Supporting Information

Effect of heteroatom (S/Se) juggling in donor-acceptordonor (D-A-D) fused systems: synthesis and electrochemical polymerization

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Formula	$C_{22}H_{22}N_4S_3$	$C_{22}H_{22}N_4SSe_2$	C ₂₂ H ₂₂ N ₄ SeS ₂
Crystal system	Monoclinic	Monoclinic	Monoclinic
space group	C2/c	C2/c	C2/c
a [Å]	20.6742(8)	24.2226(12)	24.0368(11)
b [Å]	14.3417(5)	7.8812(3)	7.8856(3)
c [Å]	16.3414(7)	25.4161(13)	24.6824(11)
α [deg]	90	90	90
β [deg]	111.545(4)	120.284(7)	118.162(6)
γ [deg]	90	90	90
V [Å3]	4506.7(3)	4189.9(3)	4124.6(4)
Ζ	8	8	8
λ[Å]	1.54184	0.71073	0.71073
pcalcd	1.293	1.694	1.5637
F[000]	1840	2128.0	1984.0
μ[mm-1]	3.123	3.647	2.040
θ [deg]	4.28-66.39	1.86-28.15	1.87-25.00
index ranges	$-24 \le h \le 22$	$-30 \le h \le 31$	$-16 \le h \le 31$
	$0 \le k \le 17$	$-10 \le k \le 7$	$-10 \le k \le 7$
	$0 \le 1 \le 19$	$-22 \le 1 \le 33$	$-32 \le 1 \le 26$
T [K]	293(2)	100.00(10)	293.15
R1	0.0386	0.0347	0.031109
wR2	0.1189	0.0856	0.116
Rmerge	0.0431	0.0405	0.035303
parameters	264	264	263
GOF	1.083	1.063	0.950288
reflns total	3945	8297	8021
unique reflns	3945	4540	3628
obsdreflns	3464	4083	3305
CCDC No.	1412607	1412747	1412608

 Table S1. Crystallographic data and structure refinement parameters.



Figure S1.Packing diagram of compound 1 along c-axis.



Figure S2.Packing diagram of compound 2 along (a) a-axis, (b) b-axis and (c) c-axis.



Figure S3.Packing diagram of compound 3along (a) a-axis, (b) b-axis and (c) c-axis.



Figure S4. (a) Bifurcated weak Se^{\cdots}Se (3.477Å) and Se^{\cdots}N (3.433Å) interactions for compound **2**, (b).Weak S^{\cdots}S interaction (3.499Å) in compound **3**.

UV-vis spectra of monomer and polymer



Figure S5.Solution state absorption spectra of compounds (a) 1, (b) 2, and (c)3.



Figure S6.Solid state absorption spectra of (a) P1, (b) P2, and (c) P3.



FigureS7.CV of (a) P1, (b) P2 and (c) P3 using ACN/TBAPC solvent/electrolyte system.

To investigate the electrochromism, thin films of the polymers P1-P3 were electrodeposited on ITO glass slides using chronoamperometry. The spectroelectrochemistry was studied using TBAPC/ACN as the electrolyte/solvent system in a comonomer free solution. The spectroelectrochemical changes were observed in the anodic region only, due to the absence of any significant reduction peaks in the CV experiment of polymers. The appearance of multiple absorption maxima was observed in the neutral state for P1-P3. Upon increase in the value of applied potential, the intensity of absorption peaks decreased with the appearance of new absorption bands from 700 nm to near IR region suggesting in the formation of singly charged species (polaron) and doubly charged species (bipolaron) (Fig. S8). The spectroelectrochemical changes of all the polymers were associated with colour change as shown in Fig. S9 in their neutral and oxidized states. For P1 depletion of peaks at 460 and 600 nm occurred with the appearance of peaks at 800 and 1335 nm due to the formation of polaron and bipolaron, respectively. P2 showed somewhat different behaviour due to the presence of more polarizable selenophene moiety; it showed sudden charge carrier formation at 650 and 1200 nm upon changing the potential from 0.7 to 0.8 V. In P3 the peaks at 430 and 500 nm due to π - π * transition started to lose its intensity with the concomitant formation of peaks at 650 and 1100 nm, respectively.



FigureS8. Spectroelectrochemistry of (a) **P1** (between -0.5 and 0.8 V), (b) **P2** (between -0.2 and +0.8 V) and (c) **P3** (between -0.2 and 1.0 V) in a comonomer free, 0.1 M TBAPC/ACN solution.

