Supplementary Materials for

New pecJ-*n* (*n* = 1, 2) basis sets for selenium atom purposed for the calculations of NMR spin-spin coupling constants involving selenium

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Table S1. Equilibrium geometries of two fitting molecules SeH_2 and Se=C and that of testing compounds **1**-**7** (the level of optimization is M06-2X/pc-3).

Molecule	Cartesian Coordinates, Å			
SeH2	Se	0.000000	0.000000	0.056114
	H	0.000000	1.037025	-0.953934
	H	0.000000	-1.037025	-0.953934
Se=C	Se	0.000000	0.000000	0.000000
	C	0.000000	0.000000	1.662334
Me_2Se_2 (**1**)	Se	1.100384	-0.314408	-0.365502
	Se	-1.100384	-0.314408	0.365502
	C	1.833865	1.105028	0.761441
	C	-1.833865	1.105028	-0.761441
	H	-2.886182	1.187824	-0.501994
	H	-1.327234	2.040257	-0.551343
	H	-1.726611	0.831620	-1.804492
	H	2.886182	1.187825	0.501994
	H	1.327233	2.040257	0.551343
	H	1.726612	0.831620	1.804492
MeSe-C≡N (**2**)	Se	0.000000	0.627734	0.000000
	C	-1.768006	-0.210961	0.000000
	C	0.960919	-0.946889	0.000000
	N	1.582618	-1.914747	0.000000
	H	-2.468657	0.618486	0.000000
	H	-1.883574	-0.805551	-0.897914
	H	-1.883574	-0.805551	0.897914
MeSeH (**3**)	Se	-0.031519	-0.420629	0.000000
	C	-0.031519	1.535877	0.000000
	H	-1.075925	1.832110	0.000000
	H	0.454225	1.910104	0.893578

	H	0.454225	1.910104	-0.893578
	H	1.428243	-0.566192	0.000000
$Me_2P(Se)Cl$ (**4**)	Se	0.604223	-1.487019	0.000000
	C	0.604223	1.472323	-1.445083
	C	0.604223	1.472323	1.445083
	P	0.074674	0.528807	0.000000
	Cl	-1.953068	0.887047	0.000000
	H	0.205180	0.992997	-2.335231
	H	0.246799	2.497551	-1.375522
	H	1.691921	1.448872	-1.479959
	H	0.205180	0.992997	2.335231
	H	1.691921	1.448872	1.479959
	H	0.246799	2.497551	1.375522
C_4H_4Se (**5**)	Se	0.000000	0.000000	0.907629
	C	0.000000	1.282615	-0.439200
	C	0.000000	0.714941	-1.669269
	C	0.000000	-0.714941	-1.669269
	C	0.000000	-1.282615	-0.439200
	H	0.000000	2.332883	-0.200899
	H	0.000000	1.299798	-2.577980
	H	0.000000	-1.299798	-2.577980
	H	0.000000	-2.332883	-0.200899
$SePMe_3$ (**6**)	Se	0.000000	0.000000	1.446013
	C	0.000000	1.657972	-1.402209
	C	-1.435846	-0.828986	-1.402209
	C	1.435846	-0.828986	-1.402209
	P	0.000000	0.000000	-0.670630
	H	0.885133	2.191102	-1.063283
	H	0.000000	1.592014	-2.489722
	H	-0.885133	2.191102	-1.063283
	H	-1.454984	-1.862098	-1.063283
	H	-2.340116	-0.329004	-1.063283
	H	-1.378725	-0.796007	-2.489722
	H	1.454984	-1.862098	-1.063283
	H	1.378725	-0.796007	-2.489722
	H	2.340116	-0.329004	-1.063283
SiH_3SeH (**7**)	Se	0.026466	-0.774339	0.000000
	Si	0.026466	1.516254	0.000000
	H	1.450595	1.886490	0.000000
	H	-0.641066	2.037802	-1.204002
	H	-0.641066	2.037802	1.204002
	H	-1.438853	-0.862133	0.000000

