SUPPORTING INFORMATION

Benzoselenadiazole Containing Donor-Acceptor-Donor Small Molecules: Nonbonding Interactions, Packing Patterns and Optoeletronic Properties

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Table 1. Absorption, emission and electrochemical properties of **1**-**3**.

Small molecules	$\lambda_{max,abs}$ (nm)		$\lambda_{max,em}$ (nm) (quantum yield)[a]	$\lambda_{max,em}$ (nm) in film	E_{ox} (V)[b]	HOMO (eV)	LUMO (eV)	Optical HOMO-LUMO gap (eV)	Theoretical HOMO-LUMO gap [c]
	sol[n]	Film							
1	318, 405	346, 427	505 (0.74)	499	1.79 (1.53)	-5.99	-3.31	2.68	3.24
2	343, 479	345, 527	597 (0.58)	631	1.18 (1.10)	-5.56	-3.32	2.24	2.57
3	332, 500	339, 541	625 (0.40)	663	1.11 (1.00)	-5.46	-3.35	2.13	2.38

[a] Quantum yield reported in benzene with respect to quinine sulfate; [b] the values in parenthesis corresponds to onset oxidation potential of small molecules; [c] the values are taken from the most stable conformations from DFT calculation in the level B3LYP/631-G(d).

Table 2. Crystallographic data and structure refinement parameters of **1**, **2** and **3**.

Compound	**1**	**2**	**3**
Formula	$C_{18}H_{12}N_2Se$	$C_{14}H_8N_2S_2Se$	$C_{14}H_8N_2Se_3$
Crystal System	Monoclinic	Monoclinic	Orthorhombic
Space group	*P2(1)/c*	*P2(1)/c*	*Pca2(1)*
a [Å]	5.877(3)	13.914(4)	16.166(5)
b [Å]	19.574(9)	5.2933(17)	12.751(4)
c [Å]	12.586(6)	18.897(6)	6.6381(17)
β[°]	97.791	110.716(6)	90.00
V [Å^3]	1434.5(12)	1301.9(7)	1368.3(7)
Z	4	4	4
λ [Å]	0.71073	0.71073	0.71073
F[000]	672	688	832
μ [mm^{-1}]	2.611	3.189	8.049
θ [°]	1.94-25.00	1.56-25.29	1.60-24.99
Index ranges	$-3 \le h \le 6$	$-16 \le h \le 16$	$-19 \le h \le 19$
	$-22 \le k \le 23$	$-6 \le k \le 6$	$-15 \le k \le 15$
	$-14 \le l \le 14$	$-22 \le l \le 22$	$-7 \le l \le 4$
T [K]	296(2)	296(2)	296(2)

R_1	0.0555	0.0846	0.0539
wR_2	0.1343	0.2350	0.1563
R_{int}	0.0797	0.1072	0.0829
Parameters	148	154	172
GOF	0.994	1.025	1.067
reflns total	10000	17185	10462
unique reflns	2502	2364	1937
obsd reflns	1268	1313	1486
CCDC no.	961059	961060	961061

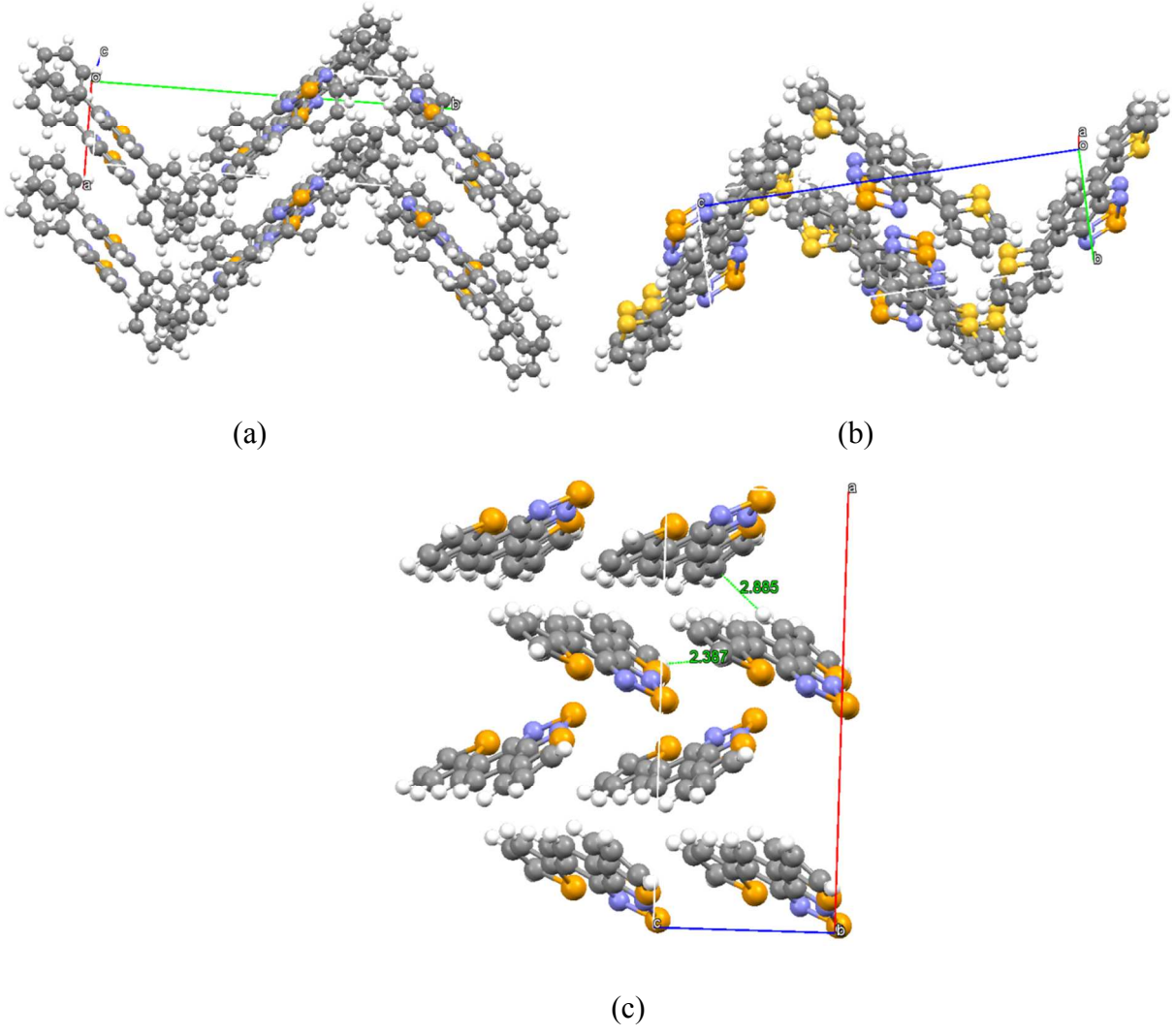


Figure S1. Packing patterns of (a) **1** and (b) **2** and (c) **3**.

