Supplementary information for: Simulating chalcogen bonding using molecular mechanics: A pseudoatom approach to model ebselen.

Thomas Fellowes, Jonathan M. White[†]

Bio21 Institute and School of Chemistry, University of Melbourne, Parkville, Australia
[*]fellowes@student.unimelb.edu.au
[†]whitejm@unimelb.edu.au

May 23, 2020

1 Fitting of classical parameters to DFT energy surfaces.

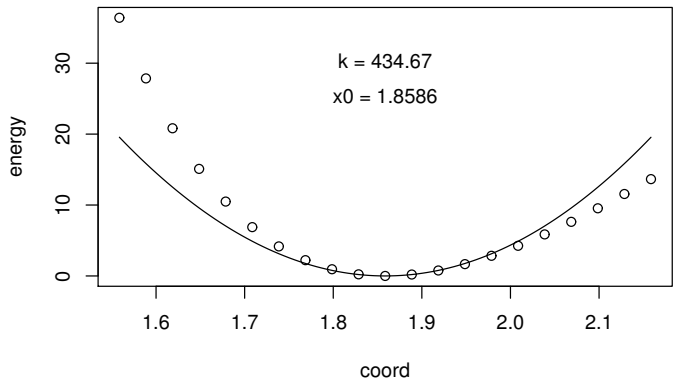

Figure 1: Harmonic potential for Se−N bond. Units are in kcal/mol and Å.

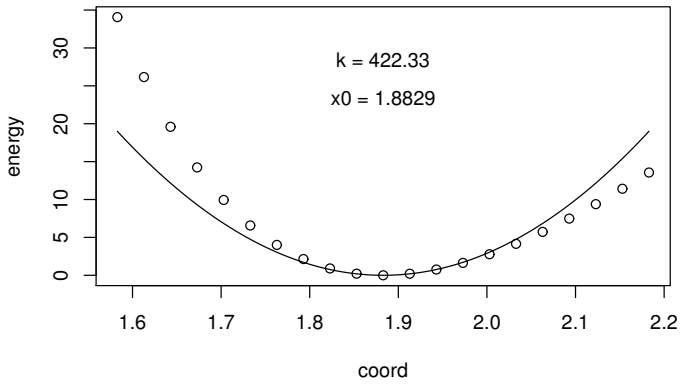

Figure 2: Harmonic potential for Se−C_{ar} bond. Units are in kcal/mol and Å.

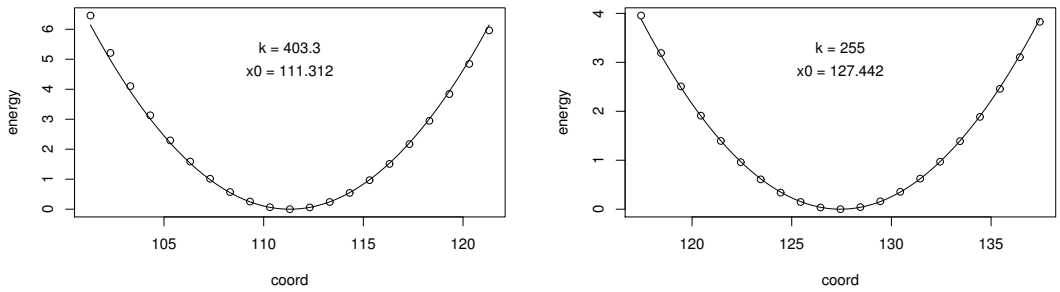

Figure 3: Harmonic potentials for Se−C_{ar}−C_{ar} bond angles. Units are in kcal and °. An average value was used for the parameter set.