Table S2. Basis set pecJ-1 for selenium, CFOUR format.

```
SE:pecJ-1
Property-energy consistent basis set

 4
  0   1   2   3
 11   7   5   3
 16  11   7   3

2.738937E+07  4.117126E+06  5.008352E+05  8.450803E+04  1.940949E+04
5.478217E+03  1.785352E+03  6.442465E+02  2.515808E+02  1.039878E+02
3.331319E+01  1.424322E+01  4.067050E+00  1.754643E+00  3.363182E-01
1.350861E-01

 1.3584E-06  4.2916E-07  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 1.7390E-05  5.4121E-06  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 2.1705E-04  6.8544E-05  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 1.6462E-03  5.1614E-04  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 8.6238E-03  2.7472E-03  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 3.5307E-02  1.1276E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 1.1465E-01  3.9306E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
```

```
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000
 0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 1.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  1.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  1.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  1.00000000

4.106684E+03  9.693471E+02  3.105258E+02  1.166637E+02  4.812571E+01
2.088559E+01  8.846983E+00  3.839338E+00  1.605191E+00  4.680879E-01
1.490880E-01

 1.4225E-03  5.7021E-04  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 1.2057E-02  4.8491E-03  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 6.1443E-02  2.4975E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 2.0152E-01  8.4407E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 4.0415E-01  1.8090E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 3.8893E-01  1.7468E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000

1.200481E+02  3.552605E+01  1.289256E+01  4.991605E+00  1.889243E+00
6.476664E-01  1.788622E-01

 1.4755E-02  0.00000000  0.00000000  0.00000000  0.00000000
 9.1608E-02  0.00000000  0.00000000  0.00000000  0.00000000
 2.7516E-01  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  1.00000000

7.528700E+00  1.282966E+00  3.328661E-01

 1.00000000  0.00000000  0.00000000
 0.00000000  1.00000000  0.00000000
 0.00000000  0.00000000  1.00000000
```

Table S3. Basis set pecJ-2 for selenium, CFOUR format.

```
SE:pecJ-2
Property-energy consistent basis set

 4
  0   1   2   3   4
 15   8   5   4   1
 22  13   8   4   1

 4.443822E+08  7.050053E+07  1.041355E+07  1.376983E+06  3.335063E+05
 9.200230E+04  2.967395E+04  1.070423E+04  4.148222E+03  1.725619E+03
```

7.670764E+02 3.540569E+02 1.675661E+02 8.094489E+01 3.573295E+01
1.748383E+01 8.669421E+00 3.664945E+00 1.624862E+00 5.344704E-01
2.507232E-01 9.266461E-02

5.6619E-08 1.7694E-08 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
3.3187E-07 1.0380E-07 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
5.7928E-06 1.8293E-06 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
5.0582E-05 1.5827E-05 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
2.4779E-04 7.8103E-05 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
1.1207E-03 3.4962E-04 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
4.0164E-03 1.2647E-03 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
1.3005E-02 4.1095E-03 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
3.7719E-02 1.2275E-02 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
1.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
0.00000000

```
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 1.00000000

1.020290E+04  2.385085E+03  7.246974E+02  2.599333E+02  1.042775E+02
4.521224E+01  2.064791E+01  9.300946E+00  4.203860E+00  1.835088E+00
6.372571E-01  2.508116E-01  8.507613E-02

 2.8852E-04  1.1040E-04  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000
 2.7773E-03  1.0953E-03  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000
 1.7261E-02  6.8573E-03  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000
 7.4340E-02  3.0010E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000
 2.1704E-01  9.1417E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000
 3.9428E-01  1.7705E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000
 3.6400E-01  1.6148E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000
 0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000
 0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
 0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
 0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
 0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000
 0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
 1.00000000

2.753441E+02  7.795287E+01  2.796792E+01  1.122825E+01  4.658535E+00
1.894959E+00  7.145110E-01  2.286113E-01

 2.8912E-03  0.00000000  0.00000000  0.00000000  0.00000000
 2.5978E-02  0.00000000  0.00000000  0.00000000  0.00000000
 1.1369E-01  0.00000000  0.00000000  0.00000000  0.00000000
 2.8390E-01  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  1.00000000

9.489329E+00  2.271550E+00  5.063583E-01  1.137481E-01

 1.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  1.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  1.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  1.00000000

2.237599E-01

 1.00000000
```