Table S3. Energy difference between syn and anti form of **2** and **3** at B3LYP/6-311G+(d,p).

Compounds	**Energy Hatrees**		**Energy difference (kcal/mole) (anti-syn)**
	Syn	**Anti**	
2	-3845.903335	-3845.904163	-0.52
3	-7852.560035	-7852.558963	0.67

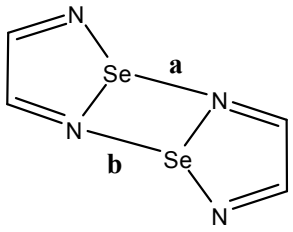
Table S4. Absolute energies of **1**, **2**, **3**, **1**-dimer, **2**-dimer and **3**-dimer at B3LYP/6-311G+(d,p).

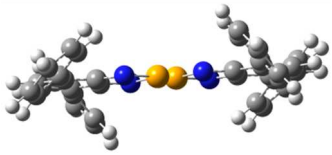
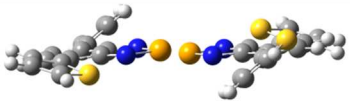
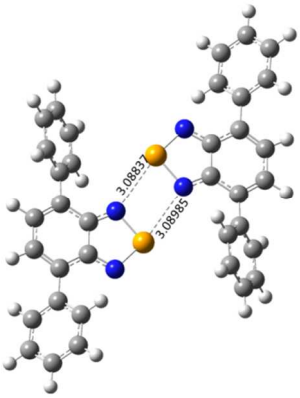
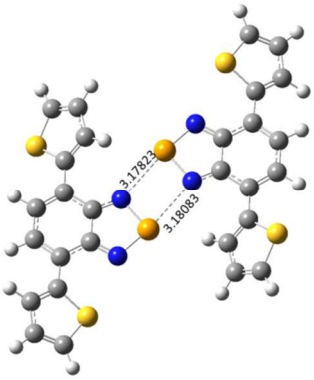
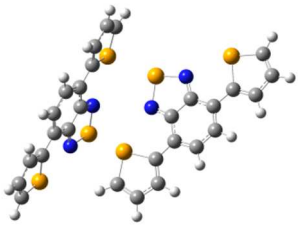
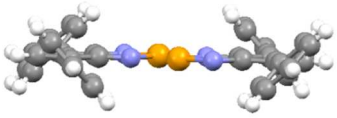
Compounds	Energy (Hatrees)
1	-3204.374683
2	-3845.904163
3	-7852.560035
1-dimer	-6408.755500
2-dimer	-7691.812343
3-dimer	-15705.1227952

Table S5. Stabilization energy by dimerization of **1**-**3**.

Dimer	Stabilization energy (kcal/mole)
1-dimer	-3.85
2-dimer	-2.52
3-dimer	-1.71

Table S6. Short contacts in selanadiazole-dimers calculated at B3LYP/6-311G+(d,p).

	**1 Dimer**	**2 Dimer**
a	3.088	3.178
b	3.089	3.180
N…N	3.173	3.295
Se…Se	3.943	3.985

		1-dimer	**2**-dimer	**3**-dimer
OPTIMIZED	**Side view**			
	Top view			
	Side view			

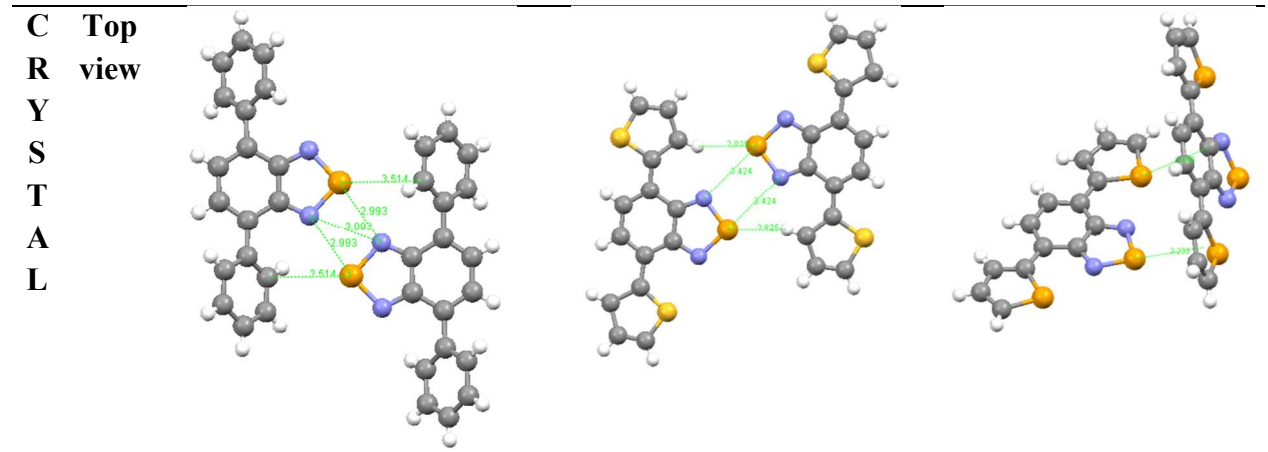


Figure S2. Side and top view of the crystal structures and optimized structures of dimers**.**