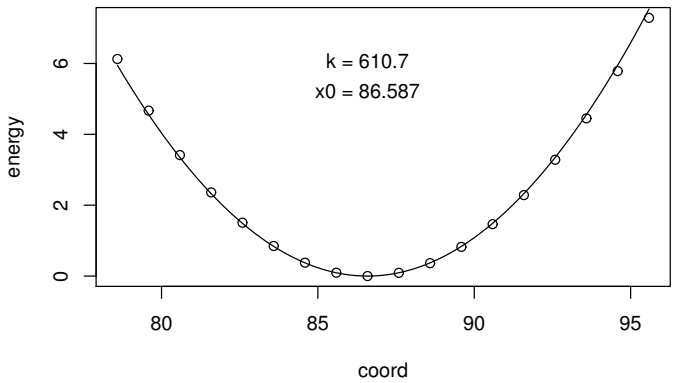

Figure 4: Harmonic potential for N−Se−C_{ar} bond angle. Units are in kcal/mol and °.

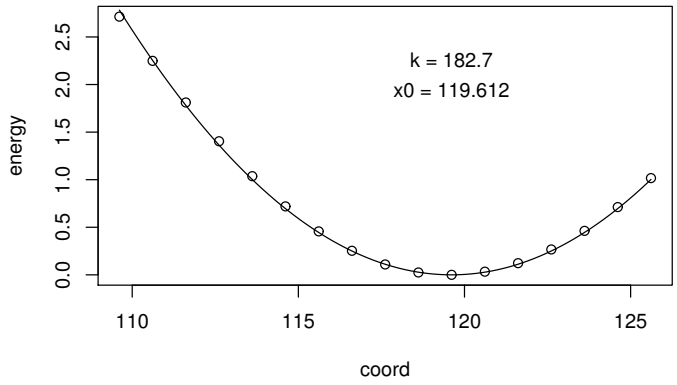

Figure 5: Harmonic potential for Se−N−C_{ar} bond angle. Units are in kcal/mol and °.

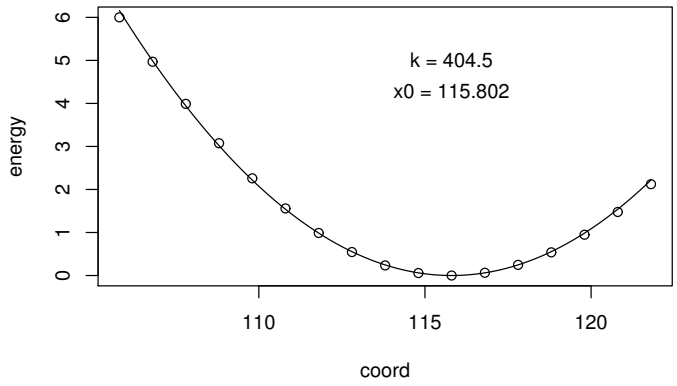

Figure 6: Harmonic potential for Se−N−C_{CO} bond angle. Units are in kcal/mol and °.

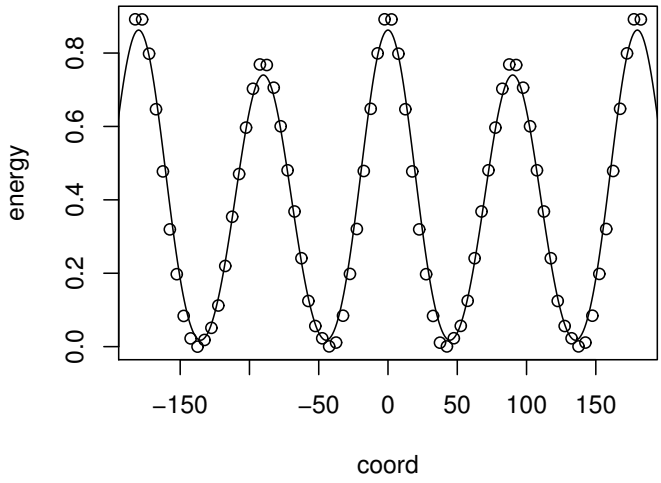

Figure 7: Torsion potential for Se−N−C−C bond angle. Units are in kcal/mol and °.

