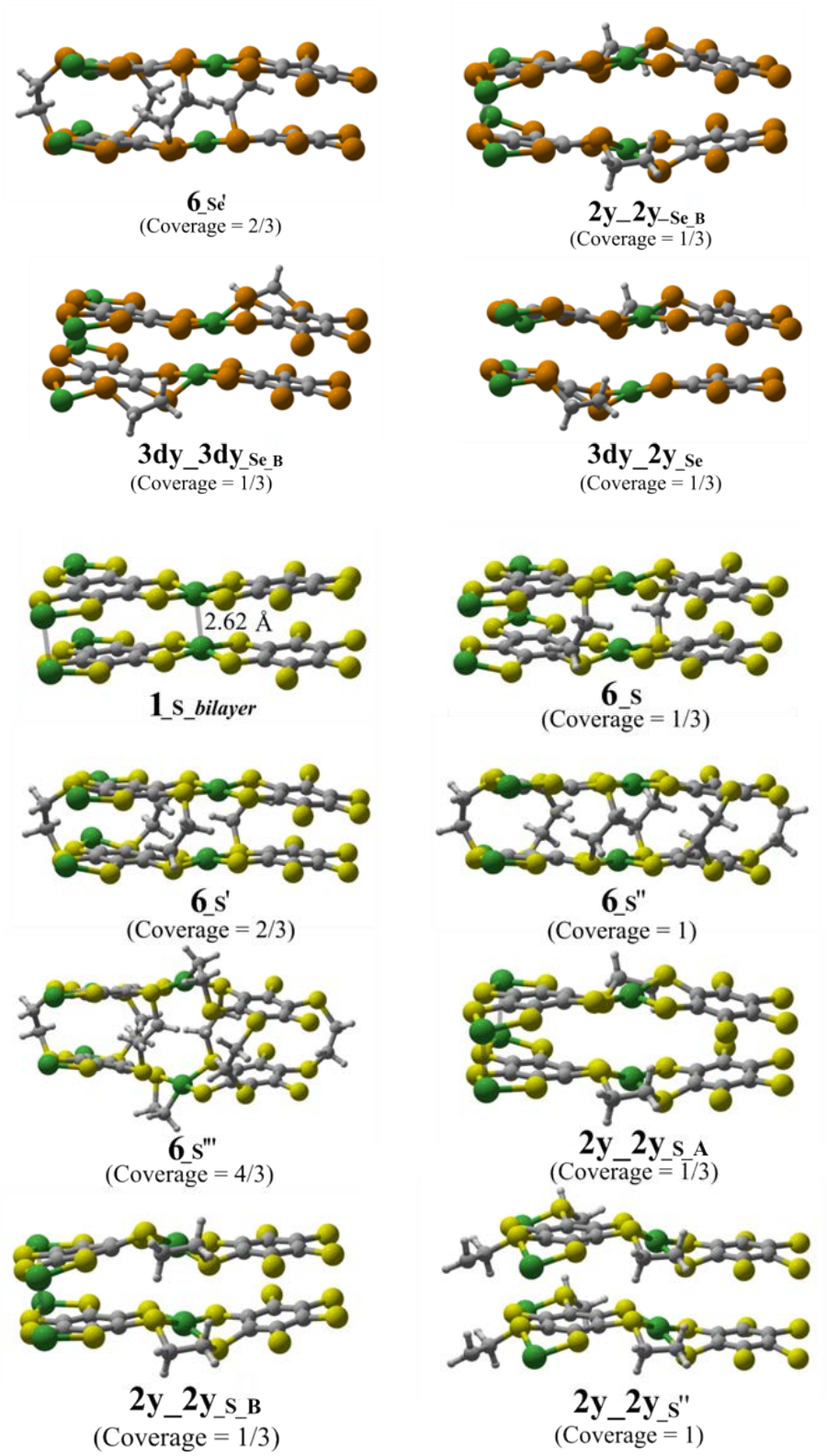

Figure S5. The optimized structures of various ethylene adducts of **1**$_{\_Se\_bilayer}$ and **1**$_{\_S\_bilayer}$ materials, calculated at the HSE06/DZ level. Ni, S, Se and C atoms are presented as green, yellow, orange-brown and gray spheres, respectively.

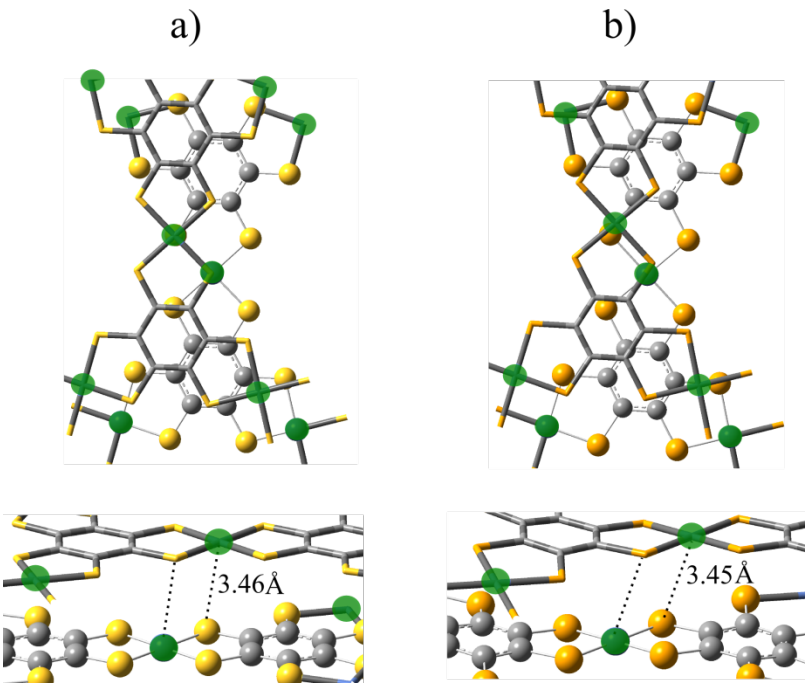

Figure S6. Two different views of a) $[Ni(SC)_4]_n$ and b) $[Ni(SeC)_4]_n$ 3D structures, constructed by displacing the sheets along the Ni – S and Ni – Se bonds, respectively. In both cases, the interlayer Ni – S and Ni – Se distances are also shown. Ni, S, and C atoms are presented as green, yellow, and gray spheres, respectively.

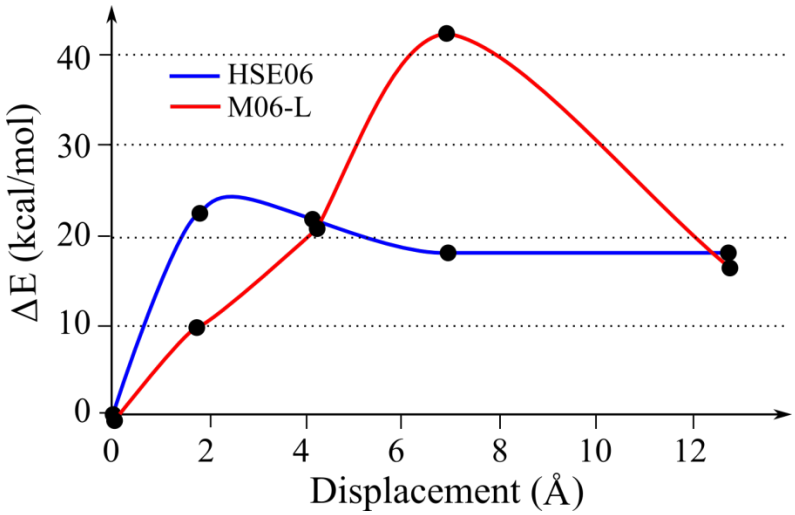

Figure S7. The relative electronic energies (kcal/mol), calculated using two different functionals, plotted as a function of the diagonal displacement between sheets, for the hypothetical $[Ni(SC)_4]_n$ 3D material.

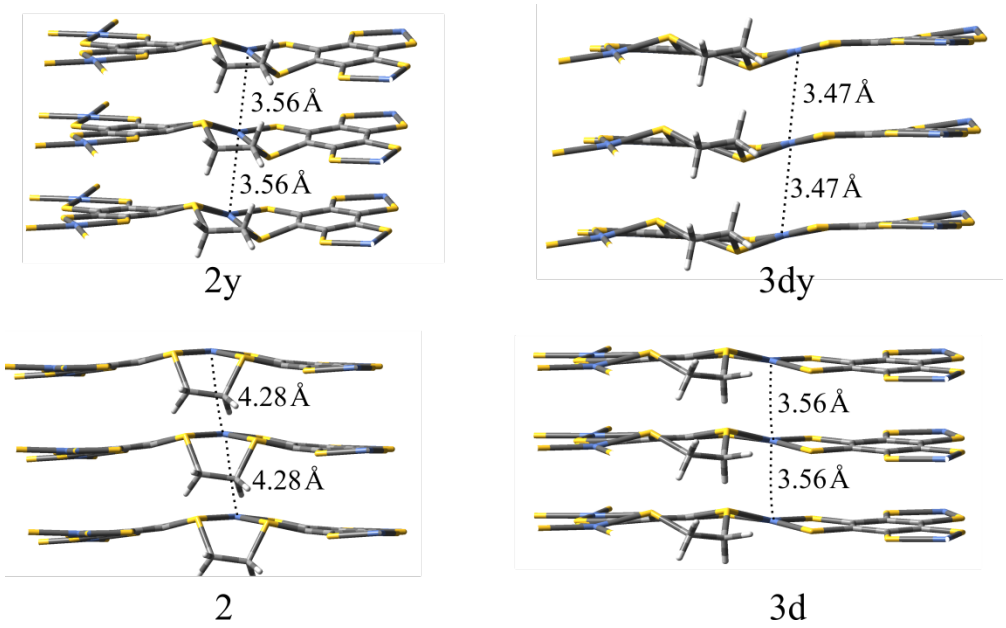

Figure S8. Optimized structures of four ethylene adducts associated with $[Ni(SC)_4]_n$ 3D sheets, calculated at the HSE06/DZ level.

1_Se

E = -33792.0476741 Hartree (Singlet)

E = -33792.0321564 Hartree (Triplet)

Ni	-7.20632000	0.24474800	0.00439700
Se	-6.67075800	-1.94662000	0.00416400
C	-4.10965100	-0.72819000	0.00116600
C	-4.81563100	-1.95070300	0.00127400
Se	-5.04079900	0.87630300	0.00332800
C	-4.09705700	-3.19500100	-0.00060200
Se	-5.02094400	-4.80378100	-0.00202000
C	-2.68537500	-3.19499800	-0.00153800
Ni	-3.39117600	-6.36346800	-0.00258300
Se	-1.76149700	-4.80377700	-0.00335500
C	-2.67276600	-0.72819000	-0.00040700
Se	-1.74161300	0.87630700	-0.00133100
C	-1.96679100	-1.95070500	-0.00128600
Se	-0.11166300	-1.94662200	-0.00226100
Ni	0.42390300	0.24474800	-0.00181700
Se	0.95946600	2.43611500	-0.00198500
Se	2.58942000	-0.38680900	-0.00080900
C	2.81459500	2.44020100	-0.00075400
C	3.52056900	1.21769000	0.00019900
C	3.53317500	3.68449700	-0.00089500
Se	2.60928000	5.29326200	-0.00204600
C	4.94485400	3.68449900	-0.00028100
Se	5.86874700	5.29327200	-0.00158900
C	5.66342900	2.44020400	0.00136600
Se	7.51855500	2.43611900	0.00304500
C	4.95745200	1.21769400	0.00180300
Se	5.88859500	-0.38679800	0.00481500
Tv	15.26043300	0.00000000	0.00000000
Tv	7.63017600	13.21645000	0.00000000

2_Se

E = -33870.5077748 Hartree (Singlet)

E = -33870.5015413 Hartree (Triplet)

Ni	-7.40904000	0.55071900	0.26796300
Se	-6.85160400	-1.63572600	0.32770200
C	-4.32896300	-0.39991500	-0.08585500
C	-5.00083700	-1.62424900	0.08219000
Se	-5.26212600	1.20287900	0.06296300
C	-4.26769600	-2.85232800	0.05031700
Se	-5.13513900	-4.47900500	0.19734600
C	-2.85701300	-2.82259100	-0.13886400
Ni	-3.48044300	-6.00754500	0.07682100
Se	-1.87930800	-4.40417700	-0.08625400
C	-2.92136500	-0.37519500	-0.38670500
Se	-2.11603200	1.26511100	-0.81458900
C	-2.22313100	-1.58286200	-0.38044200
Se	-0.44537800	-1.55658100	-1.08312100
Ni	0.07268900	0.68397600	-1.06708700
Se	0.64904900	2.88703000	-0.94460900
Se	2.27441300	0.01010800	-0.91103000
C	2.45110600	2.80266600	-0.43484200
C	3.15723800	1.60253400	-0.33808100
C	3.15653700	4.03028900	-0.17299700
Se	2.21662800	5.63483300	-0.10858700
C	4.54964100	4.02231300	0.02048100
Se	5.46775200	5.64043000	0.17740600
C	5.25695000	2.78084300	0.08383800
Se	7.09321700	2.74665500	0.29897700
C	4.54073700	1.55779800	-0.04881800
Se	5.42917700	-0.06470000	0.14433200
C	0.77368200	-2.03392700	0.42381200
C	1.73586400	-0.90534600	0.76484900
H	0.14138800	-2.29950600	1.28214100
H	1.29228300	-2.94126600	0.08462200
H	2.64629600	-1.28963000	1.25000600
H	1.27343300	-0.14363500	1.40611500
Tv	15.26043300	0.00000000	0.00000000
Tv	7.63017600	13.21645000	0.00000000

3s_Se

E = -33870.5082368 Hartree (Singlet)

E = -33870.5032788 Hartree (Triplet)

Ni	-7.00916900	0.34556000	-0.72067600
Se	-6.46848400	-1.84290300	-0.86625300
C	-3.93961800	-0.64417600	-0.37550400
C	-4.62053700	-1.86281800	-0.59655300
Se	-4.86347000	0.97935500	-0.39920400
C	-3.90231400	-3.09707600	-0.59633400
Se	-4.79846800	-4.71373200	-0.86281700
C	-2.50605100	-3.10728100	-0.37733700
Ni	-3.16245300	-6.26498100	-0.72096000
Se	-1.55032600	-4.71244600	-0.40362200
C	-2.54399800	-0.68060100	-0.13652700
Se	-1.56850200	0.90431000	0.35303400
C	-1.84792600	-1.87601300	-0.13827100
Se	0.01456000	-1.80954900	0.34218200
Ni	0.57783600	0.34116900	-0.39309300
Se	1.07686600	2.52127900	-0.71844000
Se	2.71819700	-0.30137300	-0.72877600
C	2.95233900	2.53104000	-0.75158300
C	3.65470300	1.32358800	-0.75471600
C	3.65672000	3.77372800	-0.77141400
Se	2.72043400	5.37216100	-0.82853500
C	5.07548300	3.78854700	-0.73562300
Se	5.97524700	5.40111800	-0.68445900
C	5.79782000	2.54644900	-0.73563900
Se	7.64419400	2.53070500	-0.67978900
C	5.08310100	1.32083600	-0.77460500
Se	6.00901700	-0.28344600	-0.83538500
C	-0.32799400	-1.08168600	2.15351300
C	-1.10478400	0.23233600	2.15947800
H	-0.84955000	-1.87673600	2.70365400
H	0.67970400	-0.96145900	2.57591000
H	-0.51608200	1.05158600	2.59611200
H	-2.05649400	0.15250900	2.70223300
Tv	15.26043300	0.00000000	0.00000000
Tv	7.63017600	13.21645000	0.00000000