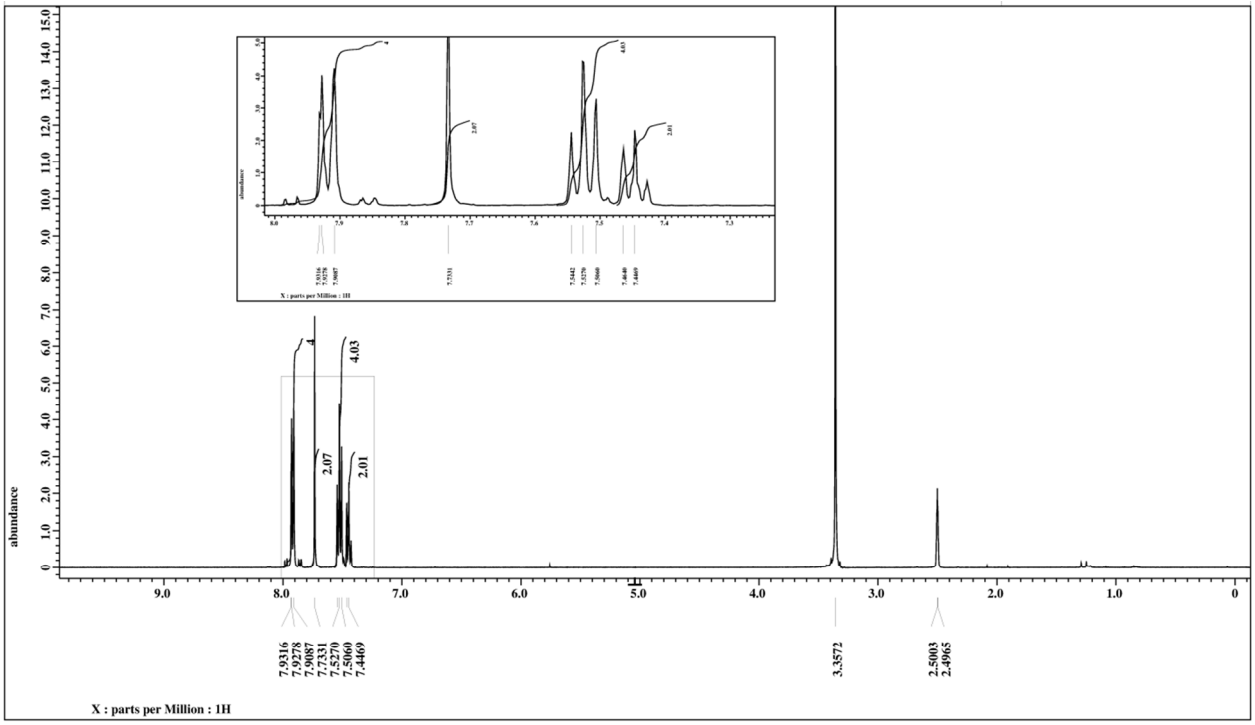


Figure S3. ^{1}H NMR spectrum of **1**.

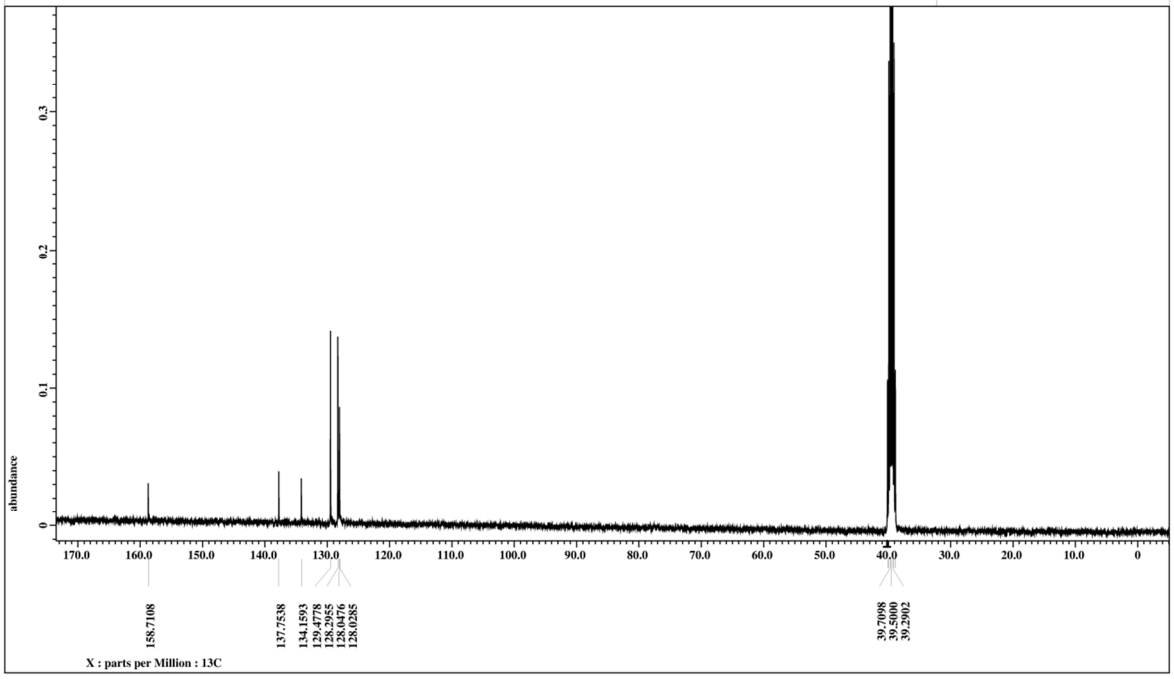


Figure S4. ^{13}C NMR spectrum of **1**.