2 FRCMOD file for ebselen

Default GAFF atom types were used. The σ-hole was given the `lp` atom type, as it behaves similarly to a lone pair.

```
Parametrization for ebselen like compounds - Thomas Fellowes
MASS
se          78.96   0.000
lp          3.0     0.000

BOND
se-n        434.67  1.8586  DFT
se-ca       422.33  1.8829  DFT
se-lp       300.0   1.32    Optimised

ANGLE
se-n-c      404.5   115.8   DFT
se-n-ca     182.7   119.6   DFT
se-ca-ca    329.2   119.4   DFT
n-se-ca     610.7   86.6    DFT
lp-se-n     50.0    180.0   Geometric
lp-se-ca    50.0    93.4    Geometric

DIHE
se-n-ca-ca    2  -0.0854    180.0     -2.0    DFT
se-n-ca-ca    2   0.7655    0.0       -4.0    DFT
se-n-ca-ca    2   0.0433    0.0       -6.0    DFT
se-n-ca-ca    2   0.0495    0.0        8.0    DFT
X-se-ca-X     1  -1.2453    180.000   -1.0    Torsello
X-se-ca-X     1   0.1235    180.000   -2.0    Torsello
X-se-ca-X     1  -1.4307    180.000   -3.0    Torsello
X-se-ca-X     1   0.1619    180.000    4.0    Torsello
X-se-n-X      1  -1.2453    180.000   -1.0    Torsello
X-se-n-X      1   0.1235    180.000   -2.0    Torsello
X-se-n-X      1  -1.4307    180.000   -3.0    Torsello
X-se-n-X      1   0.1619    180.000    4.0    Torsello

NONBON
se     2.1200    0.2910
lp     0.0       0.0
```

3 SAPT(DFT) energy decomposition analysis

Atom	x	y	z
Se1	0.1103	-0.3014	-0.026
O2	-3.0289	2.1045	-0.0599
N3	-1.6949	0.2302	-0.0513
C4	0.5087	1.5474	-0.0469
C5	1.7598	2.1522	-0.0498
H6	2.6615	1.5581	-0.038
C7	-0.6467	2.3169	-0.0605
C8	-1.9311	1.5839	-0.0541
C9	1.8252	3.5343	-0.0666
H10	2.7953	4.0158	-0.0681
C11	-2.7064	-0.7562	-0.0295
C12	0.6692	4.3127	-0.082
H13	0.7454	5.392	-0.096
C14	-0.5697	3.7033	-0.0792
H15	-1.4905	4.2727	-0.0913
C16	-3.8504	-0.5892	0.7469
H17	-3.9822	0.3191	1.3145
C18	-2.5475	-1.9213	-0.7739
H19	-1.6709	-2.0451	-1.3977
C20	-3.5143	-2.9128	-0.7341
H21	-3.3765	-3.8145	-1.3174
C22	-4.8167	-1.58	0.7676
H23	-5.7049	-1.4384	1.3704
C24	-4.6546	-2.7463	0.0343
N25	2.8164	-0.9091	0.0522
C26	3.3736	-1.2146	1.2201
C27	3.4725	-1.2228	-1.0609
C28	4.6048	-1.8402	1.3265
H29	2.805	-0.946	2.1039
C30	4.7079	-1.8489	-1.0562
H31	2.9832	-0.9598	-1.9926
C32	5.2842	-2.1631	0.1635
H33	5.0165	-2.068	2.3003
H34	5.2022	-2.0836	-1.9891
H35	-5.4133	-3.5177	0.0602
H36	6.2485	-2.6533	0.2071

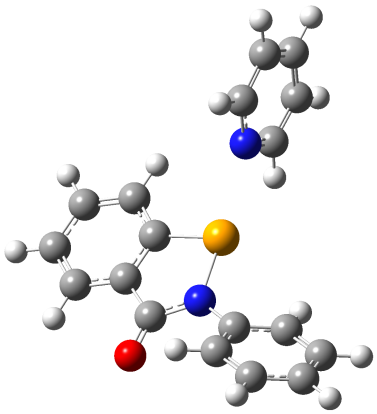

Table 1: **1**·py coordinates. Total energy = -3280.424888 a.u.