2y_Se
E = -33870.501434 Hartree

Ni	-7.55232000	0.54390800	-0.41365400
Se	-6.95593000	-1.63716300	-0.35201700
C	-4.45141900	-0.33312600	-0.05942100
C	-5.10602100	-1.57404300	-0.07959000
Se	-5.41595600	1.23623700	-0.29767500
C	-4.34377900	-2.76862600	0.12137400
Se	-5.20334800	-4.39980900	0.21128800
C	-2.92983000	-2.70091300	0.30385200
Ni	-3.54278000	-5.90254300	0.41709500
Se	-1.95778300	-4.26959400	0.55690000
C	-3.03205300	-0.25216600	0.13861600
Se	-2.25712600	1.45954900	0.22148900
C	-2.30276900	-1.43384300	0.29758000
Se	-0.50160700	-1.13249700	0.91317900
Ni	-0.06503200	0.90154800	0.00385600
Se	0.53731500	3.08294900	-0.20511500
Se	1.91456400	0.27764200	-0.91591300
C	2.40868800	2.90689000	-0.13169000
C	3.07216100	1.68773900	-0.29573500
C	3.18406100	4.09848100	0.06581300
Se	2.30150900	5.71517600	0.30636400
C	4.58625400	4.05055800	0.08326900
Se	5.56015400	5.62493100	0.35376500
C	5.24439300	2.79581800	-0.11845200
Se	7.08715500	2.73115300	-0.20485200
C	4.48325000	1.60270300	-0.30337100
Se	5.36199800	-0.01971200	-0.55950300
C	0.85141700	-2.18721900	-0.08140300
C	2.16172800	-1.42857800	0.06468200
H	0.91091800	-3.18136400	0.38323300
H	0.53657300	-2.30215400	-1.12880800
H	2.99270900	-1.97080500	-0.40779300
H	2.42290700	-1.22112700	1.11263900
Tv	15.26043300	0.00000000	0.00000000
Tv	7.63017600	13.21645000	0.00000000

3d_Se
E = -33870.50551110 Hartree

Ni	-7.24521200	0.97089800	0.20109800
Se	-6.70661600	-1.22212600	0.13879100
C	-4.15393800	0.01653200	-0.11800600
C	-4.85307200	-1.21389500	-0.08912200
Se	-5.08535300	1.62103800	0.08754300
C	-4.15103500	-2.44890400	-0.22565900
Se	-5.03072100	-4.10084100	-0.09018200
C	-2.77016700	-2.39453400	-0.46417200
Ni	-3.35801700	-5.63824800	-0.26252500
Se	-1.87098000	-4.01137400	-0.90481000
C	-2.73766700	0.03891400	-0.28978500
Se	-1.75542100	1.63602700	-0.20458500
C	-2.08751600	-1.18151300	-0.50534600
Se	-0.21335900	-1.18812800	-0.83455300
Ni	0.41782000	0.94921300	-0.27342400
Se	0.96870900	3.15290200	-0.19919300
Se	2.59446200	0.32473000	-0.09075100
C	2.82699300	3.14624900	-0.08557900
C	3.53035000	1.92838500	-0.02362300
C	3.53624500	4.38479600	-0.08493700
Se	2.59013800	5.98542300	-0.18512900
C	4.94292600	4.39323500	-0.03098100
Se	5.85523700	6.01010800	-0.10467900
C	5.66592400	3.15871900	0.07020300
Se	7.51222200	3.16321600	0.17607400
C	4.96106700	1.92857800	0.07686100
Se	5.89107500	0.33410500	0.19548800
C	0.15061500	-2.47444300	0.62558800
C	-0.27466500	-3.88720800	0.28126200
H	1.23351000	-2.42793100	0.81451100
H	-0.37934200	-2.07639200	1.50013100
H	-0.50105200	-4.45813600	1.19201100
H	0.49683700	-4.41939500	-0.29252100

4_Se
E = -33870.4783781 Hartree

Ni	-7.32827700	0.19996000	-0.28525800
Se	-6.79167400	-1.99272900	-0.35430500
C	-4.23478800	-0.77298300	-0.36205400
C	-4.93730900	-1.99629200	-0.40896400
Se	-5.15921600	0.83474800	-0.25883600
C	-4.21349600	-3.23436800	-0.49394600
Se	-5.12248000	-4.85135700	-0.55249900
C	-2.80301800	-3.22135500	-0.53546900
Ni	-3.48037200	-6.39575500	-0.60736300
Se	-1.85796400	-4.81913300	-0.61651500
C	-2.80520800	-0.76648300	-0.41104500
Se	-1.88225100	0.85330300	-0.31050300
C	-2.10032900	-1.97352400	-0.51899100
Se	-0.24305400	-1.95103600	-0.69445300
Ni	0.34873100	0.20027000	-0.07800200
Se	0.94079400	2.35158800	-0.69336700
Se	2.57981100	-0.45300200	-0.30917400
C	2.79810300	2.37375800	-0.51827100
C	3.50288200	1.16670200	-0.41029300
C	3.50088600	3.62153300	-0.53504100
Se	2.55594300	5.21933700	-0.61608800
C	4.91135700	3.63446800	-0.49374400
Se	5.82045600	5.25138600	-0.55265500
C	5.63507600	2.39634000	-0.40873500
Se	7.48942300	2.39264300	-0.35440900
C	4.93246500	1.17307900	-0.36160600
Se	5.85679900	-0.43470600	-0.25858800
C	0.17878400	-0.47629000	1.88698600
C	0.51681000	0.87427300	1.88783200
H	-0.85825500	-0.78310300	2.04775100
H	0.94791600	-1.23424700	2.06350700
H	1.55378100	1.18080100	2.04951300
H	-0.25232600	1.63217200	2.06458400
Tv	15.26043300	0.00000000	0.00000000
Tv	7.63017600	13.21645000	0.00000000

5_Se

E = -33870.4902102 Hartree

Ni	-7.29387081	0.41488762	-0.56484051
Se	-6.78375983	-1.77929826	-0.45754930
C	-4.20815279	-0.58484938	-0.49750476
C	-4.92030851	-1.79643632	-0.39057357
Se	-5.12511029	1.03041782	-0.60490697
C	-4.21930730	-3.03301889	-0.23287310
Se	-5.13918691	-4.63839202	-0.05310199
C	-2.80466170	-3.03055380	-0.21541110
Ni	-3.50649519	-6.18969614	0.05818596
Se	-1.86975805	-4.62154076	0.03870122
C	-2.77088311	-0.58722560	-0.52812294
Se	-1.85845905	1.03833538	-0.78248062
C	-2.11141881	-1.80431997	-0.38805788
Se	-0.20994104	-1.85743185	-0.50534248
Ni	0.36347316	0.41695778	-0.46134216
Se	0.90286189	2.62190907	-0.32077088
Se	2.54241717	-0.16472476	-0.90461846
C	2.78258815	2.61559756	-0.35729991
C	3.47693663	1.42500208	-0.54418020
C	3.49513104	3.84586550	-0.18768435
Se	2.55607418	5.43354148	0.02219911
C	4.90711863	3.85419497	-0.20741252
Se	5.82081463	5.46007049	-0.01398093
C	5.62319011	2.62403521	-0.37356094
Se	7.47619132	2.60403732	-0.41877173
C	4.90539361	1.41066653	-0.51531746
Se	5.81734541	-0.19630046	-0.66241697
C	0.29018041	-1.46617512	1.40307220
C	0.36816675	0.02035368	1.46376939
H	-0.47866260	-1.94114963	2.02897675
H	1.26167691	-1.96507493	1.52511107
H	1.29456032	0.42376717	1.88454159
H	-0.52225399	0.51881449	1.86109724
Tv	15.28705126	0.00000000	0.00000000
Tv	7.69068517	13.19653523	0.00000000

TS3d_Se

E = -33870.4706531 Hartree

Ni	-7.17857600	0.92370700	-0.41087200
Se	-6.63809600	-1.26744100	-0.42694600
C	-4.07297100	-0.04029400	-0.44155200
C	-4.77633700	-1.26808500	-0.43962200
Se	-5.01494600	1.56558300	-0.42808500
C	-4.06375200	-2.50851600	-0.44027800
Se	-4.95611600	-4.12979500	-0.30232400
C	-2.65182900	-2.48534200	-0.53562900
Ni	-3.28946500	-5.66879100	-0.35876800
Se	-1.69234400	-4.08182100	-0.55709900
C	-2.64250800	-0.02770100	-0.44596100
Se	-1.69430700	1.56219900	-0.31491000
C	-1.94881500	-1.25783900	-0.53928300
Se	-0.08653700	-1.27831000	-0.56723800
Ni	0.47624600	0.90187600	-0.37082000
Se	1.02053300	3.09287700	-0.27460800
Se	2.64839400	0.27277300	-0.43040900
C	2.88046500	3.09894100	-0.31993100
C	3.58455600	1.88325100	-0.36465300
C	3.59417000	4.34451700	-0.31708600
Se	2.65944700	5.95232600	-0.26339300
C	4.99903900	4.35187100	-0.36112700
Se	5.91523400	5.97398900	-0.42241900
C	5.72165000	3.11592000	-0.37662300
Se	7.57349600	3.11597000	-0.39543200
C	5.01628900	1.88484900	-0.37779500
Se	5.95249200	0.28705700	-0.39817000
C	0.08760700	-2.42950100	1.68720500
C	-0.60296400	-3.63578900	1.69204800
H	1.17600300	-2.42804300	1.59048900
H	-0.35480100	-1.54558900	2.15217200
H	-1.58777400	-3.69920500	2.16037100
H	-0.05348300	-4.57564200	1.59874800
Tv	15.28705126	0.00000000	0.00000000
Tv	7.69068517	13.19653523	0.00000000

TS3s_Se

E = -33870.4553875 Hartree

Ni	-7.008656	0.345587	-0.797105
Se	-6.467366	-1.842681	-0.943210
C	-3.938623	-0.643129	-0.455441
C	-4.619429	-1.861852	-0.675108
Se	-4.862791	0.979868	-0.478999
C	-3.901033	-3.096294	-0.675004
Se	-4.797681	-4.712657	-0.940019
C	-2.504751	-3.106532	-0.457506
Ni	-3.161978	-6.264194	-0.797859
Se	-1.549494	-4.711614	-0.483849
C	-2.542142	-0.678564	-0.218667
Se	-1.571615	0.905187	0.269554
C	-1.845439	-1.874978	-0.220541
Se	0.013537	-1.812363	0.258577
Ni	0.576987	0.340784	-0.459331
Se	1.075873	2.520668	-0.785022
Se	2.717159	-0.301583	-0.795347
C	2.951196	2.530683	-0.816557
C	3.653642	1.323231	-0.819707
C	3.655536	3.773482	-0.836113
Se	2.719249	5.371892	-0.893403
C	5.074286	3.788299	-0.800273
Se	5.974141	5.400921	-0.749953
C	5.796691	2.546251	-0.800331
Se	7.643157	2.530782	-0.745409
C	5.082118	1.320564	-0.839369
Se	6.008193	-0.283592	-0.900437
C	-0.355150	-1.026036	2.531752
C	-1.073152	0.176230	2.537012
H	-0.877023	-1.832272	3.064850
H	0.656168	-0.914851	2.947373

H	-0.491284	1.003566	2.967047
H	-2.034645	0.100933	3.062651
Tv	15.191050	0.000088	0.010640
Tv	7.503813	13.214589	0.011355

TS2y$_{Se}$

E = -33870.4602236 Hartree

Ni	-7.59648400	0.71755400	-0.73250500
Se	-7.06754300	-1.46161100	-0.47132400
C	-4.51985300	-0.21425300	-0.35430200
C	-5.22354500	-1.42304300	-0.19313300
Se	-5.43260500	1.35058200	-0.75875000
C	-4.51587000	-2.61028800	0.18465000
Se	-5.43293700	-4.19230900	0.48656800
C	-3.10967300	-2.56711400	0.36809100
Ni	-3.79233400	-5.71606700	0.74004300
Se	-2.17451800	-4.12254500	0.75941300
C	-3.09690100	-0.17116200	-0.17134800
Se	-2.18282100	1.43874900	-0.44242500
C	-2.42326000	-1.33015000	0.22385700
Se	-0.61882500	-1.12207800	0.75425700
Ni	-0.03566300	0.87234900	-0.00292800
Se	0.57891100	3.00521400	0.43980400
Se	1.97655600	0.35145800	-0.75967600
C	2.43012600	2.96493500	0.17117600
C	3.08001900	1.79275100	-0.22490700
C	3.19696800	4.16391600	0.35723000
Se	2.32148900	5.74932100	0.76331100
C	4.59583900	4.14799300	0.19792200
Se	5.57452400	5.71065100	0.47996300
C	5.25253900	2.93187100	-0.18019400
Se	7.08144600	2.90736200	-0.47906900
C	4.49425800	1.74713100	-0.36576900
Se	5.35041300	0.14627000	-0.75402200
C	1.20866400	-2.72664900	0.08422000
C	2.41238800	-2.04473500	-0.09557200
H	0.98996600	-3.17599800	1.05463100
H	0.70623300	-3.18395500	-0.77244800
H	2.90816700	-2.08548600	-1.06715500
H	3.06432300	-1.85066400	0.76039100
Tv	15.14473800	0.00000000	0.00000000
Tv	7.76698100	12.99828300	0.00000000

TS2$_{Se}$

E = -33870.4499961 Hartree

Ni	-7.51876800	0.57300300	-0.14955700
Se	-6.96717000	-1.61865200	-0.13112200
C	-4.41898400	-0.39446900	-0.29845300
C	-5.11949200	-1.62168700	-0.22957500
Se	-5.35217900	1.21481100	-0.22053900
C	-4.39408800	-2.86431500	-0.24283600
Se	-5.29214700	-4.47454000	-0.12871000
C	-2.98135400	-2.85287800	-0.35200200
Ni	-3.65609100	-6.03220000	-0.19519200
Se	-2.02858200	-4.45079600	-0.30184600
C	-3.00014400	-0.39152300	-0.44674500
Se	-2.08876300	1.23296400	-0.60001800
C	-2.29881400	-1.61524800	-0.49914100
Se	-0.46768200	-1.60508300	-0.85883300
Ni	0.09089900	0.61847100	-0.73616400
Se	0.63294300	2.82980000	-0.60068700
Se	2.29087100	0.00615700	-0.78524000
C	2.48881100	2.80928800	-0.43556600
C	3.20682300	1.58623200	-0.46812600
C	3.20296200	4.03632700	-0.30630100
Se	2.27577100	5.65147100	-0.24218100
C	4.61711900	4.03064900	-0.24534500
Se	5.53797200	5.63451900	-0.18295100
C	5.33471700	2.78459000	-0.23576700
Se	7.18294500	2.76818900	-0.12941500
C	4.62415400	1.56524600	-0.31491500
Se	5.53708000	-0.05261400	-0.21445200
C	0.81695600	-1.88290000	1.49524800
C	2.00634300	-1.17780300	1.49290100
H	-0.07658800	-1.45518900	1.95533800
H	0.80003700	-2.95725300	1.29960100
H	2.95572600	-1.69314300	1.32758600
H	2.05871500	-0.20142500	1.98100200
Tv	15.23631500	0.00000000	0.00000000
Tv	7.56809600	13.24065100	0.00000000