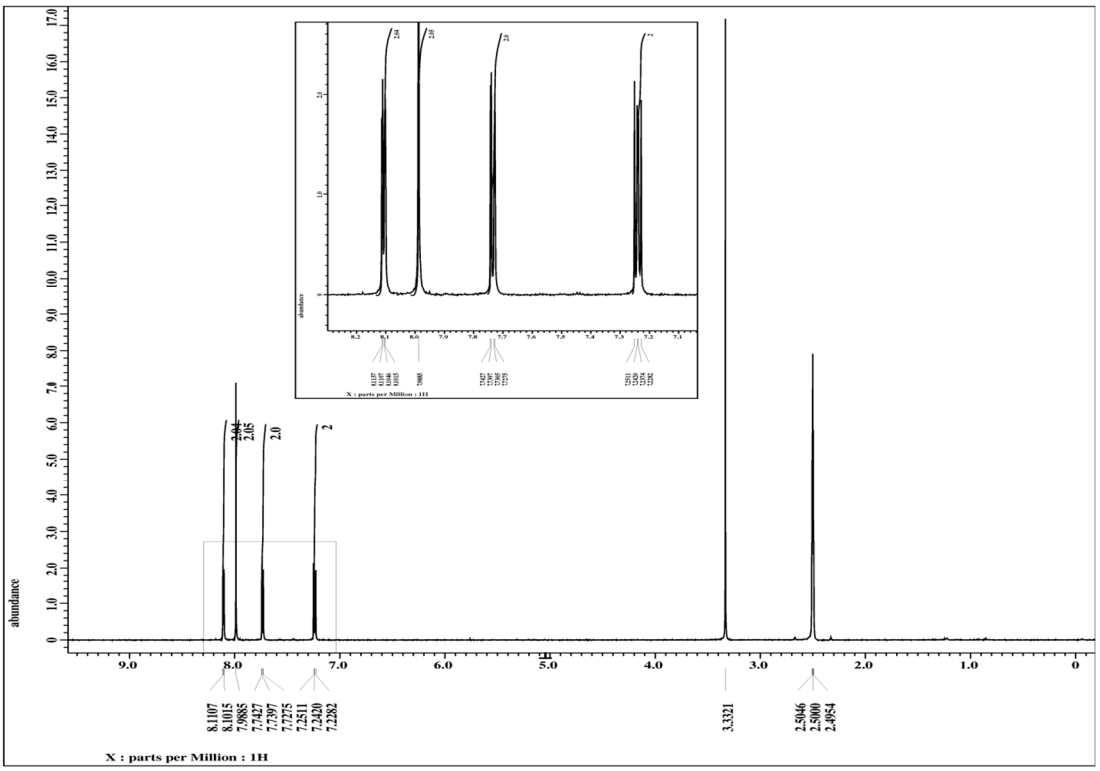


Figure S5. ^{1}H NMR spectrum of **2**.

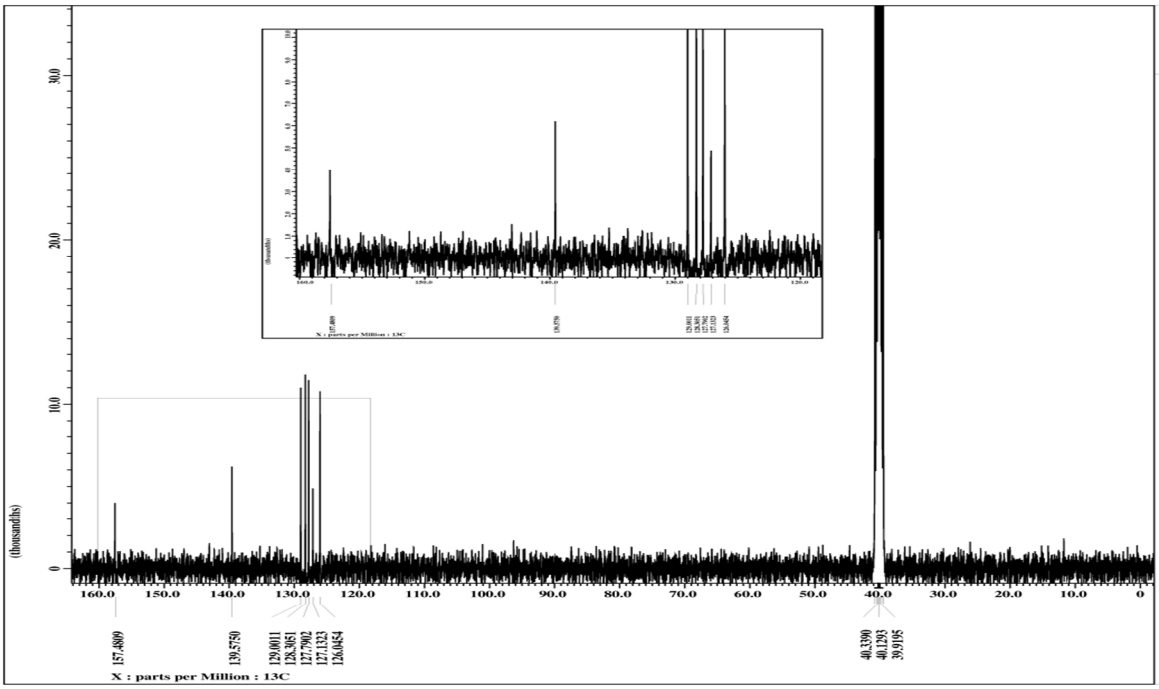


Figure S6. ^{13}C NMR spectrum of **2**.