Atom	x	y	z
Se1	0.0054	-0.1461	-0.4289
O2	-3.3159	1.8035	0.4379
N3	-1.8121	0.1369	-0.0642
C4	0.1873	1.7264	-0.2918
C5	1.341	2.4794	-0.4723
H6	2.2729	1.9967	-0.7306
C7	-1.0211	2.3349	0.0175
C8	-2.189	1.4409	0.1658
C9	1.2554	3.8524	-0.3223
H10	2.1451	4.4544	-0.4611
C11	-2.685	-0.9725	0.002
C12	0.0474	4.4724	-0.0046
H13	0.0064	5.5483	0.1047
C14	-1.0945	3.7142	0.1628
H15	-2.0511	4.1612	0.4021
C16	-3.6716	-1.0489	0.9819
H17	-3.7934	-0.2361	1.6813
C18	-2.5416	-2.014	-0.91
H19	-1.7914	-1.9472	-1.6884
C20	-3.3672	-3.124	-0.8373
H21	-3.2441	-3.9266	-1.5534
C22	-4.5001	-2.1565	1.036
H23	-5.2679	-2.2044	1.798
C24	-4.3521	-3.1998	0.1339
H25	-5.0022	-4.0636	0.1862
C26	3.4197	-0.7051	0.2768
O27	2.773	-0.3286	-0.6957
N28	4.3777	-1.6549	0.1587
C29	4.671	-2.2259	-1.1397
H30	5.7129	-2.0334	-1.4096
H31	4.5127	-3.3072	-1.12
H32	4.0172	-1.7786	-1.8813
C33	5.1973	-2.1448	1.2436
H34	5.161	-3.2368	1.2689
H35	6.2405	-1.8434	1.1077
H36	4.8535	-1.775	2.2036
C37	3.1632	-0.116	1.6452
H38	2.7896	-0.8732	2.3361
H39	4.0674	0.3202	2.0716
H40	2.4094	0.6593	1.5426

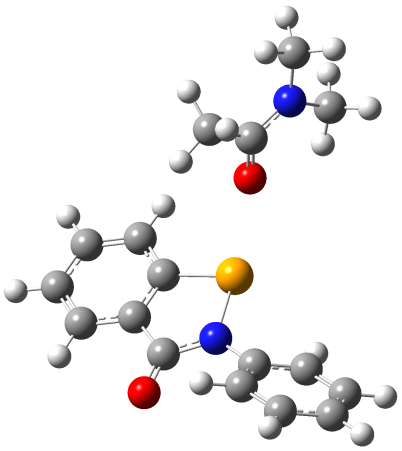

Table 2: **1**·DMAc coordinates. Total energy = -3319.951828 a.u.

Atom	x	y	z
Se1	0.3271	-0.5347	-0.0229
O2	-1.8488	2.7657	-0.0742
N3	-1.2023	0.5583	-0.063
C4	1.3072	1.0775	-0.0525
C5	2.6867	1.2317	-0.0591
H6	3.34	0.3727	-0.0495
C7	0.4723	2.1859	-0.0708
C8	-0.9819	1.9154	-0.0661
C9	3.2102	2.5121	-0.0811
H10	4.285	2.6441	-0.0858
C11	-2.4807	-0.0439	-0.0415
C12	2.3777	3.6298	-0.099
H13	2.8082	4.6223	-0.1172
C14	1.0063	3.4674	-0.0948
H15	0.328	4.3112	-0.1105
C16	-3.5014	0.4766	0.7494
H17	-3.3249	1.3696	1.3294
C18	-2.7151	-1.186	-0.8012
H19	-1.9309	-1.5783	-1.437
C20	-3.9523	-1.8083	-0.762
H21	-4.1213	-2.6966	-1.3574
C22	-4.7382	-0.1445	0.7694
H23	-5.5277	0.2705	1.3832
C24	-4.9703	-1.2893	0.0211
H25	-5.9392	-1.7709	0.0465
C26	3.4784	-2.2979	-1.0177
H27	4.1383	-3.1802	-1.0084
H28	2.8857	-2.3182	-1.9329
H29	4.1074	-1.4073	-1.0404
C30	1.7472	-3.4411	0.1639
H31	1.1614	-3.4979	-0.7548
H32	2.3328	-4.3686	0.2596
H33	1.0574	-3.3811	1.007
C34	3.3391	-2.1369	1.3768
H35	3.9965	-3.0025	1.5567
H36	3.958	-1.2393	1.3564
H37	2.6435	-2.05	2.2121
N38	2.5966	-2.2636	0.1352