TS14$_{Se}$

E = -33870.4700616 Hartree

Ni	-7.29574200	0.20625800	-0.57397300
Se	-6.73683500	-1.98405600	-0.68772900
C	-4.19502100	-0.75888100	-0.49918000
C	-4.88711900	-1.97826700	-0.62687800
Se	-5.13319100	0.85191500	-0.46159000
C	-4.15739700	-3.22227100	-0.70608500
Se	-5.07347200	-4.82532200	-0.85933300
C	-2.75137600	-3.21977700	-0.66481500
Ni	-3.43524100	-6.38538400	-0.88107500
Se	-1.80984300	-4.82089500	-0.80010300
C	-2.77060100	-0.75675100	-0.39702100
Se	-1.86319600	0.82877800	-0.12264500
C	-2.04601700	-1.98338800	-0.49693700
Se	-0.20628300	-1.96714500	-0.41272800
Ni	0.33800100	0.20415100	0.08461300
Se	0.88648500	2.40693500	-0.41484600
Se	2.55890300	-0.43076100	-0.15612700
C	2.74130300	2.39412700	-0.48509400
C	3.45741500	1.18107700	-0.39428000
C	3.44551800	3.63143700	-0.65185900
Se	2.49809500	5.22357200	-0.76963200
C	4.85587400	3.64198300	-0.70551300
Se	5.75948000	5.24554800	-0.87557700
C	5.58506800	2.39988500	-0.62426300
Se	7.42994900	2.39503200	-0.68905400
C	4.88267300	1.18057600	-0.49013000

Se	5.81042400	-0.42733200	-0.42884400
C	0.17520300	-0.49172500	2.43586100
C	0.52629300	0.81427600	2.40720300
H	-0.87079700	-0.79820400	2.52517000
H	0.93064700	-1.28056000	2.48672800
H	1.57509900	1.12041600	2.44182100
H	-0.22430100	1.60475200	2.49391500
Tv	15.23631500	0.00000000	0.00000000
Tv	7.56809600	13.24065100	0.00000000

TS45_Se

E = -33870.4756394 Hartree

Ni	-7.32781900	0.26075500	-0.39642300
Se	-6.80230600	-1.93488600	-0.40101500
C	-4.23729500	-0.72572200	-0.40124700
C	-4.94206100	-1.94592200	-0.39314800
Se	-5.16063300	0.88804000	-0.38888100
C	-4.22763400	-3.18970800	-0.37965700
Se	-5.14786300	-4.80534900	-0.35805200
C	-2.81746000	-3.18710500	-0.37950300
Ni	-3.51526500	-6.36017800	-0.34097300
Se	-1.88168000	-4.79454700	-0.34674000
C	-2.80301600	-0.72317900	-0.43198500
Se	-1.88340200	0.90354900	-0.46360000
C	-2.11461800	-1.94198600	-0.42283900
Se	-0.24481500	-1.94870900	-0.45242500
Ni	0.35084800	0.27992800	-0.24598300
Se	0.91619800	2.47240100	-0.62985500
Se	2.55068000	-0.35352500	-0.69694200
C	2.78785300	2.47046400	-0.49944700
C	3.48336600	1.26314600	-0.51865100
C	3.49292600	3.71182100	-0.41880500
Se	2.54900400	5.31017100	-0.37096800
C	4.90537500	3.71901800	-0.38939300
Se	5.81473200	5.33507700	-0.32965900
C	5.62365700	2.47672100	-0.40456300
Se	7.47638800	2.45552800	-0.36861300
C	4.91071200	1.25523100	-0.45013000
Se	5.82249900	-0.35994700	-0.44001100
C	0.21117100	-0.76952800	1.73709600
C	0.57413100	0.59672300	1.71873800
H	-0.80425500	-1.04508400	2.03556900
H	0.99085400	-1.51664400	1.91639200
H	1.62032300	0.86370500	1.89217800
H	-0.17059700	1.33974300	2.01953400
Tv	15.3257110	0.0000000	0.0000000
Tv	7.6926960	13.2437160	0.0000000

TS52_Se

E = -33870.4749789 Hartree

Ni	-7.38810100	0.48308000	-0.19494200
Se	-6.86293600	-1.70892500	-0.12125200
C	-4.29919600	-0.50357700	-0.31002900
C	-4.99959000	-1.72066600	-0.19803700
Se	-5.22473300	1.11028000	-0.28693100
C	-4.28801800	-2.96092700	-0.14414800
Se	-5.18573900	-4.57495800	0.00773500
C	-2.87107400	-2.95263200	-0.22700900
Ni	-3.54358800	-6.12245700	0.00220900
Se	-1.91515100	-4.54221600	-0.08333800
C	-2.86650000	-0.49777700	-0.44870600
Se	-1.97310400	1.13347900	-0.69889500
C	-2.19972600	-1.72083500	-0.40841500
Se	-0.33791300	-1.75000900	-0.80982500
Ni	0.26212700	0.50282800	-0.63341100
Se	0.77948200	2.73681400	-0.55372400
Se	2.43541600	-0.09035900	-0.82694000
C	2.64253900	2.70655600	-0.38569600
C	3.35483200	1.50923700	-0.44920200
C	3.36178600	3.93770100	-0.19928200
Se	2.42622600	5.53725400	-0.06105800
C	4.76913200	3.93567800	-0.14769200
Se	5.68909300	5.55009700	-0.01277700
C	5.48705500	2.69763600	-0.19991300
Se	7.33827400	2.67374700	-0.13040500
C	4.77158400	1.47643300	-0.31159500
Se	5.68821700	-0.13838600	-0.28576900
C	0.52310300	-1.77066300	0.99486400
C	1.07144500	-0.38783100	1.16660900
H	-0.26599300	-2.02697600	1.71681800
H	1.28367300	-2.56289100	0.97750500
H	2.00508400	-0.29886200	1.72890300
H	0.33229200	0.34012700	1.53434600
Tv	15.25282200	0.00000000	0.00000000
Tv	7.59741400	13.22445100	0.00000000

TS53_Se

E = -33870.4706109 Hartree

Ni	-7.192342	0.333699	-0.500250
Se	-6.680413	-1.866861	-0.501906
C	-4.106554	-0.670980	-0.398582
C	-4.814265	-1.888487	-0.420138
Se	-5.021201	0.953733	-0.445208
C	-4.106923	-3.129184	-0.375004
Se	-5.034938	-4.745706	-0.371594
C	-2.694615	-3.133919	-0.329189
Ni	-3.408108	-6.306397	-0.301656
Se	-1.764619	-4.751748	-0.259433
C	-2.679274	-0.684558	-0.362293
Se	-1.757502	0.967281	-0.281329
C	-1.999296	-1.894541	-0.340070
Se	-0.090582	-1.896762	-0.232897
Ni	0.439924	0.384343	-0.423776
Se	1.021745	2.602337	-0.596942
Se	2.621403	-0.229098	-0.777050
C	2.894487	2.584811	-0.507856
C	3.581069	1.374664	-0.566215
C	3.611545	3.818324	-0.422044
Se	2.681931	5.420907	-0.349111
C	5.026487	3.816084	-0.402002

Se	5.944979	5.420613	-0.305539
C	5.734215	2.567037	-0.455646
Se	7.580985	2.528094	-0.445093
C	5.005827	1.350962	-0.523913
Se	5.905481	-0.269863	-0.553507
C	0.027048	-1.190670	1.643693
C	-0.361517	0.250824	1.626027
H	-0.611310	-1.836074	2.262294
H	1.090191	-1.334167	1.888863
H	0.432394	0.971140	1.852383
H	-1.276254	0.484158	2.174982
Tv	15.281864	0.000000	0.000000
Tv	7.729989	13.289594	0.000000

1$_{\text{Se}}$***cluster***

E = -56324.7659026 Hartree

Se	8.81374400	4.33749100	0.00023900
Se	5.95885800	5.98706100	0.00033000
Se	5.95962300	-5.98633900	0.00060000
Se	8.81431800	-4.33639100	0.00302200
Ni	6.60555200	-3.80908400	0.00060100
Ni	-6.60610800	3.80938600	0.00083900
Se	7.23919200	-1.65191500	0.00082800
Se	-5.96007500	5.98660900	0.00188800
C	4.41260700	-1.42243500	-0.00064300
C	5.63141300	-0.71775800	0.00002200
Se	4.42066200	-3.28317800	-0.00100700
Se	-8.81485200	4.33683400	0.00415500
C	5.63132100	0.71843200	0.00000700
Se	7.23898500	1.65280200	0.00035300
Se	-5.95596000	-5.98606000	0.00580300
C	4.41242300	1.42297400	-0.00036300
Ni	6.60505700	3.80989200	0.00015100
Ni	-6.60442000	-3.80917700	-0.00345700
Se	4.42022900	3.28371900	-0.00040900
Se	-8.81128100	-4.34048100	-0.00070500
C	3.16889300	-0.70571600	-0.00109800
Se	1.55849000	-1.63003200	-0.00212600
C	3.16881200	0.70608800	-0.00081800
Se	1.55830500	1.63018100	-0.00109800
Ni	-0.00039500	-0.00002600	-0.00197800
Se	-1.55918100	-1.63014400	-0.00226400
Se	-1.55917600	1.63004800	-0.00179600
C	-3.16967900	-0.70596400	-0.00247900
C	-3.16963000	0.70584900	-0.00186100
C	-4.41336300	-1.42269200	-0.00329000
Se	-4.42138400	-3.28360900	-0.00617200
C	-5.63217900	-0.71822700	-0.00247300
Se	-7.23987900	-1.65250700	-0.00335400
C	-5.63213500	0.71797400	-0.00126200
Se	-7.23981700	1.65228900	0.00013900
C	-4.41330000	1.42260700	-0.00140800
Se	-4.42126200	3.28334200	-0.00119900
C	7.57378800	-6.85446900	0.00286000
H	7.55373400	-7.94958900	0.00337900
C	8.76068700	-6.16855300	0.00384500
H	9.71949400	-6.69801900	0.00522500
C	8.75989000	6.16964300	0.00051300
H	9.71863500	6.69924900	0.00062000
C	7.57289600	6.85540700	0.00056000
H	7.55269700	7.95053400	0.00071800
C	-7.57417000	6.85482600	0.00527200
H	-7.55402900	7.94994400	0.00654100
C	-8.76111400	6.16899500	0.00618400
H	-9.71988000	6.69853600	0.00818600
C	-8.75609800	-6.17243600	0.00890600
H	-9.71442000	-6.70278900	0.01233500
C	-7.56856500	-6.85689500	0.01194500
H	-7.54681800	-7.95194800	0.01835200

2$_{\text{Se}}$***cluster***

E = -56403.2280038 Hartree

C	8.29614700	-6.02500100	-0.98798000
Se	8.30221500	-4.19012000	-1.07677600
C	7.25697800	-6.71296400	-0.42420800
Se	5.79601300	-5.84869300	0.27802700
Ni	6.07999800	3.93253400	-0.65361400
Se	6.71136300	1.78001300	-0.81443900
C	4.14394300	1.54856200	0.37448300
C	5.27257400	0.84218500	-0.08680900
Se	4.10078900	3.40596100	0.26385100
C	5.31773500	-0.58378300	0.00934300
Se	6.81066300	-1.53087900	-0.56426300
C	4.21763500	-1.27654200	0.56940400
Ni	6.30403900	-3.67308600	-0.12576200
Se	4.29610200	-3.13263100	0.76440200
C	3.01569300	0.84568400	0.92108200
Se	1.52271000	1.82643100	1.52020300
C	3.07954900	-0.54403000	0.98083100
Se	1.65319800	-1.43066900	1.89915400
Ni	-0.01105300	0.16573600	1.86800100
Se	-1.69368400	1.72072900	1.78332700
Se	-1.52959000	-1.56483200	1.67615800
C	-3.08985000	0.71029400	1.02792100
C	-3.03836300	-0.67690400	0.91060100
C	-4.27281600	1.37970300	0.55889300
Se	-4.37863600	3.23478100	0.66391800
C	-5.34401000	0.64333900	0.01435400
Se	-6.86752400	1.53955400	-0.58134900
C	-5.26647500	-0.78162400	-0.07844600
Se	-6.67486700	-1.77138700	-0.77929900
C	-4.10476300	-1.44357200	0.38457300
Se	-3.99970100	-3.30563000	0.29525400
C	0.85096600	-2.62241600	0.51980700
C	-0.51860200	-2.14680700	0.07786300
H	1.56018900	-2.66896300	-0.31831000
H	0.81932300	-3.61463000	0.99193200
H	-1.08957400	-2.95426100	-0.40694100
H	-0.46362300	-1.28210400	-0.59678900
Ni	-5.98016000	-3.90096500	-0.62102800
Se	-5.29909500	-6.06104000	-0.46455900
C	-7.83018900	-6.29881200	-1.65650700

C	-6.72538500	-6.95976300	-1.19434900
Se	-7.96352200	-4.46846600	-1.57374700
H	9.16263800	-6.54827000	-1.40618400
H	7.26319800	-7.80697900	-0.37298900
H	-6.65574400	-8.05162300	-1.24487500
H	-8.67492100	-6.84207600	-2.09333100
Se	5.44349900	6.10435300	-0.46912200
Se	8.08771600	4.46923200	-1.56675400
C	8.00681600	6.29945800	-1.59579400
C	6.90692200	6.97958200	-1.13933000
H	8.87603500	6.83389400	-1.99399000
H	6.87012900	8.07404400	-1.16176000
Ni	-6.40286500	3.70365900	-0.18303600
Se	-8.44928500	4.18213300	-1.04136100
Se	-5.92443800	5.88654100	0.22009800
C	-8.49520500	6.00823700	-0.89972900
C	-7.44530800	6.71720600	-0.37439200
H	-9.39919500	6.51629400	-1.25242200
H	-7.48481100	7.80886400	-0.29422900

3s$_{Se}$*cluster*

E = -56403.2199828 Hartree

C	-8.03711800	-6.18157900	-1.48346000
Se	-8.08284900	-4.35140600	-1.51692900
C	-7.00261500	-6.86615600	-0.89743000
Se	-5.59727900	-5.99565800	-0.10983100
Ni	-6.15177400	3.81884700	-0.44525200
Se	-6.71301400	1.66235300	-0.78151600
C	-4.24143200	1.42403200	0.59531600
C	-5.30591500	0.71498500	-0.00306500
Se	-4.23860100	3.29089700	0.61531900
C	-5.30666400	-0.71344200	-0.00205400
Se	-6.71478600	-1.66041400	-0.77914400
C	-4.24288700	-1.42275000	0.59725300
Ni	-6.15530700	-3.81703800	-0.44079000
Se	-4.24191800	-3.28958700	0.61970300
C	-3.17227600	0.69187500	1.17091700
Se	-1.68107100	1.57071100	2.01668500
C	-3.17299700	-0.69088000	1.17191000
Se	-1.68152900	-1.57023200	2.01652300
Ni	-0.07069000	0.00015900	1.37957800
Se	1.41636200	1.62759700	0.91847500
Se	1.41549700	-1.62777100	0.91740000
C	2.99514200	0.69701400	0.50050800
C	2.99478600	-0.69775100	0.50009700
C	4.18594900	1.41515300	0.18053100
Se	4.18165400	3.27556100	0.18729300
C	5.37116800	0.71559800	-0.14171500
Se	6.91382400	1.66313800	-0.55998200
C	5.37078500	-0.71717900	-0.14220200
Se	6.91288400	-1.66525400	-0.56131800
C	4.18521800	-1.41630900	0.17967600
Se	4.17999500	-3.27671800	0.18544100
C	-2.00018600	-0.76129800	3.79678500
C	-2.00631500	0.76189600	3.79588700
H	-2.94964900	-1.18236100	4.15414700
H	-1.18345800	-1.16701300	4.41064400
H	-1.19831100	1.17475100	4.41650600
H	-2.96210900	1.17607600	4.14421600
Ni	6.29289000	-3.81711800	-0.38560100
Se	5.66879500	-5.99166700	-0.20196500
C	8.37567900	-6.18494400	-0.92653400
C	7.23194100	-6.86643900	-0.61307100
Se	8.42692400	-4.34828500	-0.95764400
H	-8.87239300	-6.71282100	-1.95232600
H	-6.98522100	-7.96122300	-0.88389900
H	7.21172300	-7.96145300	-0.59764000
H	9.30240900	-6.71543000	-1.17032000
Se	-8.07897300	4.35375000	-1.52172200
Se	-5.59298700	5.99735700	-0.11456500
C	-8.03291900	6.18391800	-1.48796800
C	-6.99825100	6.86822200	-0.90190900
H	-8.86809700	6.71535500	-1.95678100
H	-6.98065800	7.96328500	-0.88818700
Ni	6.29507700	3.81518300	-0.38251300
Se	8.42980900	4.34557100	-0.95269300
Se	5.67233000	5.98995100	-0.19674400
C	8.37984700	6.18222900	-0.91921700
C	7.23639100	6.86413300	-0.60563600
H	9.30711500	6.71235100	-1.16173200
H	7.21692600	7.95914200	-0.58885000