Table S4. Basis set pecJ-1 for selenium, Dalton format.

```
$ Se
a 34
$ s functions
  16   11    0
```

```
   2.738937E+07  1.3584E-06  4.2916E-07  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   4.117126E+06  1.7390E-05  5.4121E-06  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   5.008352E+05  2.1705E-04  6.8544E-05  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   8.450803E+04  1.6462E-03  5.1614E-04  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   1.940949E+04  8.6238E-03  2.7472E-03  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   5.478217E+03  3.5307E-02  1.1276E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   1.785352E+03  1.1465E-01  3.9306E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   6.442465E+02  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   2.515808E+02  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   1.039878E+02  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   3.331319E+01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   1.424322E+01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
0.00000000
   4.067050E+00  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
0.00000000
   1.754643E+00  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
0.00000000
   3.363182E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000
0.00000000
   1.350861E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
1.00000000
$ p functions
   11    7    0
   4.106684E+03  1.4225E-03  5.7021E-04  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   9.693471E+02  1.2057E-02  4.8491E-03  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   3.105258E+02  6.1443E-02  2.4975E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   1.166637E+02  2.0152E-01  8.4407E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   4.812571E+01  4.0415E-01  1.8090E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   2.088559E+01  3.8893E-01  1.7468E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   8.846983E+00  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   3.839338E+00  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
   1.605191E+00  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
   4.680879E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
   1.490880E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000
$ d functions
   7    5    0
   1.200481E+02  1.4755E-02  0.00000000  0.00000000  0.00000000  0.00000000
   3.552605E+01  9.1608E-02  0.00000000  0.00000000  0.00000000  0.00000000
   1.289256E+01  2.7516E-01  0.00000000  0.00000000  0.00000000  0.00000000
   4.991605E+00  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
   1.889243E+00  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
   6.476664E-01  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
   1.788622E-01  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000
$ f functions
   3    3    0
   7.528700E+00  1.00000000  0.00000000  0.00000000
   1.282966E+00  0.00000000  1.00000000  0.00000000
   3.328661E-01  0.00000000  0.00000000  1.00000000
```