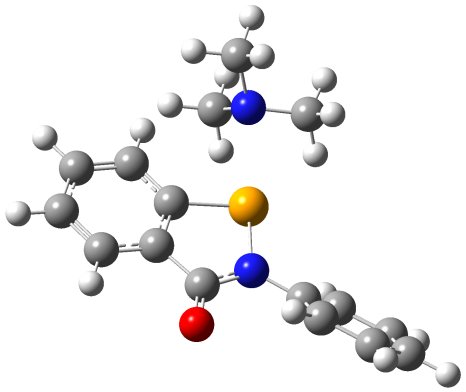

Table 3: **1**·TMA coordinates. Total energy = -3206.593859 a.u.

Atom	x	y	z
Se1	0.3065	-0.5154	-0.4
O2	-1.6865	2.7999	0.3621
N3	-1.1594	0.6101	-0.0963
C4	1.3641	1.0435	-0.2832
C5	2.7386	1.1523	-0.4498
H6	3.3403	0.2878	-0.6942
C7	0.5897	2.1611	-0.0082
C8	-0.867	1.9387	0.1184
C9	3.3194	2.4011	-0.3155
H10	4.3899	2.5017	-0.4436
C11	-2.4564	0.0507	-0.0281
C12	2.5504	3.5276	-0.0274
H13	3.027	4.494	0.0711
C14	1.1825	3.4101	0.122
H15	0.5525	4.2644	0.3353
C16	-3.3589	0.4607	0.9492
H17	-3.0781	1.2378	1.6436
C18	-2.8253	-0.9381	-0.9348
H19	-2.134	-1.2402	-1.7121
C20	-4.0801	-1.5202	-0.8584
H21	-4.355	-2.2887	-1.5696
C22	-4.6154	-0.1173	1.0065
H23	-5.3136	0.2114	1.7658
C24	-4.9816	-1.1109	0.1104
H25	-5.9647	-1.5601	0.1655
S26	2.9125	-2.4561	-0.0815
C27	3.0637	-1.9613	1.6424
H28	3.7192	-1.0921	1.6749
H29	2.0898	-1.6829	2.0461
H30	3.5034	-2.7613	2.2375
C31	1.7527	-3.8193	0.0936
H32	1.5578	-4.2111	-0.9034
H33	2.1795	-4.6108	0.709
H34	0.8151	-3.4741	0.5323

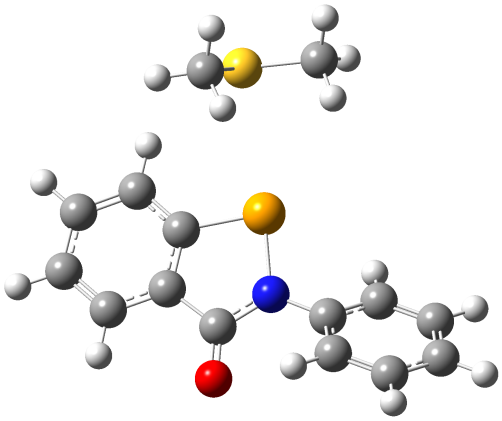

Table 4: **1**·DMS coordinates. Total energy =-3510.182468 a.u.

Complex	E_{tot}	E_{elst}	E_{ind}	E_{dis}	E_{exch}
1·DMAc	-7.551	-11.641	-4.431	-5.447	+13.967
1·TMA	-6.627	-12.067	-5.200	-6.777	+17.417
1·py	-7.093	-14.093	-5.605	-5.750	+18.358
1·DMS	-5.646	-8.703	-3.669	-5.571	+12.297

Table 5: SAPT(DFT) analysis of complexes with four Lewis bases. All energies are given in kcal/mol.