3d$_{Se}$*cluster*

E = -56403.2160681 Hartree

C	8.21560400	-6.11430400	-1.48229600
Se	8.40675300	-4.32609200	-1.05901500
C	7.06951700	-6.79451300	-1.21515000
Se	5.61376400	-5.96814000	-0.42986100
Ni	6.53054100	3.84321500	-0.15187000
Se	7.12848200	1.67869100	-0.25962800
C	4.37287600	1.49179300	0.42582500
C	5.55619900	0.76403500	0.15850400
Se	4.39614700	3.35565300	0.35605500
C	5.55267000	-0.66456000	0.19180500
Se	7.06335800	-1.66409800	-0.27631800
C	4.36377600	-1.30636500	0.57695000
Ni	6.34557900	-3.81243700	-0.21981700
Se	4.41923400	-3.18901400	0.86301100
C	3.15297000	0.80928000	0.72822600
Se	1.53012200	1.71880500	0.91192400
C	3.20352500	-0.58787700	0.84528700
Se	1.61875200	-1.53317100	1.31848800
Ni	-0.02181200	0.04364200	0.96772300
Se	-1.58184000	1.67882100	0.77319900
Se	-1.60465400	-1.57951200	0.81627900
C	-3.17125400	0.75675100	0.44490000
C	-3.18544100	-0.64601100	0.46876000
C	-4.37600300	1.48065600	0.17423600
Se	-4.35573100	3.34082800	0.12878700
C	-5.58045700	0.78566800	-0.05808300
Se	-7.14034200	1.73420400	-0.40557000
C	-5.59464000	-0.64940900	-0.02436400

Se	-7.17291700	-1.58187400	-0.32039500
C	-4.40167100	-1.35720100	0.23604000
Se	-4.41906600	-3.21861600	0.27589500
C	1.72401400	-2.71279000	-0.26442100
C	2.79818000	-3.76970500	-0.13787000
H	0.72842000	-3.16987600	-0.36535800
H	1.88959900	-2.04097100	-1.11618200
H	3.13843100	-4.10833300	-1.12556400
H	2.45363100	-4.63889800	0.43953100
Ni	-6.57066300	-3.73977700	-0.13559500
Se	-5.96138800	-5.91865100	0.06209200
C	-8.71228100	-6.09172500	-0.47311200
C	-7.55735900	-6.78148800	-0.21935700
Se	-8.74419600	-4.25776000	-0.54828500
H	6.96169800	-7.85692000	-1.45658300
H	9.07265300	-6.60080400	-1.95979800
H	-7.54982900	-7.87587600	-0.17552400
H	-9.65943500	-6.61592200	-0.63969800
Ni	-6.49351600	3.88479000	-0.32166200
Se	8.68918300	4.33995000	-0.65598900
Se	5.92946300	6.02993400	-0.02724700
C	8.66164200	6.17020700	-0.65240500
C	7.51268100	6.87385400	-0.39034800
H	9.60298300	6.68690000	-0.86840500
H	7.50903200	7.96917200	-0.39054900
Se	-8.65242500	4.42561300	-0.77805300
Se	-5.83970600	6.05698500	-0.22940800
C	-8.58229400	6.25941700	-0.79644000
C	-7.41433800	6.93675900	-0.56847700
H	-9.51665700	6.79418500	-0.99805800
H	-7.38341700	8.03154100	-0.58147500

TS2$_{Se}$*cluster*

E = -56403.1649311 Hartree

Se	8.87677500	4.15733800	0.27820100
Se	6.15509600	5.90172200	-0.37762900
Se	5.50385100	-6.01046100	0.67813100
Se	8.38838800	-4.46229700	1.07223700
Ni	6.26360000	-3.87604800	0.51809800
Ni	-6.40611000	3.90466600	0.56409900
Se	7.01118200	-1.76075700	0.41204500
Se	-5.73557100	6.07187100	0.63550000
C	4.25906000	-1.42109400	-0.19222600
C	5.49117000	-0.76922800	0.00788800
Se	4.15211300	-3.27149000	0.00668200
Se	-8.53660200	4.41588800	1.16772200
C	5.56544200	0.66047500	-0.10199000
Se	7.19057800	1.52727600	0.15013400
Se	-5.92544800	-5.85287000	-0.54023700
C	4.41042500	1.41429300	-0.39328100
Ni	6.68489200	3.70654200	-0.11177800
Ni	-6.52258800	-3.69326300	-0.17304500
Se	4.52125200	3.27080300	-0.50160200
Se	-8.66090500	-4.24768900	0.36055300
C	3.09721500	-0.65606500	-0.52750900
Se	1.49335400	-1.52042500	-0.86624700
C	3.15136800	0.76015200	-0.61019600
Se	1.64473300	1.75997400	-1.02133700
Ni	-0.00340800	0.15140000	-1.07007500
Se	-1.63128200	-1.45467500	-1.34814800
Se	-1.53299900	1.77553200	-0.87159900
C	-3.18701300	-0.55139500	-0.73922000
C	-3.15636200	0.82804500	-0.58627000
C	-4.38307100	-1.27873400	-0.50588000
Se	-4.40163100	-3.13422300	-0.69662200
C	-5.56128500	-0.59406900	-0.12199900
Se	-7.11889700	-1.55691400	0.19649600
C	-5.53726600	0.82825600	0.01914400
Se	-7.07336200	1.75996500	0.50039400
C	-4.33298600	1.53479900	-0.21011800
Se	-4.28994300	3.38812800	-0.01490100
C	7.02144900	-6.91200000	1.17879300
H	6.93151200	-7.99141100	1.34121500
C	8.21877100	-6.26858900	1.34552000
H	9.11808800	-6.81533200	1.64870800
C	8.91094600	5.98342100	0.14743400
H	9.87637900	6.47893200	0.29622100
C	7.77896900	6.70930500	-0.12577900
H	7.81319800	7.80143000	-0.20195600
C	-7.28052600	6.92621800	1.13569400
H	-7.23615600	8.01456500	1.25068500
C	-8.44389900	6.23855900	1.35778800
H	-9.36034400	6.75832300	1.65718300
C	-8.62898600	-6.07380600	0.18420100
H	-9.55988500	-6.61312400	0.38966000
C	-7.49243500	-6.74077700	-0.18877600
H	-7.48413800	-7.83127800	-0.29100100
C	-0.74466200	-2.18452700	1.25274100
C	0.63060700	-2.13021700	1.38178700
H	-1.36836200	-1.33273100	1.53214600
H	-1.26340000	-3.12506000	1.05641000
H	1.21894800	-3.05216900	1.39758400
H	1.09055800	-1.25020900	1.84001400

TS2y$_{Se}$*cluster*

E = -56403.1822619 Hartree

Se	9.11434200	3.66503000	1.75933800
Se	6.40725300	5.44913500	2.35633400
Se	5.41268400	-5.44312500	-2.53734800
Se	8.38397800	-4.21260000	-1.81788100
Ni	6.23072000	-3.50961600	-1.67520500
Ni	-6.87824100	3.42045900	-1.45317000
Se	7.05641700	-1.61542900	-0.79111700
Se	-6.40704900	5.44940200	-2.35601000
C	4.26456900	-1.11040700	-0.72486600
C	5.54390600	-0.59804300	-0.41927700
Se	4.09679400	-2.79682900	-1.49436500
Se	-9.11417000	3.66511800	-1.75970600
C	5.66232400	0.70413200	0.16552100
Se	7.34013600	1.40088100	0.57734400
Se	-5.41289100	-5.44300500	2.53744100
C	4.50715500	1.46778400	0.42970400

Ni	6.87839800	3.42047600	1.45282900
Ni	-6.23086500	-3.50947000	1.67529900
Se	4.66281600	3.16797600	1.16649600
Se	-8.38411300	-4.21258100	1.81749200
C	3.10874600	-0.33238200	-0.43681200
Se	1.38582200	-0.92142600	-0.93063700
C	3.20708600	0.93835500	0.13475200
Se	1.66999300	1.95540900	0.49584800
Ni	0.00001100	0.51378800	0.00016600
Se	-1.38588400	-0.92129300	0.93104200
Se	-1.66992600	1.95541300	-0.49567900
C	-3.10877900	-0.33229600	0.43704800
C	-3.20705500	0.93838900	-0.13463700
C	-4.26462800	-1.11028700	0.72507100
Se	-4.09693400	-2.79661400	1.49480000
C	-5.54393200	-0.59797000	0.41926400
Se	-7.05648100	-1.61532500	0.79104100
C	-5.66228800	0.70413700	-0.16569700
Se	-7.34004900	1.40079100	-0.57788900
C	-4.50709400	1.46778700	-0.42977400
Se	-4.66268100	3.16793500	-1.16668200
C	6.94825400	-6.41155500	-2.81001100
H	6.83763600	-7.41941900	-3.22425200
C	8.18225700	-5.90103000	-2.51029900
H	9.09332500	-6.48610400	-2.67516100
C	9.20384800	5.31398300	2.55478800
H	10.19757000	5.68690000	2.82520000
C	8.07815900	6.05536500	2.80410900
H	8.14339700	7.03919000	3.28108900
C	-8.07795200	6.05589900	-2.80342800
H	-8.14317700	7.03994500	-3.27995300
C	-9.20365500	5.31444600	-2.55438500
H	-10.19737700	5.68752000	-2.82458300
C	-8.18242300	-5.90111600	2.50966600
H	-9.09348400	-6.48628700	2.67421500
C	-6.94845100	-6.41159700	2.80958200
H	-6.83785400	-7.41952100	3.22368100
C	-0.65576900	-3.24204300	0.23434300
C	0.65542100	-3.24211000	-0.23373600
H	-0.85342200	-3.49719700	1.27744600
H	-1.48448200	-3.41167500	-0.45832900
H	0.85303900	-3.49727800	-1.27684700
H	1.48412500	-3.41181300	0.45893100

TS3s$_{Se}$*cluster*

E = -56403.1860192 Hartree

Se	-8.53555000	-4.34056000	-0.90414000
Se	-5.77796900	-5.98770100	-0.15736700
Se	-5.77801400	5.98766400	-0.15718700
Se	-8.53557500	4.34052300	-0.90403400
Ni	-6.40055200	3.81221200	-0.33719600
Ni	6.29410000	-3.81323500	-0.39360200
Se	-7.01673100	1.65850100	-0.50758700
Se	5.69564600	-5.98796400	-0.13318000
C	-4.28787300	1.41827500	0.23403900
C	-5.46863800	0.71662900	-0.08744300
Se	-4.28763200	3.27839200	0.22661800
Se	8.36429600	-4.34758000	-1.15866100
C	-5.46863100	-0.71666600	-0.08747000
Se	-7.01671800	-1.65853700	-0.50764000
Se	5.69550100	5.98800600	-0.13333500
C	-4.28785800	-1.41831300	0.23397700
Ni	-6.40052200	-3.81224900	-0.33732200
Ni	6.29400400	3.81328500	-0.39370800
Se	-4.28759900	-3.27843000	0.22648500
Se	8.36417200	4.34766000	-1.15882200
C	-3.09419300	0.70018700	0.56642900
Se	-1.53313900	1.63350900	1.00851700
C	-3.09418400	-0.70022800	0.56639300
Se	-1.53311400	-1.63355600	1.00841500
Ni	-0.00292900	-0.00002100	1.26104700
Se	1.59544200	1.59057500	1.49067400
Se	1.59547400	-1.59059400	1.49070300
C	3.08638100	0.69717700	0.77162800
C	3.08639300	-0.69718000	0.77163600
C	4.24181800	1.42123800	0.34320300
Se	4.23707200	3.28412500	0.34489400
C	5.38217200	0.71650700	-0.09016200
Se	6.88767900	1.65926000	-0.65283800
C	5.38219000	-0.71647100	-0.09014400
Se	6.88772700	-1.65920200	-0.65277700
C	4.24184900	-1.42122000	0.34322800
Se	4.23714600	-3.28410700	0.34495800
C	-7.34196900	6.85910000	-0.56321400
H	-7.32372900	7.95413600	-0.54777400
C	-8.48660800	6.17529700	-0.87383300
H	-9.41436500	6.70500700	-1.11538600
C	-8.48657500	-6.17533400	-0.87396800
H	-9.41433400	-6.70504400	-1.11551200
C	-7.34192700	-6.85913700	-0.56338000
H	-7.32368300	-7.95417400	-0.54795600
C	7.20883400	-6.86065900	-0.68431500
H	7.19314500	-7.95557300	-0.65978500
C	8.31875000	-6.17809400	-1.11279300
H	9.21705800	-6.71069000	-1.44307700
C	8.31858000	6.17817400	-1.11300600
H	9.21686800	6.71078400	-1.44332400
C	7.20865500	6.86072300	-0.68452600
H	7.19293900	7.95563700	-0.66002800
C	2.31308900	-0.69461900	3.78104700
C	2.31299700	0.69469100	3.78101800
H	1.47929500	-1.23322900	4.23796700
H	3.25380200	-1.24500200	3.70156700
H	3.25362300	1.24522100	3.70153000
H	1.47910800	1.23320000	4.23787900

TS3d$_{Se}$*cluster*

E = -56403.1851898 Hartree

Se	8.81975000	4.38111200	0.41129800
Se	5.96664200	6.02971300	0.29424700
Se	6.00011500	-5.93187900	-0.28195200
Se	8.84205900	-4.28655300	0.01571900