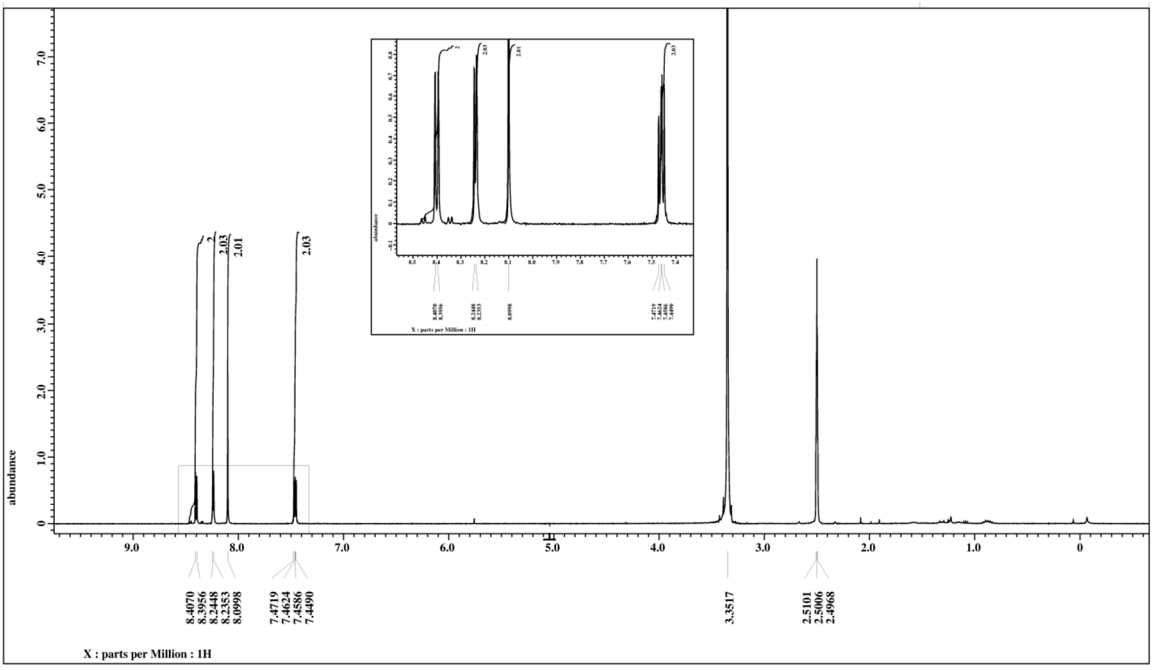


Figure S7. ^{1}H NMR spectrum of **3**.

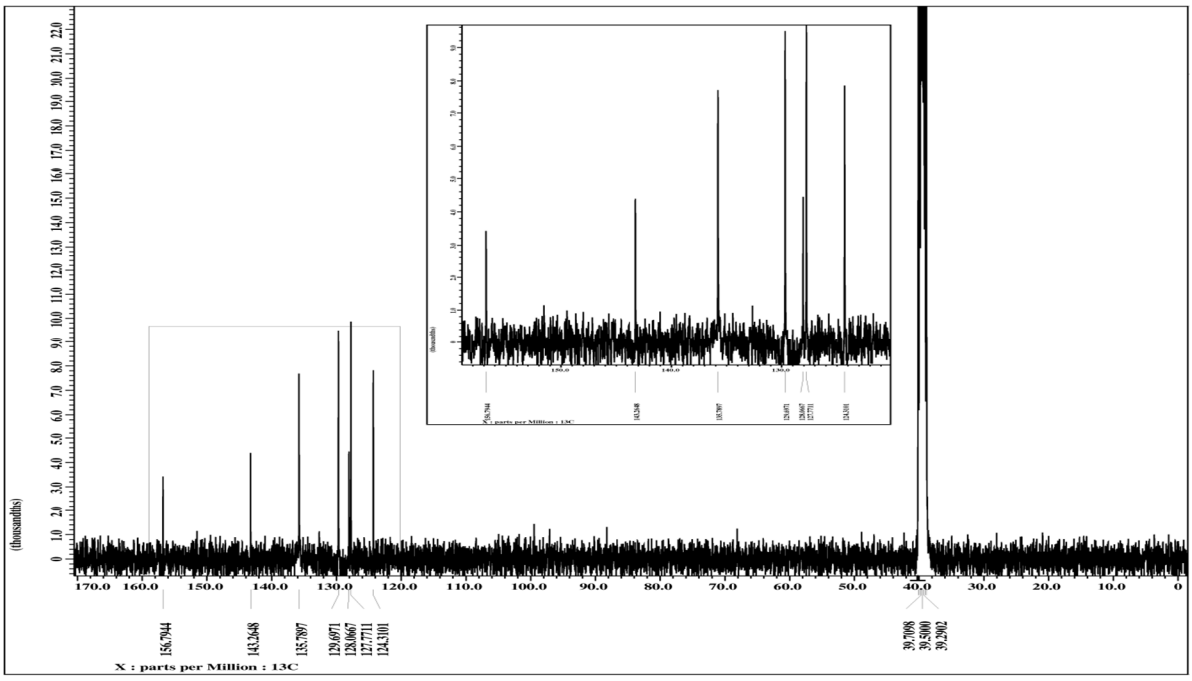


Figure S8. ^{13}C NMR spectrum of **3**.

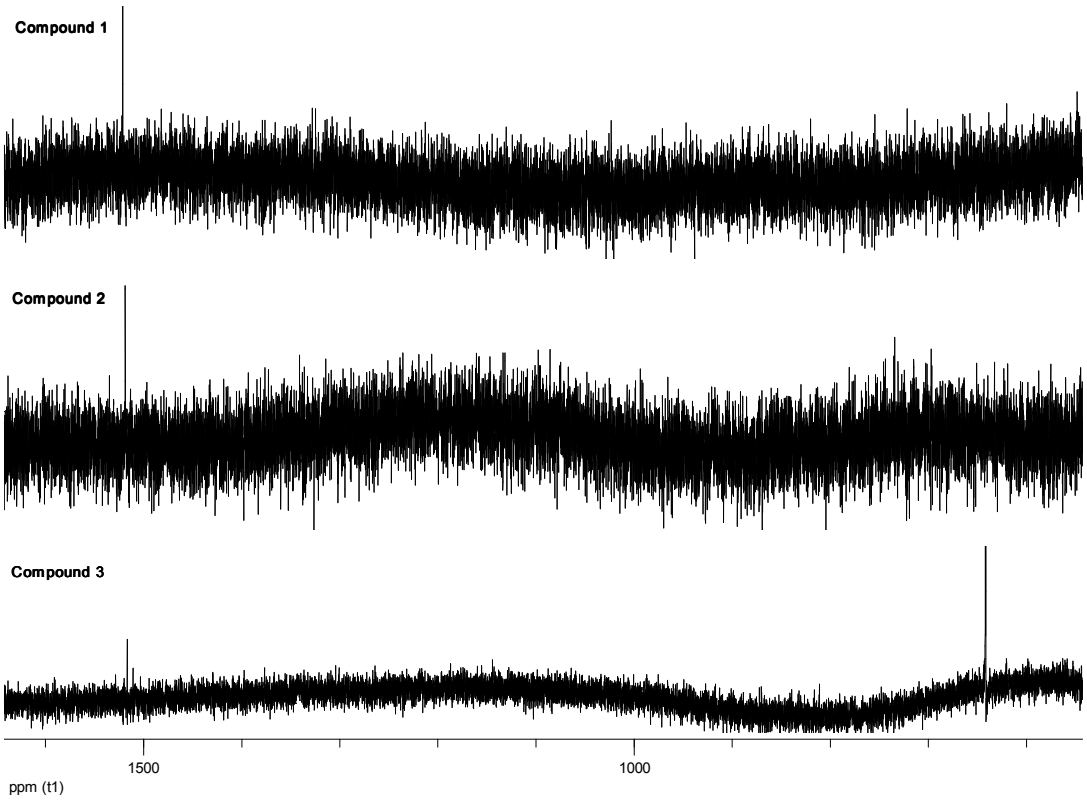


Figure S9. ^{77}Se-NMR spectrum of **1**, **2** and **3**.