Table S5. Basis set pecJ-2 for selenium, Dalton format.

```
$ Se
a 34
$ s functions
   22   15    0
   4.443822E+08  5.6619E-08  1.7694E-08  0.00000000  0.00000000  0.00000000  0.00000000
   0.00000000     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   0.00000000     0.00000000
   7.050053E+07  3.3187E-07  1.0380E-07  0.00000000  0.00000000  0.00000000  0.00000000
   0.00000000     0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   0.00000000     0.00000000
```

```
  1.041355E+07  5.7928E-06  1.8293E-06  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  1.376983E+06  5.0582E-05  1.5827E-05  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  3.335063E+05  2.4779E-04  7.8103E-05  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  9.200230E+04  1.1207E-03  3.4962E-04  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  2.967395E+04  4.0164E-03  1.2647E-03  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  1.070423E+04  1.3005E-02  4.1095E-03  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  4.148222E+03  3.7719E-02  1.2275E-02  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  1.725619E+03  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  7.670764E+02  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  3.540569E+02  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  1.675661E+02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  8.094489E+01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  1.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  3.573295E+01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    1.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  1.748383E+01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  8.669421E+00  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  3.664945E+00  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  1.624862E+00  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
  0.00000000    0.00000000
  5.344704E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000
  0.00000000    0.00000000
  2.507232E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  1.00000000    0.00000000
  9.266461E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    1.00000000
$ p functions
  13    8    0
  1.020290E+04  2.8852E-04  1.1040E-04  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  2.385085E+03  2.7773E-03  1.0953E-03  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  7.246974E+02  1.7261E-02  6.8573E-03  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
  2.599333E+02  7.4340E-02  3.0010E-02  0.00000000  0.00000000  0.00000000  0.00000000
  0.00000000    0.00000000
```

```
   1.042775E+02  2.1704E-01  9.1417E-02  0.00000000  0.00000000  0.00000000  0.00000000
   0.00000000     0.00000000
   4.521224E+01  3.9428E-01  1.7705E-01  0.00000000  0.00000000  0.00000000  0.00000000
   0.00000000     0.00000000
   2.064791E+01  3.6400E-01  1.6148E-01  0.00000000  0.00000000  0.00000000  0.00000000
   0.00000000     0.00000000
   9.300946E+00  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
   0.00000000     0.00000000
   4.203860E+00  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
   0.00000000     0.00000000
   1.835088E+00  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
   0.00000000     0.00000000
   6.372571E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000
   0.00000000     0.00000000
   2.508116E-01  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   1.00000000     0.00000000
   8.507613E-02  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
   0.00000000     1.00000000
$ d functions
    8    5    0
   2.753441E+02  2.8912E-03  0.00000000  0.00000000  0.00000000  0.00000000
   7.795287E+01  2.5978E-02  0.00000000  0.00000000  0.00000000  0.00000000
   2.796792E+01  1.1369E-01  0.00000000  0.00000000  0.00000000  0.00000000
   1.122825E+01  2.8390E-01  0.00000000  0.00000000  0.00000000  0.00000000
   4.658535E+00  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
   1.894959E+00  0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
   7.145110E-01  0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
   2.286113E-01  0.00000000  0.00000000  0.00000000  0.00000000  1.00000000
$ f functions
    4    4    0
   9.489329E+00  1.00000000  0.00000000  0.00000000  0.00000000
   2.271550E+00  0.00000000  1.00000000  0.00000000  0.00000000
   5.063583E-01  0.00000000  0.00000000  1.00000000  0.00000000
   1.137481E-01  0.00000000  0.00000000  0.00000000  1.00000000
$ g functions
    1    1    0
   2.237599E-01  1.00000000
```