Ni	6.63741500	-3.75839800	-0.12135800
Ni	-6.60738400	3.85872800	-0.12367400
Se	7.26556600	-1.60610300	0.03710500
Se	-5.98542500	6.04252300	-0.21246100
C	4.44589200	-1.36890200	-0.15810000
C	5.66250900	-0.66758800	-0.03228000
Se	4.45524300	-3.22753600	-0.25413000
Se	-8.81628600	4.36871800	0.03131400
C	5.65824000	0.76543100	0.04186900
Se	7.25719000	1.70163600	0.20059200
Se	-5.80419200	-5.95518400	0.08960100
C	4.43765600	1.46783900	-0.00617100
Ni	6.61593300	3.85467500	0.25517000
Ni	-6.46328200	-3.77584900	0.15297300
Se	4.43522600	3.32585400	0.09213000
Se	-8.61862000	-4.32433300	0.61315700
C	3.20804800	-0.65138700	-0.21073400
Se	1.59850100	-1.57344700	-0.40648500
C	3.20231300	0.75127000	-0.13113000
Se	1.58595200	1.67805500	-0.18825500
Ni	0.02623400	0.05553100	-0.34942100
Se	-1.54935400	-1.55866500	-0.48226000
Se	-1.52774700	1.71286100	-0.28909100
C	-3.15556400	-0.61611300	-0.37932800
C	-3.14264700	0.79650500	-0.31390200
C	-4.36907600	-1.33421300	-0.27975200
Se	-4.32397400	-3.20214900	-0.26359600
C	-5.59652100	-0.65843600	-0.11056300
Se	-7.15694100	-1.62725500	0.17660600
C	-5.60496600	0.77186600	-0.14463700
Se	-7.21895700	1.69586000	-0.04060900
C	-4.39193000	1.49082100	-0.24684800
Se	-4.42262400	3.35369400	-0.27818100
C	7.61366900	-6.80151600	-0.20537700
H	7.59672600	-7.89514600	-0.26342500
C	8.79422600	-6.11795300	-0.08151200
H	9.75221400	-6.64704200	-0.03716200
C	8.76293700	6.21383800	0.46433700
H	9.71925900	6.74280000	0.53719800
C	7.57753000	6.89873700	0.41551800
H	7.55497600	7.99333600	0.44757300
C	-7.60263900	6.89600200	-0.10619500
H	-7.59399000	7.99108000	-0.12736500
C	-8.78016700	6.19975700	-0.00472100
H	-9.74112600	6.72168200	0.05744500
C	-8.54002500	-6.16358200	0.68735300
H	-9.47453900	-6.69192400	0.90394000
C	-7.37381600	-6.83869400	0.48053000
H	-7.33011500	-7.93190300	0.52686900
C	-3.00907400	-3.28182700	1.88380700
C	-1.81892300	-2.56221300	1.77900300
H	-3.86287800	-2.84655800	2.40770200
H	-2.98746300	-4.37272500	1.82884400
H	-0.87460500	-3.09843500	1.65725700
H	-1.74637700	-1.56956300	2.22938300

3s_Se_A"

E = -34027.4181052 Hartree

Ni	-8.44246403	-0.48954699	-1.24535017
Se	-7.87711362	-2.60613954	-1.81179058
C	-5.32875506	-1.43680453	-1.26082069
C	-6.00929796	-2.64285803	-1.51083462
Se	-6.28926899	0.19659513	-1.17896121
C	-5.31636173	-3.87238879	-1.50731157
Se	-6.25189833	-5.49084738	-1.79988803
C	-3.93256648	-3.91355715	-1.25522589
Ni	-4.73222791	-7.06860658	-1.23428029
Se	-3.03167695	-5.58017958	-1.16851372
C	-3.94495130	-1.48582240	-1.05154609
Se	-2.96123864	0.06465526	-0.50398885
C	-3.25846511	-2.70345296	-1.04906149
Se	-1.42224530	-2.66310393	-0.50464978
Ni	-0.77386931	-0.49803515	-1.10429139
Se	-0.23062430	1.69869470	-1.27554760
Se	1.38539675	-1.17179657	-1.28511450
C	1.64465886	1.67994830	-1.08419790
C	2.34272729	0.43988470	-1.08818636
C	2.37544411	2.86164117	-0.89773582
Se	1.49287496	4.57805224	-0.78797490
C	3.75148379	2.84881311	-0.64156273
Se	4.57101442	4.51635216	-0.15124693
C	4.43612622	1.63198705	-0.64405996
Se	6.28614665	1.46275189	-0.14985974
C	3.73245028	0.45025256	-0.90390314
Se	4.74138142	-1.19578639	-0.80843416
C	-1.82264315	-1.96847905	1.31126271
C	-2.58182569	-0.64226272	1.31142917
H	-2.38242135	-2.76844990	1.81498597
H	-0.83450823	-1.87157036	1.78280902
H	-2.00252760	0.15726153	1.79451037
H	-3.56082943	-0.72204843	1.80362175
C	3.41723843	4.78119581	1.44496562
C	1.92004284	4.78389644	1.13658411
H	3.69026131	3.99682159	2.16474242
H	3.75486272	5.75380319	1.82930464
H	1.45503318	5.74401795	1.40008199
H	1.38684900	3.97280752	1.65131683
C	5.90544083	0.33047999	1.43782043
C	5.14454005	-0.95586160	1.11712576
H	6.90898771	0.12057879	1.83358839
H	5.36373772	0.96516392	2.15301143
H	4.17799271	-1.00833809	1.63700933
H	5.73581774	-1.84817580	1.36533474
Tv	15.36996781	0.00000000	0.00000000
Tv	7.95866456	13.14937868	0.00000000

3s_Se_B"

E = -34027.3654290 Hartree

Ni	-8.72673644	-0.66225289	-1.41758453
Se	-8.23576288	-2.83592057	-1.75797337

C	-5.63865620	-1.63916228	-1.73291385
C	-6.33690711	-2.84858764	-1.73066260
Se	-6.59930808	-0.00118789	-1.76094748
C	-5.63218759	-4.06947487	-1.72582226
Se	-6.57051570	-5.72031023	-1.73847947
C	-4.23574361	-4.06927261	-1.72590597
Ni	-4.93270041	-7.23093834	-1.39869590
Se	-3.29692562	-5.71974072	-1.74577740
C	-4.22897910	-1.63904299	-1.73090794
Se	-3.26821216	-0.00126182	-1.75496855
C	-3.53086183	-2.84850757	-1.72808544
Se	-1.63211488	-2.83640510	-1.74809633
Ni	-1.14131554	-0.66280908	-1.40819606
Se	-0.71913940	1.40620144	-0.44276157
Se	0.85817907	-1.32802419	-0.43666895
C	1.21940393	1.51349030	-0.49834171
C	1.92172553	0.29628736	-0.49968534
C	1.91685262	2.72023092	-0.49550468
Se	1.04229254	4.45383866	-0.42313368
C	3.32206295	2.71972557	-0.49940214
Se	4.19929496	4.45178419	-0.44194465
C	4.01843873	1.51244137	-0.50380719
Se	5.95739679	1.40401122	-0.45006313
C	3.31552627	0.29561602	-0.50228776
Se	4.37820694	-1.32991310	-0.44805915
C	0.06263059	-0.84176191	1.31988313
C	-0.70505862	0.47817586	1.31542417
H	-0.59941342	-1.69611305	1.51732707
H	0.88212038	-0.84325908	2.05212835
H	-0.30720684	1.19161044	2.05070562
H	-1.77680476	0.32564290	1.50315369
C	3.39524736	4.90107274	1.31988920
C	1.86861671	4.89452864	1.33065319
H	3.81804254	4.20036310	2.05348013
H	3.79878969	5.90581061	1.50660422
H	1.45992478	5.89419937	1.53309007
H	1.46137362	4.18351626	2.06312019
C	5.94153807	0.47380271	1.30696082
C	5.18438017	-0.85217899	1.30595673
H	7.01335017	0.32933892	1.50098896
H	5.53414092	1.18355895	2.04050452
H	4.37255451	-0.86663499	2.04662417
H	5.85506629	-1.70314690	1.48828513
Tv	15.10630144	0.00000000	0.00000000
Tv	7.54803014	13.08566402	0.00000000

3d$_{Se''}$

E = -34027.3947966 Hartree

Ni	-5.72604865	1.02076715	-0.33153572
Se	-5.31344732	-1.08412597	-1.19850569
C	-2.68460243	0.04817329	-1.09844314
C	-3.38982045	-1.16270932	-1.09992715
Se	-3.64276226	1.71364713	-1.05052312
C	-2.68993763	-2.36916668	-1.10620608
Se	-3.65023483	-4.03158350	-1.07957454
C	-1.28913412	-2.37278353	-1.08760883
Ni	-2.01586650	-5.50534159	-0.36787362
Se	-0.37764134	-4.06654973	-1.15913399
C	-1.28975812	0.05203242	-1.08513524
Se	-0.27257409	1.68431100	-1.17536739
C	-0.59305928	-1.16365985	-1.08774827
Se	1.32563267	-1.17137808	-1.02568247
Ni	1.78120127	0.99257734	-0.35188256
Se	2.24393133	3.13949620	0.22732956
Se	3.88319338	0.33015936	0.19835211
C	4.14062603	3.17187431	0.31149035
C	4.84461071	1.96422357	0.32008345
C	4.83871571	4.39043318	0.30408980
Se	3.90748596	6.04093860	0.16935508
C	6.23662604	4.39535116	0.31831148
Se	7.15948828	6.05149978	0.21610037
C	6.94248283	3.18211769	0.33808782
Se	8.84194821	3.16408865	0.27317007
C	6.24818874	1.96902842	0.33984847
Se	7.22485306	0.34017829	0.29056252
C	1.35735609	-2.36351048	0.55236598
C	1.05525368	-3.79944105	0.20243733
H	2.37197603	-2.25804044	0.96738320
H	0.64428433	-1.93447591	1.26797070
H	0.73931800	-4.37352651	1.08621665
H	1.91771891	-4.29926085	-0.25887222
C	-1.23600534	2.82811195	0.14498500
C	-2.61871809	2.35463572	0.51439582
H	-0.57994259	2.88791474	1.02671389
H	-1.25772204	3.80717148	-0.35261774
H	-3.22146178	3.17485197	0.93540785
H	-2.61343418	1.52410980	1.23220508
C	-5.84977132	-2.52502475	0.07060228
C	-4.74717898	-3.47227342	0.46732954
H	-6.27410177	-2.01132152	0.94721895
H	-6.65575458	-3.03996183	-0.46939210
H	-5.15689691	-4.40651959	0.88294122
H	-4.04795915	-3.04508440	1.19783627
Tv	15.02860596	0.00000000	0.00000000
Tv	7.55337466	13.03307197	0.00000000

TMP[7]

E = -19157.7720339 Hartree

Ni	-2.56961100	3.32066200	-0.00039600
Se	-0.34442200	3.31907300	-0.00013900
C	-1.31106500	0.52668700	-0.00015500
C	-0.19868900	1.39412500	-0.00006400
Se	-3.14200000	1.13020800	-0.00036500
C	1.11214800	0.87242000	0.00009000
Se	2.55091800	2.15617500	0.00020000
C	1.30694100	-0.52488100	0.00015000
Ni	4.16070700	0.56434100	0.00040000
Se	3.04676800	-1.36166400	0.00036100
C	-1.10753600	-0.86925200	-0.00009800
Se	-2.70230700	-1.95653900	-0.00021600
C	0.19975600	-1.39920500	0.00005300
Se	0.59166900	-3.28734300	0.00016500

Ni	-1.59219100	-3.88487000	-0.00000700

DMP[5]

E = -17728.3225449 Hartree

Ni	3.77296000	-1.67076500	-0.07112800
Se	3.32523100	0.51614500	0.00025800
Se	1.74748300	-2.68257300	0.01394200
C	1.41485000	0.24702300	-0.03860500
C	0.78593800	-1.01416500	-0.00854900
C	0.62721200	1.41090500	-0.10781700
Se	1.46376800	3.12798700	-0.13734800
C	-0.77391700	1.32784200	-0.11943900
Se	-1.87333800	2.85617200	-0.45106500
C	-1.41207500	0.07439800	-0.01585100
Se	-3.33591200	0.10106800	0.05537000
C	-0.62645600	-1.09486200	0.02138300
Se	-1.37171000	-2.87246300	0.11998000
Ni	-3.48771600	-2.15743300	-0.00603700
C	-1.08854000	4.21322900	0.74258500
C	0.29229800	3.87276200	1.24636800
H	-1.07396100	5.12846200	0.13249600
H	-1.78093800	4.36199800	1.58594500
H	0.80224700	4.77126200	1.62765100
H	0.26217000	3.12958600	2.05545300

MMP[3]

E = -16298.8701241 Hartree

Se	-3.21244200	1.38759800	-0.07635300
Se	-0.07871400	3.32814300	-0.06487100
C	-1.41888500	0.69101600	-0.08321300
C	-0.21724300	1.41613300	-0.01763000
C	-1.36187900	-0.71709700	-0.13487300
Se	-2.98313800	-1.72891800	-0.22398100
C	-0.13523200	-1.39348900	-0.09586700
Se	-0.03071000	-3.28312400	-0.35604200
C	1.06980900	-0.66957300	0.02189400
Se	2.69242600	-1.70856100	0.11217200
C	1.02516100	0.73625700	0.04931800
Se	2.59743800	1.83913700	0.19634200
Ni	3.99201200	0.09152300	-0.19269700
C	-1.45123300	-3.95354600	0.83706600
C	-2.46586900	-2.91469000	1.24866600
H	-1.92218200	-4.75928700	0.25478100
H	-0.96722700	-4.39463000	1.72224800
H	-3.39272700	-3.39133900	1.60376600
H	-2.08848200	-2.26387400	2.04946400
C	-1.83592800	3.84613800	0.59395400
H	-1.94485300	3.54095300	1.64463400
H	-1.79963500	4.94720100	0.55707900
C	-2.94748400	3.31078100	-0.27149400
H	-3.92410200	3.71874800	0.03905000
H	-2.78965300	3.56263400	-1.32951800

BHSe_Et

E = -14869.41783760 Hartree

Se	-2.76051300	-1.83740400	-0.21465700
Se	-2.76410000	1.83202000	0.21466100
C	-1.23090300	-0.69450600	-0.07088400
C	-1.23225700	0.69213600	0.07085400
C	0.00053100	-1.37644400	-0.12933600
Se	0.01872500	-3.26475800	-0.33531200
C	1.21345300	-0.69831700	-0.05779200
Se	2.87432700	-1.60843100	-0.20545200
C	1.21208700	0.70066000	0.05786000
Se	2.87115400	1.61406700	0.20555600
C	-0.00215100	1.37645300	0.12930800
Se	0.01235000	3.26480500	0.33524400
C	2.58646000	-3.15064500	0.99427700
C	1.13456900	-3.49932800	1.26101400
H	3.09544300	-3.97535400	0.48955200
H	3.09876600	-2.93422600	1.93494600
H	1.03533100	-4.54062400	1.57745600
H	0.69077700	-2.86863300	2.03354100
C	-4.19073800	0.54166800	0.52434000
H	-4.12133000	0.13499700	1.53517000
H	-5.09720100	1.15260500	0.45612900
C	-4.18972600	-0.54985400	-0.52420400
H	-5.09498200	-1.16256400	-0.45586800
H	-4.12121800	-0.14307100	-1.53504800
C	1.12771900	3.50150900	-1.26111200
H	0.68506600	2.87003500	-2.03365100
H	1.02655100	4.54264300	-1.57747800
C	2.58028700	3.15550400	-0.99448300
H	3.09284500	2.93979800	-1.93517700
H	3.08787200	3.98122400	-0.49000600

1_Se_*bilayer*

E = -67584.1598453 Hartree

Ni	-7.40805922	-0.15327683	2.03143642
C	-4.34101945	-1.21374149	1.84669325
C	-5.09487823	-2.41122251	1.83941123
C	-4.45483055	-3.67703008	1.64646135
C	-3.06094884	-3.72082047	1.53277544
Ni	-3.89933367	-6.91558904	1.28017506
C	-2.91292963	-1.27481662	1.77964678
C	-2.27588053	-2.53140382	1.66108907
Ni	0.19117010	-0.47515512	1.27598125
C	2.54424859	1.84182021	1.53810904
C	3.27643035	0.65445827	1.64798877
C	3.18516846	3.11485037	1.66700035
C	4.59224977	3.18779087	1.78112910
C	5.35601203	1.97932361	1.84818530
C	4.69267565	0.72933089	1.84241855
Ni	-6.94613605	0.65217051	-2.02932348
C	-3.83602664	-0.23026470	-1.83941074
C	-4.49929391	-1.48029538	-1.84509758
C	-3.73547825	-2.68870363	-1.77763167