Coordinate of optimized geometry in level B3LYP/6-311+G(d,p) level.

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.737146	0.393343	-0.005171
2	6	0	0.737182	0.393364	0.005249
3	6	0	1.469067	-0.853168	0.002278
4	6	0	0.712235	-1.999134	0.002165
5	6	0	-0.712135	-1.999123	-0.002151
6	6	0	-1.468991	-0.853176	-0.002244
7	1	0	1.216951	-2.958396	0.019743
8	1	0	-1.216860	-2.958383	-0.019611
9	7	0	1.315440	1.585381	0.003354
10	7	0	-1.315456	1.585330	-0.003322
11	34	0	-0.000164	2.814354	-0.000009
12	6	0	-2.950353	-0.905573	0.011730
13	6	0	-3.610778	-1.836842	0.828357
14	6	0	-3.726924	-0.065512	-0.801084
15	6	0	-4.999477	-1.934511	0.825581
16	1	0	-3.031210	-2.472669	1.488103
17	6	0	-5.114656	-0.168619	-0.807151
18	1	0	-3.240203	0.665633	-1.432169
19	6	0	-5.757766	-1.101983	0.004645
20	1	0	-5.488601	-2.654703	1.472075
21	1	0	-5.696106	0.483776	-1.449193
22	1	0	-6.839459	-1.175393	0.001914
23	6	0	2.950475	-0.905502	-0.011708
24	6	0	3.727018	-0.065446	0.801098
25	6	0	3.610880	-1.836783	-0.828340
26	6	0	5.114776	-0.168502	0.807125
27	1	0	3.240327	0.665608	1.432283
28	6	0	4.999577	-1.934383	-0.825631
29	1	0	3.031273	-2.472674	-1.487993
30	6	0	5.757869	-1.101792	-0.004741
31	1	0	5.696193	0.483892	1.449193
32	1	0	5.488724	-2.654512	-1.472178
33	1	0	6.839566	-1.175140	-0.002131

2 anti

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.756481	0.343505	0.036652
2	6	0	-0.711543	0.492038	0.025520
3	6	0	-1.565787	-0.679113	-0.009127
4	6	0	-0.902981	-1.890282	-0.043798
5	6	0	0.505071	-2.028743	-0.042498
6	6	0	1.376850	-0.961105	0.014592
7	1	0	-1.482256	-2.805566	-0.086002
8	1	0	0.904388	-3.033473	-0.103126
9	6	0	-3.022358	-0.592171	-0.018089

10	6	0	-3.845593	0.514129	0.008523
11	16	0	-4.003485	-2.056390	-0.066267
12	6	0	-5.231239	0.198927	-0.009874
13	1	0	-3.453630	1.518158	0.040161
14	6	0	-5.472604	-1.144359	-0.050058
15	1	0	-6.015917	0.943766	0.006216
16	1	0	-6.421010	-1.659071	-0.071283
17	6	0	2.823082	-1.159650	0.059267
18	6	0	3.482229	-2.327443	0.392207
19	16	0	3.991297	0.074757	-0.379863
20	6	0	4.892264	-2.244988	0.280859
21	1	0	2.967699	-3.217425	0.728651
22	6	0	5.311930	-1.011320	-0.136795
23	1	0	5.564324	-3.060879	0.511642
24	1	0	6.323050	-0.666390	-0.292492
25	7	0	-1.155845	1.738605	0.045212
26	7	0	1.450382	1.468129	0.063811
27	34	0	0.275641	2.828922	0.076379

2 syn

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.736040	0.261434	-0.057949
2	6	0	-0.736031	0.261367	-0.057974
3	6	0	-1.475302	-0.977913	0.007525
4	6	0	-0.708034	-2.121584	0.105153
5	6	0	0.708203	-2.121520	0.105147
6	6	0	1.475360	-0.977789	0.007499
7	1	0	-1.203593	-3.078417	0.213582
8	1	0	1.203906	-3.078290	0.213532
9	6	0	-2.934121	-1.040369	-0.025935
10	6	0	-3.702565	-2.148765	-0.324686
11	16	0	-3.976889	0.310234	0.385167
12	6	0	-5.097872	-1.930319	-0.209066
13	1	0	-3.276012	-3.091755	-0.639384
14	6	0	-5.396133	-0.651935	0.177118
15	1	0	-5.845708	-2.684616	-0.414949
16	1	0	-6.368977	-0.208636	0.327686
17	6	0	2.934162	-1.040249	-0.026045
18	6	0	3.702522	-2.148527	-0.325331
19	16	0	3.976937	0.310129	0.385754
20	6	0	5.097855	-1.930164	-0.209669
21	1	0	3.275896	-3.091341	-0.640472
22	6	0	5.396141	-0.652006	0.177225
23	1	0	5.845661	-2.684358	-0.416037
24	1	0	6.369003	-0.208856	0.328102
25	7	0	-1.311263	1.450784	-0.114415
26	7	0	1.311165	1.450910	-0.114375
27	34	0	-0.000047	2.682313	-0.169510