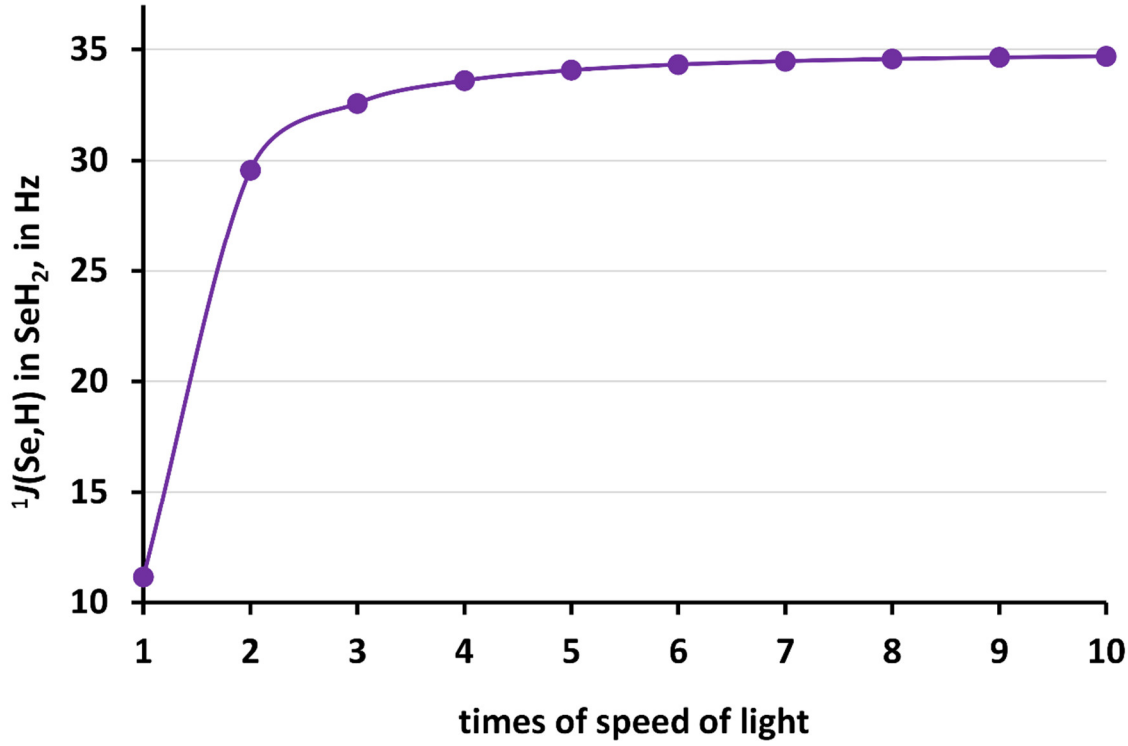

Figure S1. The convergence of ^{1}J(Se,H) in SeH_2 calculated at the 4-component DFT(SVWN5)//pecJ-2(uc) level with increasing the speed of light by 1 (totally relativistic calculation) to 10 ("10c limit scheme") times.

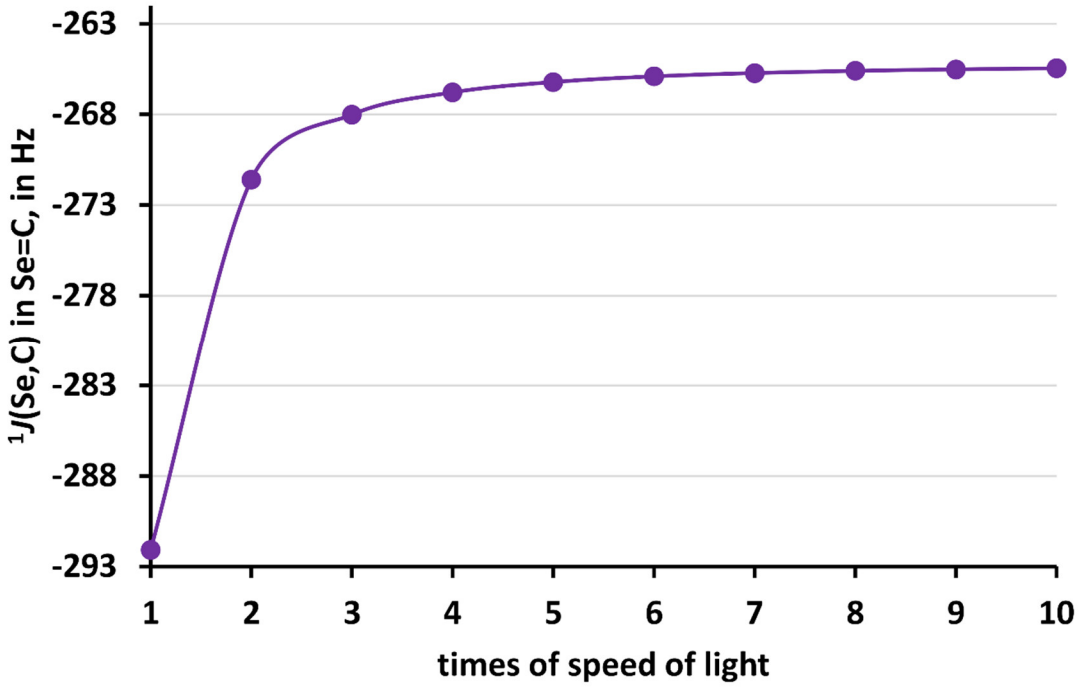

Figure S2. The convergence of ^{1}J(Se,C) in Se=C calculated at the 4-component DFT(SVWN5)//pecJ-2(uc) level with increasing the speed of light by 1 (totally relativistic calculation) to 10 ("10c limit scheme") times.