C	-2.32842355	-2.61565939	-1.66331585
Ni	-2.88285208	-5.77832383	-1.27619843
C	-2.41985114	-0.15527192	-1.64450674
C	-1.68762564	-1.34257956	-1.53441785
Ni	0.66536811	0.97450744	-1.27203659
C	3.13262753	3.03061492	-1.65709576
C	3.76958434	1.77399092	-1.77590298
C	3.91781515	4.21996539	-1.52876474
C	5.31169146	4.17610384	-1.64271145
C	5.95160957	2.91028444	-1.83615429
C	5.19766967	1.71283423	-1.84336721
Se	0.72591364	1.76302012	1.10243381
Se	2.47078479	-1.01001846	1.39931600
Se	-0.42102137	-2.64231029	1.69520300
Se	-1.88730266	0.27575837	1.88027242
Se	-5.22015038	0.42606303	1.92014662
Se	-2.22534411	-5.33762923	1.09471030
Se	-6.93152717	-2.35281377	2.06223687
Se	-5.49764997	-5.20564993	1.40879145
Se	2.16596379	4.66881169	1.70637638
Se	5.42807132	4.84790220	1.88033173
Se	7.21604384	2.03248289	1.92007076
Se	5.65781359	-0.83405168	2.06778170
Se	0.13065181	-1.26367333	-1.09854597
Se	-1.61433260	1.50923734	-1.39553168
Se	2.74380203	0.22351259	-1.87647151
Se	1.27775945	3.14165548	-1.69104403
Se	-1.30907365	-4.16954071	-1.70244443
Se	-4.57111221	-4.34891910	-1.87657368
Se	-4.80118457	1.33297835	-2.06568396
Se	-6.35930925	-1.53354939	-1.91748004
Se	6.07671417	0.07298457	-1.91745644
Se	7.78814679	2.85176702	-2.06001714
Se	6.35462817	5.70463541	-1.40487620
Se	3.08235699	5.83680293	-1.09058056
Tv	15.21081052	0.00000000	0.00000000
Tv	7.63924665	13.19303485	0.00000000

6_**Se**

E = -67741.0638986 Hartree

Ni	-7.23851458	0.14503920	1.31352956
Se	-6.70883472	-2.08640688	1.62734172
C	-4.12453062	-0.88678864	1.68563259
C	-4.85016542	-2.10125473	1.58233368
Se	-5.02359535	0.73291682	1.59137347
C	-4.13539236	-3.33223605	1.50690258
Se	-5.06486315	-4.91988763	1.26003907
C	-2.71390131	-3.35337317	1.60595744
Ni	-3.46786286	-6.53575218	1.41150861
Se	-1.79360309	-4.98157359	1.66283378
C	-2.70356213	-0.90761126	1.82271482
Se	-1.80362608	0.68250735	2.21043195
C	-2.02610426	-2.13284869	1.73870580
Se	-0.14662014	-2.07471775	2.17165288
Ni	0.43155839	0.15099818	2.09075305
Se	1.02295101	2.36891780	2.26967189
Se	2.67073301	-0.38838502	2.17238163
C	2.88484900	2.44203859	1.75948923
C	3.56070604	1.21161409	1.79276344
C	3.57257281	3.66207842	1.63039978
Se	2.67055839	5.29765289	1.76296507
C	4.99029675	3.63842034	1.48217485
Se	5.91704313	5.22432159	1.22129753
C	5.70152618	2.40349033	1.52275032
Se	7.55863886	2.38359357	1.50373306
C	4.97673206	1.19118630	1.61998523
Se	5.86493970	-0.42807209	1.41238174
Ni	-7.39268854	0.25328988	-1.33384796
Se	-6.87661141	-1.97219729	-1.67249482
C	-4.29417278	-0.77499500	-1.57597625
C	-5.02183323	-1.98751737	-1.67876891
Se	-5.18354115	0.83020249	-1.32559823
C	-4.31558526	-3.21759005	-1.79265470
Se	-5.22201638	-4.83347449	-1.66467569
C	-2.89863025	-3.22433042	-1.92128484
Ni	-3.61805952	-6.43739550	-1.97317203
Se	-2.02200355	-4.83286386	-2.34316740
C	-2.86863295	-0.78315548	-1.59421615
Se	-1.94260085	0.84143181	-1.43333417
C	-2.20848813	-2.00749098	-1.76852697
Se	-0.30048921	-1.92197589	-1.96508156
Ni	0.27839101	0.25755744	-1.50161138
Se	0.85250386	2.45838518	-1.87033696
Se	2.49420965	-0.33211548	-1.47198060
C	2.76777753	2.51616788	-1.76881597
C	3.42669687	1.28709280	-1.63748680
C	3.45661831	3.73324487	-1.92427237
Se	2.56435770	5.34649529	-2.28593619
C	4.87645485	3.72304410	-1.83755926
Se	5.79025635	5.33666675	-1.72799695
C	5.58204804	2.49010724	-1.74697914
Se	7.43688182	2.46856797	-1.78067563
C	4.85222135	1.27477957	-1.65271540
Se	5.74050406	-0.34211192	-1.51063809
C	0.27483785	-3.24943956	-0.62299600
H	1.01605305	-3.84336059	-1.18043928
H	-0.59901932	-3.90144715	-0.49174260
C	0.89624837	-2.87843908	0.69009848
H	1.25650212	-3.81782017	1.13742883
H	1.75452298	-2.19676852	0.58840856
C	0.39847605	3.71652681	-0.42135076
H	-0.38582875	4.33894114	-0.88023885
H	1.28525772	4.35847832	-0.33588748
C	-0.10557689	3.28810483	0.92406065
H	-0.39820056	4.20971136	1.45040629
H	-0.98874036	2.63417432	0.85946557
Tv	15.33276882	0.00000000	0.00000000
Tv	7.79782935	13.38063233	0.00000000

6_**Se"**

E = -68054.8739727 Hartree

Ni	-7.13801371	0.18564504	1.95840526

Se	-6.56082532	-2.03268158	2.20015914
C	-3.94737791	-0.87093212	2.04313454
C	-4.66939232	-2.07409882	2.06920300
Se	-4.91794983	0.77516309	1.89704367
C	-3.95755843	-3.29132236	2.12677276
Se	-4.90318808	-4.93201485	2.46452356
C	-2.55442434	-3.30032238	2.24196128
Ni	-3.22706376	-6.54122607	2.55844737
Se	-1.59448261	-4.89019733	2.62294159
C	-2.54668871	-0.84253034	2.14565734
Se	-1.62935481	0.80227024	2.34828533
C	-1.86848899	-2.06890665	2.18280341
Se	0.04578860	-2.02762620	2.23405922
Ni	0.61069106	0.22149843	2.30479231
Se	1.21713695	2.44310435	2.36319366
Se	2.83616710	-0.42320961	2.33696590
C	3.12628623	2.43611826	2.18780092
C	3.78233917	1.20295185	2.10084179
C	3.83243196	3.65332554	2.24294876
Se	2.95148998	5.25280826	2.73967987
C	5.21928518	3.62544266	2.00715819
Se	6.18408400	5.28136900	2.08805225
C	5.91526711	2.40629367	1.87335340
Se	7.80686914	2.40070452	1.72480323
C	5.18232052	1.20507673	1.91998823
Se	6.15374931	-0.43397081	2.11055699
Ni	-7.91247044	0.10705792	-2.61182230
Se	-7.31555688	-2.11208441	-2.45303174
C	-4.69532706	-0.89669145	-2.51676132
C	-5.42380489	-2.09473330	-2.41333468
Se	-5.68032889	0.72571796	-2.73064226
C	-4.71843450	-3.30391180	-2.32185366
Se	-5.67805177	-4.94360821	-2.15449692
C	-3.32128337	-3.34882264	-2.38630738
Ni	-4.06230310	-6.59682249	-2.21821574
Se	-2.39816628	-5.00664980	-2.41913090
C	-3.28730525	-0.89934441	-2.57758991
Se	-2.32238626	0.71050004	-2.86625175
C	-2.62607834	-2.13259766	-2.46062447
Se	-0.71024464	-2.14172600	-2.44861453
Ni	-0.13027899	0.08896902	-2.41926720
Se	0.42125048	2.32193312	-2.23865295
Se	2.08705192	-0.53279834	-2.42241880
C	2.33249934	2.34366418	-2.20793115
C	3.00819830	1.11582193	-2.30777458
C	3.03039164	3.56810582	-2.25474455
Se	2.10017237	5.21560214	-2.07154293
C	4.41933821	3.52556133	-2.43869631
Se	5.38415367	5.17310288	-2.55872105
C	5.13146818	2.31590079	-2.54098340
Se	6.98280163	2.30447633	-2.96498755
C	4.40811566	1.12928069	-2.39505446
Se	5.36977147	-0.52806247	-2.44760373
C	-0.48552253	-2.84493870	-0.58026633
H	-0.20091624	-3.89373642	-0.72170074
H	-1.50497773	-2.81081677	-0.17264479
C	0.49203860	-2.08443280	0.26955011
H	1.49173970	-2.53861828	0.27725547
H	0.61068580	-1.04124974	-0.04424496
C	-0.12705053	2.54010903	-0.32915149
H	-0.37209963	1.53470185	0.03043751
H	-1.07574136	3.08195374	-0.44599660
C	0.82141953	3.28435106	0.58095964
H	1.81922848	3.43794061	0.15093732
H	0.42972154	4.27185027	0.85159675
C	-5.51924953	1.61671685	-0.92630859
H	-6.51926553	1.49129961	-0.49750121
H	-5.39051260	2.67099105	-1.20108731
C	-4.41756122	1.12550771	-0.01143388
H	-4.01149223	0.15466922	-0.32130748
H	-3.59092401	1.84093382	0.06373482
C	-6.30584473	-4.69124820	-0.27042603
H	-7.38787812	-4.85831623	-0.35040186
H	-6.16437280	-3.62259217	-0.06009681
C	-5.67721774	-5.62965042	0.74287639
H	-6.42382499	-6.30296963	1.18293369
H	-4.91107148	-6.27251028	0.29590895
C	6.41097106	4.94608701	-0.85795650
H	7.46674246	4.97437854	-1.15489169
H	6.16948941	3.91619678	-0.56452359
C	6.06259080	5.94847904	0.20448946
H	6.74475043	6.80853679	0.23802190
H	5.05195974	6.35435617	0.07517021
C	4.92660631	-1.12147315	-0.58302489
H	4.31830034	-2.01483712	-0.77365251
H	4.23441673	-0.34927290	-0.22214524
C	6.04254246	-1.45243853	0.38282732
H	5.91959851	-2.47448203	0.76624614
H	7.05329575	-1.40131438	-0.05113353
Tv	15.51802491	0.00000000	0.00000000
Tv	7.81881345	13.41559129	0.00000000

2y_2y$_{\text{Se\_A}}$

E = -67741.0736399 Hartree

Ni	-7.44347196	1.00570820	1.14462773
Se	-6.93601183	-1.24581673	0.96568940
C	-4.35601481	-0.15260362	1.48859723
C	-5.13890045	-1.32930322	1.47132911
Se	-5.13460698	1.51531999	1.16514011
C	-4.54058829	-2.59807457	1.71169159
Se	-5.58069897	-4.14851459	1.75257587
C	-3.15279067	-2.68944371	1.95141214
Ni	-3.99230004	-5.77562385	1.48206475
Se	-2.34290968	-4.35385228	2.15970444
C	-2.96734781	-0.27393186	1.72145753
Se	-1.70168813	1.06804353	1.21050953
C	-2.35635741	-1.50517275	2.00003149
Se	-0.52574641	-1.66611757	2.43300014
Ni	0.21524385	0.47806081	2.22654397
Se	0.68556790	2.60868831	2.82972660
Se	2.44256418	-0.04597236	2.30499980
C	2.44928877	2.85051587	2.10608213
C	3.20592970	1.66999158	2.07444278
C	3.01761161	4.12042502	1.86914430

Se	1.94601101	5.64944940	1.72213325
C	4.41138177	4.19782583	1.66500659
Se	5.19717848	5.83713617	1.24363579
C	5.22170700	3.03193290	1.71530708
Se	7.08574906	3.15672073	1.60620986
C	4.61774904	1.76947310	1.87368394
Se	5.66531550	0.22765049	1.83517070
Ni	-7.00903234	-0.60020903	-1.45014915
Se	-6.38093767	-2.78693274	-1.71358418
C	-3.91268048	-1.39979089	-1.92752532
C	-4.51908567	-2.65043119	-1.68182221
Se	-4.95945232	0.12707821	-2.13687893
C	-3.71169488	-3.79805804	-1.44398498
Se	-4.52543374	-5.40043651	-0.93031680
C	-2.30180973	-3.70050237	-1.46998079
Ni	-2.82196500	-6.95626368	-1.11643704
Se	-1.23576609	-5.20285118	-1.15188963
C	-2.48978661	-1.29392919	-1.98269807
Se	-1.72511118	0.37574227	-2.42051380
C	-1.72124867	-2.43411171	-1.70680668
Se	0.07353654	-2.00051147	-1.20290234
Ni	0.50472924	-0.03634185	-2.20977649
Se	1.15063910	2.15932115	-2.27468644
Se	2.59112390	-0.67563043	-2.81251729
C	3.01986858	1.97360202	-2.04257496
C	3.67140826	0.73197222	-2.07382881
C	3.80478759	3.15108379	-1.84071889
Se	2.98517448	4.82589037	-1.80381089
C	5.20069843	3.05103020	-1.68248676
Se	6.23318427	4.60793770	-1.57857233
C	5.81267576	1.76997896	-1.63098398
Se	7.62691018	1.64235797	-1.21564588
C	5.05595925	0.59714517	-1.83478311
Se	5.85392097	-1.09111257	-1.68951102
C	1.46454971	-3.13705230	-2.02466038
H	1.47170127	-4.09955156	-1.49519960
H	1.24493410	-3.30806309	-3.08828386
C	2.75276237	-2.36993537	-1.79004661
H	3.62250463	-2.91124123	-2.18475444
H	2.92350677	-2.13353152	-0.72917185
C	-2.00326337	2.84673041	2.01662622
H	-2.83141891	3.32593174	1.47689993
H	-2.26864354	2.74962673	3.07912371
C	-0.69599744	3.58219625	1.78648340
H	-0.73718739	4.60941795	2.17169268
H	-0.39622164	3.60312109	0.72784019
Tv	15.14371101	0.00000000	0.00000000
Tv	7.49279649	13.16429737	0.00000000