3 anti

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.806169	0.397646	0.032226
2	6	0	-0.634203	0.713521	0.048866
3	6	0	-1.617198	-0.351418	0.098297
4	6	0	-1.092582	-1.629337	0.131924
5	6	0	0.289199	-1.927997	0.112806
6	6	0	1.280949	-0.967172	0.069112
7	1	0	-1.771487	-2.473129	0.186770
8	1	0	0.564075	-2.974698	0.138812
9	6	0	-3.052330	-0.098904	0.107704
10	6	0	-3.735316	1.076504	0.311384
11	6	0	-5.157679	0.990355	0.276843
12	1	0	-3.211998	2.004778	0.485836
13	6	0	-5.661633	-0.251349	0.035605
14	1	0	-5.792916	1.854451	0.430965
15	1	0	-6.697500	-0.546292	-0.036666
16	6	0	2.698530	-1.309985	0.064208
17	6	0	3.238302	-2.575776	0.146963
18	6	0	4.655248	-2.664083	0.109846
19	1	0	2.622928	-3.461960	0.239506
20	6	0	5.299964	-1.466598	-0.004069
21	1	0	5.178699	-3.610808	0.169865
22	1	0	6.365960	-1.297883	-0.047288
23	7	0	-0.933684	2.002061	0.009166
24	7	0	1.621475	1.435955	-0.021169
25	34	0	0.609911	2.923265	-0.053919
26	34	0	-4.299769	-1.515288	-0.188347
27	34	0	4.102304	-0.030713	-0.073442

3 syn

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.735372	0.133643	-0.000040
2	6	0	0.735390	0.133652	-0.000030
3	6	0	1.481550	-1.102912	0.000015
4	6	0	0.706877	-2.249028	0.000080
5	6	0	-0.706856	-2.249035	0.000078
6	6	0	-1.481532	-1.102922	-0.000008
7	1	0	1.194387	-3.215715	0.000140
8	1	0	-1.194360	-3.215726	0.000160
9	6	0	2.938866	-1.146230	0.000012
10	6	0	3.729472	-2.275670	-0.000008
11	6	0	5.134153	-2.065780	-0.000013
12	1	0	3.311243	-3.274553	-0.000013
13	6	0	5.516976	-0.755875	0.000016
14	1	0	5.842587	-2.885560	-0.000031
15	1	0	6.524838	-0.367525	-0.000014
16	6	0	-2.938846	-1.146239	-0.000054
17	6	0	-3.729444	-2.275683	-0.000227
18	6	0	-5.134127	-2.065804	-0.000192
19	1	0	-3.311208	-3.274563	-0.000394
20	6	0	-5.516959	-0.755901	-0.000010
21	1	0	-5.842555	-2.885588	-0.000319

22	1	0	-6.524823	-0.367558	0.000044
23	7	0	1.307902	1.325372	-0.000052
24	7	0	-1.307882	1.325366	-0.000061
25	34	0	-0.000040	2.561895	-0.000075
26	34	0	4.047378	0.402506	0.000033
27	34	0	-4.047371	0.402490	0.000144

1-dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.283521	0.153438	-0.021020
2	6	0	6.296461	1.347754	-0.757835
3	1	0	5.422934	1.632173	-1.328286
4	6	0	7.422391	2.165633	-0.763813
5	1	0	7.415487	3.079914	-1.346937
6	6	0	8.553580	1.817449	-0.026905
7	1	0	9.426610	2.460354	-0.029308
8	6	0	8.550214	0.640311	0.718885
9	1	0	9.418412	0.365529	1.307628
10	6	0	7.427037	-0.182128	0.720925
11	1	0	7.425685	-1.083599	1.323276
12	34	0	1.628829	1.097048	0.191417
13	7	0	1.421458	-0.696688	0.109892
14	7	0	3.422066	0.992951	0.134884
15	6	0	0.804010	-3.629719	1.003059
16	1	0	0.826989	-2.848025	1.752056
17	6	0	-0.185748	-4.607268	1.052058
18	1	0	-0.928527	-4.579008	1.841740
19	6	0	-0.223028	-5.621087	0.094862
20	1	0	-0.998130	-6.378157	0.131437
21	6	0	0.741580	-5.652252	-0.910258
22	1	0	0.716539	-6.430646	-1.664754
23	6	0	1.737519	-4.679080	-0.955066
24	1	0	2.476122	-4.699882	-1.748663
25	6	0	1.784951	-3.654274	0.000863
26	6	0	2.881161	-2.655132	-0.025779
27	6	0	2.632695	-1.235622	0.052575
28	6	0	3.756083	-0.286276	0.050186
29	6	0	5.118122	-0.762870	-0.037833
30	6	0	5.282040	-2.123480	-0.131839
31	1	0	6.284298	-2.525369	-0.226378
32	6	0	4.194462	-3.042951	-0.122665
33	1	0	4.422920	-4.101701	-0.175210
34	6	0	-6.282811	-0.155439	0.012758
35	6	0	-6.297365	-1.349225	0.750399
36	1	0	-5.425542	-1.632610	1.323963
37	6	0	-7.422724	-2.167908	0.753209
38	1	0	-7.417112	-3.081766	1.337010
39	6	0	-8.551694	-1.821068	0.012274
40	1	0	-9.424264	-2.464601	0.012213
41	6	0	-8.546678	-0.644463	-0.734344
42	1	0	-9.413098	-0.370732	-1.326189
43	6	0	-7.424091	0.178786	-0.733220
44	1	0	-7.421372	1.079830	-1.336207
45	34	0	-1.626821	-1.095956	-0.184381
46	7	0	-1.420929	0.698026	-0.103403

47	7	0	-3.420285	-0.993034	-0.133307
48	6	0	-0.802751	3.631234	-0.996142
49	1	0	-0.822686	2.849116	-1.744782
50	6	0	0.186300	4.609633	-1.042502
51	1	0	0.931630	4.581608	-1.829787
52	6	0	0.219607	5.624031	-0.085771
53	1	0	0.994145	6.381775	-0.120307
54	6	0	-0.748234	5.654891	0.916246
55	1	0	-0.726299	6.433731	1.670379
56	6	0	-1.743449	4.680865	0.958394
57	1	0	-2.484629	4.701449	1.749589
58	6	0	-1.786932	3.655498	0.002875
59	6	0	-2.882453	2.655522	0.026562
60	6	0	-2.632713	1.236133	-0.050157
61	6	0	-3.755460	0.286006	-0.050598
62	6	0	-5.118110	0.761698	0.032758
63	6	0	-5.283292	2.122246	0.125333
64	1	0	-6.286128	2.523489	0.216407
65	6	0	-4.196329	3.042466	0.119049
66	1	0	-4.425688	4.101089	0.170251