2y_2y$_{\textbf{Se\_B}}$

E = -67741.0583707 Hartree

Ni	-7.85174964	1.14602143	1.18076523
Se	-7.23580946	-1.05255344	0.81219742
C	-4.77080837	0.12255698	1.57482415
C	-5.43274879	-1.09396269	1.35025002
Se	-5.60697644	1.75602382	1.28647562
C	-4.71502348	-2.32126163	1.50464687
Se	-5.60474116	-3.93630727	1.32210269
C	-3.33383113	-2.31009700	1.87763394
Ni	-3.91249145	-5.51459552	1.38198189
Se	-2.40285468	-3.91170634	2.11294286
C	-3.38907554	0.14495246	1.92369941
Se	-2.59364306	1.83231432	2.18582003
C	-2.70218746	-1.06562153	2.07761290
Se	-0.99029227	-0.75522489	2.96434916
Ni	-0.41559785	1.20060123	1.93750609
Se	0.15397606	3.34561286	1.46666193
Se	1.64511336	0.50230146	1.27247750
C	2.02183247	3.24753000	1.64758965
C	2.73165762	2.03816240	1.71569901
C	2.75674659	4.47171637	1.61423301
Se	1.85769013	6.04050100	1.20068342
C	4.15707376	4.47066952	1.73398594
Se	5.10247835	6.07347336	1.61917999
C	4.85569260	3.23090926	1.81168299
Se	6.70563095	3.23066166	1.94013654
C	4.14099391	2.00119654	1.74176350
Se	5.10063082	0.39551316	1.65132104
Ni	-7.29487514	0.07373577	-1.50546570
Se	-6.61243459	-2.05445421	-2.06098619
C	-4.15854733	-0.63446428	-1.82374802
C	-4.76820068	-1.90777053	-1.84826283
Se	-5.19899316	0.90369077	-1.90371575
C	-3.97036670	-3.07639812	-1.68629034
Se	-4.81715578	-4.68879507	-1.40440190
C	-2.55999250	-2.99357018	-1.58569347
Ni	-3.12793064	-6.22289481	-1.17858194
Se	-1.52900493	-4.52311218	-1.27651621
C	-2.73510030	-0.53324813	-1.75288443
Se	-1.96492264	1.18606804	-1.69525431
C	-1.97889601	-1.71293083	-1.67547279
Se	-0.14481087	-1.39883828	-1.23688012
Ni	0.22902528	0.66644441	-2.05248655
Se	0.82084614	2.86307135	-2.22246500
Se	2.23009919	0.10785722	-2.97950505
C	2.68307444	2.67007052	-2.00700593
C	3.33963947	1.43400878	-2.12228606
C	3.46001214	3.83873031	-1.74311664
Se	2.62056117	5.48448585	-1.77836551
C	4.85672757	3.73929004	-1.52238772
Se	5.87208652	5.28278239	-1.29616210
C	5.46172270	2.44714168	-1.53543552
Se	7.24750768	2.26668610	-1.06218510
C	4.72087884	1.29094317	-1.88764694
Se	5.55244808	-0.38556519	-1.97585751
C	1.10935099	-2.41571890	-2.37418185
H	1.14926030	-3.44995418	-2.00357364
H	0.74201620	-2.42235665	-3.41073533
C	2.44638501	-1.71277681	-2.21431104
H	3.23730030	-2.21533584	-2.78742079
H	2.76986313	-1.63003261	-1.16676016
C	0.56155472	-1.86313618	2.39228032
H	0.59394741	-2.74169044	3.05179017
H	0.41608438	-2.19614546	1.35612891

C	1.80091294	-0.99263855	2.57351084
H	2.71486684	-1.55577576	2.33259238
H	1.89664081	-0.58599992	3.59092569
Tv	15.09662281	0.00000000	0.00000000
Tv	7.39077367	13.18194730	0.00000000

2y_2y_Se"

E = -68054.8359570 Hartree

Ni	-7.15256726	1.23904686	2.27176668
Se	-6.52418013	-0.89361223	2.86245439
C	-4.01171863	0.54014688	2.81541585
C	-4.62548929	-0.72461078	2.83464329
Se	-5.23183135	1.96764079	3.22815022
C	-3.78898331	-1.85188435	2.84361037
Se	-4.38295090	-3.61473075	3.31972497
C	-2.38376557	-1.75140474	2.83908656
Ni	-2.83269502	-4.92325853	2.30749911
Se	-1.27515546	-3.30259675	2.79639006
C	-2.61711208	0.69844354	2.83219527
Se	-1.82404589	2.43259580	2.82488533
C	-1.82414371	-0.46509433	2.86520463
Se	-0.02726757	-0.08379645	3.43477420
Ni	0.36746485	1.88059286	2.37919928
Se	1.00865011	4.01662759	1.81597460
Se	2.31209751	1.13414392	1.49856396
C	2.90374975	3.83817974	1.84674706
C	3.52180349	2.57320609	1.86478778
C	3.73683270	4.96610991	1.82345757
Se	3.11388740	6.72651855	1.36426417
C	5.14452220	4.86926650	1.80184579
Se	6.24751977	6.42465876	1.80172871
C	5.70591618	3.58156527	1.76645642
Se	7.50931235	3.20472281	1.19882912
C	4.91393240	2.41876716	1.80684888
Se	5.70586392	0.68266030	1.75455210
Ni	-4.67736865	0.15520714	-2.19685486
Se	-4.07281676	-1.98378094	-1.58430876
C	-1.55205380	-0.56442856	-1.72725979
C	-2.17490050	-1.82752486	-1.69198252
Se	-2.74809927	0.85893968	-1.22537132
C	-1.35706117	-2.96862624	-1.70611785
Se	-2.01439624	-4.72128488	-1.26491996
C	0.04955277	-2.87651314	-1.71078434
Ni	-0.39130068	-6.03699651	-2.16246405
Se	1.14762169	-4.42713856	-1.57171379
C	-0.15675265	-0.41986489	-1.80140722
Se	0.64205241	1.30521872	-1.89598828
C	0.62238587	-1.59677494	-1.77851128
Se	2.47225815	-1.26341108	-1.37010897
Ni	2.83682197	0.76216933	-2.30845231
Se	3.47632061	2.92487717	-2.78453967
Se	4.76693938	0.09393949	-3.28859551
C	5.37461278	2.75290649	-2.78255011
C	5.99143571	1.48787382	-2.78190187
C	6.20606228	3.88420303	-2.77770612
Se	5.63728183	5.65175167	-3.28825370
C	7.61236651	3.78202044	-2.74901627
Se	8.70683111	5.34592099	-2.68145579
C	8.17629391	2.49728844	-2.75847022
Se	10.00307904	2.13069224	-3.24305209
C	7.38580360	1.33243488	-2.75960713
Se	8.18751803	-0.39587204	-2.72421527
C	3.74537863	-2.35312195	-2.41646745
H	3.79974714	-3.34501418	-1.94860110
H	3.38540289	-2.46857437	-3.44906758
C	5.06141443	-1.60284467	-2.31581198
H	5.87657780	-2.13990665	-2.81888510
H	5.36046859	-1.38504296	-1.27929846
C	1.34975299	-1.22862551	2.59710985
H	1.41176920	-2.15215404	3.18819019
H	1.06258893	-1.48845592	1.56803200
C	2.63034437	-0.42196796	2.67352884
H	3.48539956	-0.97948151	2.26806879
H	2.87495644	-0.08789427	3.69224681
C	-4.90240922	3.55814740	2.10468849
H	-4.07981225	4.12541884	2.56037971
H	-4.58925554	3.23577977	1.10154153
C	-6.19448992	4.34841796	2.10561222
H	-6.10304128	5.26882122	1.51256997
H	-6.54139872	4.60689416	3.11569331
C	-2.43614828	2.50165012	-2.28426488
H	-1.63992428	3.06475885	-1.77933995
H	-2.09569288	2.23569610	-3.29478509
C	-3.74826083	3.26041988	-2.28211888
H	-3.65963948	4.20550819	-2.83552704
H	-4.11870189	3.49277139	-1.27391308
C	-5.98813542	-4.16636973	2.31099001
H	-6.86550888	-3.73338624	2.81000267
H	-5.93038590	-3.76948036	1.28709510
C	-6.00288566	-5.67976058	2.37188604
H	-6.88104497	-6.10211438	1.86605067
H	-5.95852713	-6.07757502	3.39574171
C	-3.51726088	-5.23364012	-2.44755092
H	-4.43520565	-4.79975350	-2.02866498
H	-3.35970322	-4.81676033	-3.45300375
C	-3.55649554	-6.74827835	-2.42721769
H	-4.38962704	-7.13748798	-3.02813777
H	-3.62701177	-7.16523521	-1.41309450
Tv	15.03823041	0.00000000	0.00000000
Tv	7.51434628	12.97541439	0.00000000

2y_3dy_Se

E = -67741.0583988 Hartree

Ni	-6.59554555	0.54508883	1.17361624
Se	-6.20046709	-1.59700935	1.97011923
C	-3.56576545	-0.55761261	1.75701014
C	-4.35735943	-1.73705469	1.92536642
Se	-4.37484171	1.10656022	1.58336676
C	-3.69838719	-3.00421536	2.06468251
Se	-4.67719819	-4.59696417	2.08519127
C	-2.29010437	-3.08820973	2.08697645
Ni	-3.06370171	-6.24165076	2.11587692

Se	-1.40144020	-4.69135611	2.38422924
C	-2.15591602	-0.68434911	1.72889149
Se	-1.01976413	0.70781588	1.04444065
C	-1.50570047	-1.91262535	1.86026489
Se	0.35554323	-2.12038189	1.60317905
Ni	1.03359167	0.05127247	1.73574902
Se	1.53212556	2.05409537	2.65667927
Se	3.25817412	-0.46131504	1.67345473
C	3.27731825	2.42269025	1.93466368
C	4.01901329	1.25396639	1.67346285
C	3.85515158	3.70247439	1.92895193
Se	2.84162973	5.23620125	2.29878561
C	5.25091411	3.81082664	1.65560238
Se	6.02565042	5.48827646	1.57872603
C	6.04917977	2.64410180	1.45451850
Se	7.87971047	2.78172724	1.16392639
C	5.42521714	1.37698251	1.44749520
Se	6.41241965	-0.13814988	1.06569916
Ni	-7.58445884	0.27834763	-1.38343046
Se	-6.94129234	-1.93849269	-1.17272313
C	-4.45307134	-0.63420728	-1.60208011
C	-5.09878899	-1.87363721	-1.38947435
Se	-5.39017876	0.94846376	-1.37742570
C	-4.30732359	-3.05981064	-1.30024335
Se	-5.09642168	-4.67956509	-0.80542396
C	-2.92697172	-2.99206094	-1.57880589
Ni	-3.47578261	-6.22479267	-1.35355993
Se	-1.90692536	-4.53223151	-1.09635424
C	-3.07115150	-0.58905968	-1.95377872
Se	-2.24136367	1.03653439	-2.40306237
C	-2.34778672	-1.79510224	-1.99293007
Se	-0.65650558	-1.61324994	-2.88410734
Ni	0.01881867	0.44860773	-2.14426228
Se	0.57655808	2.65860287	-1.90665729
Se	2.14587957	-0.19328736	-1.72328274
C	2.45274973	2.62036678	-1.79302756
C	3.12547151	1.37699606	-1.78056943
C	3.19490980	3.81921347	-1.71326459
Se	2.28485327	5.45201978	-1.59710362
C	4.60662539	3.78543024	-1.72898152
Se	5.56383347	5.37109911	-1.65853656
C	5.29996418	2.53185371	-1.79532558
Se	7.14238162	2.47215136	-1.91832431
C	4.55368188	1.33050496	-1.77988428
Se	5.43164599	-0.30318433	-1.82867728
C	-0.48154939	-4.45009634	-2.43590156
H	0.13470225	-5.33679216	-2.21974882
H	-0.90690403	-4.55642730	-3.44307526
C	0.32008674	-3.18070780	-2.23493226
H	1.23226341	-3.19324582	-2.85179497
H	0.60134054	-3.02356574	-1.18261914
C	-1.18876316	2.39763556	2.06617796
H	-2.03735008	2.95031742	1.63976039
H	-1.39560128	2.17076253	3.12237502
C	0.10676007	3.15975924	1.85631481
H	0.09108263	4.12136070	2.38742162
H	0.32950383	3.32859329	0.79104042
Tv	15.19433082	0.00000000	0.00000000
Tv	7.43748154	13.19478073	0.00000000

3dy_3dy$_{Se\_A}$

E = -67741.0553720 Hartree

Ni	-6.90475036	0.55856674	1.59065194
Se	-6.36705669	-1.68339173	1.55093475
C	-3.76786178	-0.51901105	1.82301247
C	-4.50056364	-1.71636824	1.76433678
Se	-4.70656469	1.00099612	1.15942807
C	-3.79342841	-2.94092094	1.90027191
Se	-4.70696466	-4.54622358	1.65738408
C	-2.40152437	-2.97537433	2.15150510
Ni	-3.07034436	-6.12879172	1.79047406
Se	-1.51168882	-4.58923472	2.50212170
C	-2.39243218	-0.54947490	2.06570398
Se	-1.35351409	0.97622753	2.56247331
C	-1.68134137	-1.75424949	2.17691447
Se	0.21569080	-1.75493214	2.26160725
Ni	0.74283865	0.46176997	1.82567559
Se	1.27271915	2.63618923	1.39393425
Se	2.93843439	-0.16908996	1.65322021
C	3.11906685	2.67257656	1.54399826
C	3.84408681	1.45230341	1.60414709
C	3.81107621	3.91755353	1.56837643
Se	2.86695750	5.50486189	1.49726131
C	5.23151110	3.94403363	1.65118627
Se	6.13093566	5.56785847	1.78320136
C	5.95491952	2.72299100	1.63751341
Se	7.82480879	2.75339756	1.65983096
C	5.26837669	1.48852935	1.61224179
Se	6.23412293	-0.10285082	1.59162373
Ni	-6.91403247	0.39484983	-1.93726687
Se	-6.35413560	-1.79594339	-1.67505125
C	-3.81282884	-0.58365679	-2.04967401
C	-4.49126134	-1.79492095	-1.77338315
Se	-4.75851570	0.99633166	-2.37343729
C	-3.74933026	-2.99009627	-1.54422756
Se	-4.61870343	-4.60185508	-1.13388621
C	-2.34277871	-2.96875482	-1.65256328
Ni	-2.93321310	-6.21032366	-1.36175217
Se	-1.44011353	-4.50489789	-0.95588385
C	-2.39313064	-0.56942262	-2.09592624
Se	-1.45316720	1.06033258	-2.23712196
C	-1.68930117	-1.78465095	-1.98565268
Se	0.12039742	-1.66307934	-2.60066196
Ni	0.76139151	0.42101893	-1.93750625
Se	1.31148585	2.62551148	-1.70687654
Se	2.94464497	-0.21093712	-1.68438096
C	3.16821016	2.62949774	-1.74649380
C	3.87338777	1.39761235	-1.74378063
C	3.88721351	3.85909934	-1.73154166
Se	2.97173753	5.47653107	-1.72075482
C	5.30522372	3.85919746	-1.74510248
Se	6.23191187	5.48231560	-1.73662753
C	6.00992376	2.62528392	-1.78535025
Se	7.87414697	2.60582182	-1.86457396

C	5.29581600	1.40137452	-1.75987414
Se	6.22132910	-0.21085814	-1.72445405
C	0.22491834	-4.45901090	-1.97982350
H	0.78848629	-5.32591560	-1.60008990
H	0.02461853	-4.61264119	-3.04944818
C	0.96064719	-3.16891520	-1.67523416
H	1.98361955	-3.19433760	-2.08286034
H	1.00924028	-2.95095067	-0.59698531
C	-3.77043256	2.45036559	2.07649970
H	-4.26530468	3.36394481	1.71116228
H	-3.92465250	2.37845274	3.16220649
C	-2.30976419	2.43496852	1.66876657
H	-1.79363108	3.34188030	2.02147150
H	-2.17408593	2.34621287	0.57988703
Tv	15.31473112	0.00000000	0.00000000
Tv	7.52952831	13.24624245	0.00000000

3dy_3dy$_{Se_B}$

E = -67741.0678868 Hartree

Ni	-6.88121938	0.27792540	1.28082809
Se	-6.33741528	-1.89437925	1.81379049
C	-3.76294876	-0.72378442	1.49355775
C	-4.49598753	-1.93272859	1.68031095
Se	-4.65202046	0.89395424	1.37812808
C	-3.79752112	-3.17157395	1.82498262
Se	-4.73297801	-4.76922317	1.98828838
C	-2.38526346	-3.19047064	1.85408718
Ni	-3.09219639	-6.35555703	1.90086576
Se	-1.46587456	-4.78317374	2.22039896
C	-2.33356628	-0.77451586	1.44338504
Se	-1.33623279	0.75978503	1.11103653
C	-1.65809672	-1.99993447	1.63550332
Se	0.21779823	-2.06977273	1.58742001
Ni	0.82718876	0.14204211	1.46371901
Se	1.39361994	2.15536396	2.47150564
Se	3.03503974	-0.46791554	2.02333964
C	3.21717556	2.38593787	1.93505274
C	3.93374180	1.17368295	1.88956462
C	3.86710980	3.60442240	1.76970869
Se	2.96473549	5.23006385	1.34317791
C	5.27004106	3.67669560	1.64096034
Se	6.11827799	5.34563562	1.49322027
C	6.01365715	2.46410664	1.60237205
Se	7.84528281	2.50924152	1.26725915
C	5.34236075	1.22593108	1.71139907
Se	6.27160514	-0.36780298	1.49956169
Ni	-7.76569799	0.12356740	-1.27136976
Se	-7.15160065	-2.11084355	-1.25774333
C	-4.64768186	-0.82897484	-1.70874758
C	-5.32070746	-2.06643403	-1.59205673
Se	-5.57893092	0.76533151	-1.51491700
C	-4.57597559	-3.27862133	-1.62311163
Se	-5.42531463	-4.94537791	-1.46722178
C	-3.17283016	-3.20672088	-1.75283908
Ni	-3.74176481	-6.47882423	-1.88213645
Se	-2.26908144	-4.83231838	-1.32573731
C	-3.23898053	-0.77686943	-1.88163917
Se	-2.34093051	0.86545364	-2.01641216
C	-2.52228404	-1.98997263	-1.92228374
Se	-0.69850240	-1.75824628	-2.45689619
Ni	-0.13224796	0.25685287	-1.46037743
Se	0.47559094	2.46959492	-1.58410598
Se	2.03412885	-0.35806384	-1.10496129
C	2.35100044	2.40127983	-1.63552112
C	3.02815851	1.17519728	-1.44854435
C	3.07818662	3.59288171	-1.85017029
Se	2.15797350	5.18632496	-2.21325593
C	4.49071061	3.57521894	-1.81520294
Se	5.42586829	5.17330789	-1.97340378
C	5.18939472	2.33643352	-1.67225209
Se	7.03294407	2.30383406	-1.78075115
C	4.45675445	1.12515406	-1.50275389
Se	5.34541725	-0.49446737	-1.41594822
C	-0.64825518	-4.63366759	-2.40075609
H	-0.08750384	-5.56578750	-2.22899401
H	-0.91535805	-4.57950417	-3.46565851
C	0.14192063	-3.43965704	-1.90868693
H	1.12962219	-3.39338803	-2.39483002
H	0.28861508	-3.44318231	-0.81611561
C	0.55197586	3.83720187	1.92432162
H	0.40146161	3.83920729	0.83251145
H	-0.43366393	3.79018026	2.41413201
C	1.34015020	5.03474293	2.41220959
H	1.59915739	4.99277401	3.47932984
H	0.77877503	5.96358486	2.22440607
Tv	15.33998574	0.00000000	0.00000000
Tv	7.52560234	13.23518899	0.00000000

1$_{Se_3D}$ (Eclipsed)

E = -33792.1159526 Hartree

Ni	-7.26722300	0.24708600	-0.00152900
Se	-6.70893500	-1.98045400	-0.04003400
C	-4.12737700	-0.75524800	0.02088700
C	-4.83346700	-1.97673800	-0.00755600
Se	-5.05879000	0.87243800	0.04640900
C	-4.12486300	-3.20259600	-0.01424100
Se	-5.06703300	-4.82387300	-0.06086100
C	-2.71358100	-3.20267900	0.00408100
Ni	-3.41946400	-6.42331100	0.00221500
Se	-1.77056000	-4.82391800	-0.01141300
C	-2.71166200	-0.75519400	0.03481300
Se	-1.78090900	0.87232300	0.07995100
C	-2.00509200	-1.97682000	0.02480000
Se	-0.12966100	-1.98122400	0.04526100
Ni	0.42747300	0.24704500	-0.00051100
Se	0.98459600	2.47532600	-0.04551100
Se	2.63586000	-0.37819200	-0.08185100
C	2.86003700	2.47090500	-0.02462400
C	3.56661600	1.24929800	-0.03613000
C	3.56849200	3.69674800	-0.00229200
Se	2.62543600	5.31796100	0.01513400
C	4.97977900	3.69667400	0.01571700

Se	5.92191700	5.31791100	0.06406100
C	5.68840800	2.47084900	0.00685800
Se	7.56390400	2.47459700	0.03829300
C	4.98234300	1.24937500	-0.02269200
Se	5.91375500	-0.37828900	-0.04923600
Tv	15.38942600	0.00000000	0.00000000
Tv	7.69377200	13.34068200	0.00000000
Tv	-0.06744800	-0.11590200	3.22603900

1$_{\text{Se\_3D}}$ **(Int#1)**

E = -33792.03515 Hartree

Ni	-7.26722300	0.24708600	-0.00152900
Se	-6.70893500	-1.98045400	-0.04003400
C	-4.12737700	-0.75524800	0.02088700
C	-4.83346700	-1.97673800	-0.00755600
Se	-5.05879000	0.87243800	0.04640900
C	-4.12486300	-3.20259600	-0.01424100
Se	-5.06703300	-4.82387300	-0.06086100
C	-2.71358100	-3.20267900	0.00408100
Ni	-3.41946400	-6.42331100	0.00221500
Se	-1.77056000	-4.82391800	-0.01141300
C	-2.71166200	-0.75519400	0.03481300
Se	-1.78090900	0.87232300	0.07995100
C	-2.00509200	-1.97682000	0.02480000
Se	-0.12966100	-1.98122400	0.04526100
Ni	0.42747300	0.24704500	-0.00051100
Se	0.98459600	2.47532600	-0.04551100
Se	2.63586000	-0.37819200	-0.08185100
C	2.86003700	2.47090500	-0.02462400
C	3.56661600	1.24929800	-0.03613000
C	3.56849200	3.69674800	-0.00229200
Se	2.62543600	5.31796100	0.01513400
C	4.97977900	3.69667400	0.01571700
Se	5.92191700	5.31791100	0.06406100
C	5.68840800	2.47084900	0.00685800
Se	7.56390400	2.47459700	0.03829300
C	4.98234300	1.24937500	-0.02269200
Se	5.91375500	-0.37828900	-0.04923600
Tv	15.30250569	0.00000000	0.00000000
Tv	7.79499030	13.16471335	0.00000000
Tv	1.66900000	0.964000000	3.20000000

1$_{\text{Se\_3D}}$ **(Int#2)**

E = -33792.03054 Hartree

Ni	-7.26722300	0.24708600	-0.00152900
Se	-6.70893500	-1.98045400	-0.04003400
C	-4.12737700	-0.75524800	0.02088700
C	-4.83346700	-1.97673800	-0.00755600
Se	-5.05879000	0.87243800	0.04640900
C	-4.12486300	-3.20259600	-0.01424100
Se	-5.06703300	-4.82387300	-0.06086100
C	-2.71358100	-3.20267900	0.00408100
Ni	-3.41946400	-6.42331100	0.00221500
Se	-1.77056000	-4.82391800	-0.01141300
C	-2.71166200	-0.75519400	0.03481300
Se	-1.78090900	0.87232300	0.07995100
C	-2.00509200	-1.97682000	0.02480000
Se	-0.12966100	-1.98122400	0.04526100
Ni	0.42747300	0.24704500	-0.00051100
Se	0.98459600	2.47532600	-0.04551100
Se	2.63586000	-0.37819200	-0.08185100
C	2.86003700	2.47090500	-0.02462400
C	3.56661600	1.24929800	-0.03613000
C	3.56849200	3.69674800	-0.00229200
Se	2.62543600	5.31796100	0.01513400
C	4.97977900	3.69667400	0.01571700
Se	5.92191700	5.31791100	0.06406100
C	5.68840800	2.47084900	0.00685800
Se	7.56390400	2.47459700	0.03829300
C	4.98234300	1.24937500	-0.02269200
Se	5.91375500	-0.37828900	-0.04923600
Tv	15.26906795	0.00000000	0.00000000
Tv	7.54791250	13.27347445	0.00000000
Tv	3.84900000	2.22220000	3.20000000

1$_{\text{Se\_3D}}$ **(Int#3)**

E = -33792.05685 Hartree

Ni	-7.26722300	0.24708600	-0.00152900
Se	-6.70893500	-1.98045400	-0.04003400
C	-4.12737700	-0.75524800	0.02088700
C	-4.83346700	-1.97673800	-0.00755600
Se	-5.05879000	0.87243800	0.04640900
C	-4.12486300	-3.20259600	-0.01424100
Se	-5.06703300	-4.82387300	-0.06086100
C	-2.71358100	-3.20267900	0.00408100
Ni	-3.41946400	-6.42331100	0.00221500
Se	-1.77056000	-4.82391800	-0.01141300
C	-2.71166200	-0.75519400	0.03481300
Se	-1.78090900	0.87232300	0.07995100
C	-2.00509200	-1.97682000	0.02480000
Se	-0.12966100	-1.98122400	0.04526100
Ni	0.42747300	0.24704500	-0.00051100
Se	0.98459600	2.47532600	-0.04551100
Se	2.63586000	-0.37819200	-0.08185100
C	2.86003700	2.47090500	-0.02462400
C	3.56661600	1.24929800	-0.03613000
C	3.56849200	3.69674800	-0.00229200
Se	2.62543600	5.31796100	0.01513400
C	4.97977900	3.69667400	0.01571700
Se	5.92191700	5.31791100	0.06406100
C	5.68840800	2.47084900	0.00685800
Se	7.56390400	2.47459700	0.03829300
C	4.98234300	1.24937500	-0.02269200
Se	5.91375500	-0.37828900	-0.04923600
Tv	15.36537159	0.00000000	0.00000000
Tv	7.71049699	13.25424724	0.00000000
Tv	6.31680000	3.64700000	3.20000000

1$_{Se_3D}$ (max_displaced)

E = -33792.06107 Hartree

Ni	-7.27773050	0.19449091	0.00010623
Se	-6.69156033	-2.01081544	0.26514625
C	-4.14554232	-0.73710170	0.26881000
C	-4.83998270	-1.97506459	0.32662568
Se	-5.09452913	0.84035712	0.11682680
C	-4.10504259	-3.20339536	0.32288260
Se	-5.01646526	-4.81102497	0.27410757
C	-2.68450497	-3.18257543	0.27371138
Ni	-3.36758754	-6.38710009	0.02037422
Se	-1.74265042	-4.77293894	0.14048993
C	-2.71310861	-0.71361717	0.25095335
Se	-1.80739217	0.89773892	0.16165623
C	-1.97852840	-1.93599768	0.26573480
Se	-0.13142609	-1.91751884	0.26770405
Ni	0.40584411	0.29404584	-0.01528428
Se	0.99825212	2.50803820	-0.20483834
Se	2.58831989	-0.36044231	-0.28257163
C	2.84674989	2.46730371	-0.29145181
C	3.54077373	1.22135270	-0.30414412
C	3.59193803	3.69176138	-0.30053699
Se	2.69349010	5.30066076	-0.17752528
C	5.01118411	3.66942907	-0.33338668
Se	5.96514692	5.25153375	-0.20275829
C	5.70900518	2.42139298	-0.34156099
Se	7.55859379	2.40298006	-0.30190542
C	4.97248073	1.20581343	-0.30526657
Se	5.87902993	-0.39987156	-0.13353199
Tv	15.36537159	0.00000000	0.00000000
Tv	7.71049699	13.25424724	0.00000000
Tv	7.45740839	4.34077203	2.71873496

3dy$_{Se_3D}$

E = -33870.53304 Hartree

Ni	-7.35548957	1.00211695	-0.01340252
Se	-6.78377345	-1.20654626	0.16541970
C	-4.23144617	0.02804533	-0.12641190
C	-4.92862963	-1.19479874	0.06914392
Se	-5.16702612	1.62842017	-0.24754841
C	-4.20671734	-2.41467785	0.20923320
Se	-5.09224138	-4.04697954	0.46746423
C	-2.79904336	-2.37631308	0.13292647
Ni	-3.38482631	-5.62659055	0.25342648
Se	-1.96169917	-3.94236238	0.83660373
C	-2.81286085	0.02944355	-0.25609190
Se	-1.86178409	1.62182409	-0.53170405
C	-2.12663399	-1.19798928	-0.15369682
Se	-0.33659181	-1.12652746	-0.81651770
Ni	0.36545787	0.97335911	-0.26957685
Se	0.89649575	3.17734451	-0.03963404
Se	2.53376391	0.34586362	0.08095025
C	2.75529784	3.17662254	-0.01741196
C	3.47101727	1.95711268	0.01450480
C	3.45817729	4.41573244	0.00236123
Se	2.50190199	6.01056504	-0.01897194
C	4.87272271	4.42871509	-0.00739120
Se	5.77392992	6.06145867	-0.05575955
C	5.59490781	3.20352903	-0.01646460
Se	7.44936097	3.21460126	-0.09708186
C	4.89307544	1.96722826	0.02832260
Se	5.83311846	0.36976695	0.12721052
C	-0.18816863	-3.93831101	-0.00642051
C	0.55051869	-2.62162855	0.09508452
H	0.35729748	-4.72848970	0.53606569
H	-0.30561586	-4.27509258	-1.03981499
H	1.52743942	-2.68960272	-0.41221370
H	0.74073582	-2.31912471	1.12851256
Tv	15.38052418	0.00000000	0.00000000
Tv	7.49691996	13.22524893	0.00000000
Tv	0.22951593	0.56599239	3.57574439

2y$_{Se_3D}$

E = -33870.52184 Hartree

Ni	-7.63141526	0.56714799	-0.24198939
Se	-7.01905856	-1.64084145	-0.14195608
C	-4.49178491	-0.33732810	-0.14687973
C	-5.15005948	-1.58528499	-0.09025169
Se	-5.45871469	1.23346953	-0.32679941
C	-4.38540337	-2.77806819	0.04626311
Se	-5.24417094	-4.41572888	0.17658622
C	-2.96627745	-2.71459793	0.16555203
Ni	-3.54685270	-5.94699031	0.22824991
Se	-1.96411058	-4.28117180	0.33200474
C	-3.07148982	-0.26493937	-0.03393278
Se	-2.26996026	1.43785463	-0.10457110
C	-2.34468345	-1.45365141	0.14019784
Se	-0.56172694	-1.11509998	0.78464390
Ni	-0.06626873	0.90172821	-0.06076647
Se	0.54935974	3.08215209	-0.12305070
Se	1.96879879	0.28756039	-0.78030927
C	2.42615821	2.93916374	-0.07419476
C	3.11044546	1.71721202	-0.17684334
C	3.18242981	4.14230871	0.05257840
Se	2.28138367	5.75916525	0.13440251
C	4.59403997	4.10349670	0.06246141
Se	5.55599425	5.70463767	0.13920340
C	5.26150550	2.85061625	-0.04770892
Se	7.11114979	2.79449043	-0.14432101
C	4.51371987	1.64206912	-0.16184377
Se	5.39258811	-0.00343839	-0.25753442
C	0.90032596	-2.24700328	0.03596130
C	2.20586485	-1.47300729	0.12965753
H	0.93368325	-3.16393029	0.64300406
H	0.64074355	-2.53961751	-0.98475860
H	3.01768400	-1.99623936	-0.39705229
H	2.53866301	-1.30027850	1.15660040
Tv	15.24722866	0.00000000	0.00000000
Tv	7.47720943	13.26881519	0.00000000
Tv	0.27918060	0.36979215	3.59645495