2 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	-1.612964	1.141273	-0.278907
2	7	0	-1.492375	-0.660568	-0.229874
3	7	0	-3.408300	1.120373	-0.214763
4	16	0	-2.180690	-5.082957	0.707745
5	16	0	-6.107578	2.123923	0.339509
6	6	0	-0.707237	-5.706255	0.049033
7	1	0	-0.362556	-6.687576	0.336970
8	6	0	-0.119576	-4.812623	-0.801771
9	1	0	0.808055	-5.010297	-1.322872
10	6	0	-0.858850	-3.604587	-0.932015
11	1	0	-0.564878	-2.782971	-1.568617
12	6	0	-2.015171	-3.582649	-0.187776
13	6	0	-3.047964	-2.550897	-0.112417
14	6	0	-2.726269	-1.143016	-0.174263
15	6	0	-3.801480	-0.140203	-0.151536
16	6	0	-4.384370	-2.862105	0.020713
17	1	0	-4.674953	-3.905379	0.070695
18	6	0	-5.415661	-1.891715	0.073466
19	1	0	-6.429873	-2.248247	0.203045
20	6	0	-5.187401	-0.535758	-0.039120
21	6	0	-6.290816	0.422105	-0.048567
22	6	0	-7.619303	0.142398	-0.303883
23	1	0	-7.966933	-0.838646	-0.598457
24	6	0	-8.478999	1.261103	-0.173435
25	1	0	-9.546416	1.225142	-0.346468
26	6	0	-7.805410	2.398186	0.181453
27	1	0	-8.203097	3.390242	0.334232
28	34	0	1.609688	-1.139187	0.269375
29	7	0	1.491502	0.662917	0.222239
30	7	0	3.405281	-1.120356	0.211462

31	16	0	2.189713	5.086160	-0.706758
32	16	0	6.105162	-2.126678	-0.333510
33	6	0	0.713976	5.710159	-0.053869
34	1	0	0.371932	6.692457	-0.341623
35	6	0	0.121148	4.815738	0.792506
36	1	0	-0.808680	5.013688	1.309576
37	6	0	0.858234	3.606512	0.924046
38	1	0	0.560214	2.784125	1.557748
39	6	0	2.018073	3.584437	0.185287
40	6	0	3.049837	2.551479	0.112777
41	6	0	2.726169	1.143902	0.171612
42	6	0	3.800239	0.139806	0.151445
43	6	0	4.387149	2.861191	-0.014728
44	1	0	4.679244	3.904165	-0.062147
45	6	0	5.417437	1.889609	-0.064881
46	1	0	6.432574	2.245094	-0.190011
47	6	0	5.187063	0.533771	0.044813
48	6	0	6.289228	-0.425499	0.056994
49	6	0	7.617187	-0.147767	0.317179
50	1	0	7.965065	0.832512	0.613996
51	6	0	8.475903	-1.267426	0.188501
52	1	0	9.542764	-1.232999	0.365244
53	6	0	7.802094	-2.403273	-0.169913
54	1	0	8.199046	-3.395672	-0.322372

3 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	-6.155416	-1.412042	-0.156388
2	34	0	-3.299732	1.256523	-2.565404
3	34	0	-0.291660	4.142824	-0.633746
4	7	0	-4.150031	0.363938	-1.255541
5	7	0	-2.242005	2.145595	-1.413326
6	6	0	-7.070441	-2.478111	1.080275
7	1	0	-7.864250	-3.136479	0.759217
8	6	0	-6.595290	-2.311156	2.348468
9	1	0	-6.991302	-2.850468	3.200599
10	6	0	-5.532083	-1.376740	2.468159
11	1	0	-5.070029	-1.170532	3.425513
12	6	0	-5.119861	-0.762488	1.305201
13	6	0	-4.073642	0.244763	1.175555
14	6	0	-3.434884	0.792241	2.273537
15	1	0	-3.732816	0.482572	3.267232
16	6	0	-2.402270	1.754447	2.187537
17	1	0	-1.987621	2.112196	3.121641
18	6	0	-1.911446	2.255213	0.995868
19	6	0	-0.822431	3.224208	0.948550
20	6	0	-0.046813	3.646648	2.007536
21	1	0	-0.163159	3.242581	3.005493
22	6	0	0.929427	4.638772	1.720606
23	1	0	1.591817	5.036628	2.480147
24	6	0	0.968919	5.043080	0.417454
25	1	0	1.631637	5.774019	-0.022138
26	6	0	-3.629782	0.749854	-0.102747
27	6	0	-2.557015	1.749640	-0.191729
28	34	0	6.847704	0.298587	0.229929

29	34	0	2.344529	1.141700	0.398289
30	34	0	-0.867089	-2.137037	0.087679
31	7	0	3.959837	0.363295	0.241296
32	7	0	1.465718	-0.408951	0.151615
33	6	0	8.596584	-0.349187	0.068247
34	1	0	9.442614	0.313270	0.178020
35	6	0	8.622036	-1.687596	-0.196706
36	1	0	9.542465	-2.243934	-0.328542
37	6	0	7.344023	-2.300728	-0.290177
38	1	0	7.242563	-3.357924	-0.501353
39	6	0	6.252598	-1.479881	-0.103323
40	6	0	4.848569	-1.872179	-0.141214
41	6	0	4.452051	-3.183581	-0.334595
42	1	0	5.205715	-3.952179	-0.451394
43	6	0	3.102560	-3.601505	-0.384023
44	1	0	2.922338	-4.659478	-0.528120
45	6	0	2.023242	-2.746072	-0.251000
46	6	0	0.645190	-3.214443	-0.333872
47	6	0	0.222729	-4.476753	-0.691623
48	1	0	0.915206	-5.253823	-0.990906
49	6	0	-1.179249	-4.706820	-0.663616
50	1	0	-1.615220	-5.661570	-0.932942
51	6	0	-1.929202	-3.632897	-0.280789
52	1	0	-3.004739	-3.574326	-0.199908
53	6	0	3.769160	-0.928138	0.026702
54	6	0	2.366770	-1.361675	-0.025466