Neutral	Oxidized	Neutral	Oxidized	Neutral	Oxidized
(P1)	(P1)	(P2)	(P2)	(P3)	(P3)

Figure S9. Colour of the polymers in their neutral and oxidized states

Compounds	Energy (Hartree)
2	-6267.528359
3	-4266.33418
Dimer2	-12535.06345
Dimer3	-8532.686751

Table S2. Absolute energies of 2 and 3, 2-dimer and 3-dimer at B3LYP/6-311G+(d,p).

 Table S3. Stabilization energy by dimerization of 2 and 3.

Dimer	Stabilization Energy (Hartree)	Stabilization Energy (kcal/mol)
2	0.006732	4.2
3	0.018391	11.5



Figure S10. View of optimized structures of dimers of 2 and 3.



Figure S11. (a)HOMO, (b) LUMO for P1; (c) HOMO, (d) LUMO for P2 and (e) HOMO, (f) LUMO for P3.



Figure S12. ¹H NMR of compound **1**.



Figure S13. ¹³C NMR of compound 1.



Figure S14. ¹H NMR of compound 5b.



Figure S15. ¹³C NMR of compound 5b.



Figure S16. ¹H NMR of compound 6b.



Figure S17. ¹³C NMR of compound 6b.



Figure S18. ¹H NMR of compound 2.



Figure S19. ¹³C NMR of compound 2.





Reference

T. L. Tam, H. Li, Y. M. Lam, S. G. Mhaisalkar and A. C. Grimsdale, Org. Lett., 2011, 13, 4613.

Coordinates for optimized geometry P1

Center Number	Atomic Number	Atomic Type	Coord X	dinates (Angs Y	stroms) Z
1	 7	0	-4.622470	3.666171	0.014693
2	7	0	-7.133660	3.651453	-0.302792
3	7	0	-4.230057	-1.068947	-0.042818
4	7	0	-7.514535	-1.067252	0.103544
5	6	0	-7.306656	-2.378916	0.703728
6	1	0	-7.246709	-3.175651	-0.045623
7	1	0	-6.393057	-2.373753	1.299840
8	1	0	-8.143892	-2.595180	1.373194
9	6	0	-4.433022	-2.419294	-0.552453
10	1	0	-4.491589	-3.163349	0.249305
11	1	0	-5.345861	-2.457465	-1.148489
12	1	0	-3.594251	-2.677863	-1.204780
13	6	0	-0.719607	0.046857	0.074924
14	6	0	-11.027722	0.029575	-0.087790
15	6	0	-1.634694	-0.990065	0.005170
16	1	0	-1.343594	-2.031492	-0.070575
17	6	0	-10.110416	-0.997752	0.055925
18	1	0	-10.399384	-2.031160	0.209628
19	6	0	-8.670706	0.860100	-0.203123
20	6	0	-8.782536	-0.515957	-0.019282
21	6	0	-6.589071	-0.026841	-0.015869
22	6	0	-7.298258	1.194791	-0.177941
23	6	0	-5.157945	-0.024514	-0.002570
24	6	0	-4.451878	1.207386	0.070193
25	6	0	-3.0/86/9	0.8/8/18	0.122/80
26	6	0	-2.963515	-0.5068/3	0.041481
27	6	0	-5.156060	2.449825	-0.008662
28	6	0	-6.59/099	2.441397	-0.190635
29	16	0	-1.510097	1 607007	0.10/2/3
3U 21	TO	0	-10.232040	1.00/22/	-0.319091
32	6	0	1 635362	-0.034631	-0.060705
33	16	0	1 516072	-1 612231	0.000703
34	1	0	1 345487	2 027140	-0 212196
35	6	0	2 963660	0 513004	0.212190
36	6	0	3 076723	-0.863313	0.195217
37	7	0	4.231228	1.065840	-0.106524
38	6	0	4.449521	-1.196616	0.170354
39	6	0	4.438207	2.378507	-0.704929
40	6	0	5.157605	0.026020	0.011259
41	6	0	5.151894	-2.442558	0.180970
42	1	0	4.496986	3.174323	0.045483
43	1	0	5.352157	2.374974	-1.300524
44	1	0	3.601146	2.594850	-1.374589
45	6	0	6.588732	0.025128	-0.001141
46	7	0	4.616437	-3.653353	0.290326
47	6	0	6.593056	-2.449212	-0.000123
48	7	0	7.515559	1.070357	0.041959
49	6	0	7.296070	-1.205929	-0.076022
50	7	0	7.127835	-3.664995	-0.025631

51	6	0	7.310838	2.419685	0.553511
52	6	0	8.782698	0.509753	-0.042830
53	6	0	8.668970	-0.875789	-0.127108
54	1	0	7.252140	3.164923	-0.247144
55	1	0	6.397503	2.456007	1.148901
56	1	0	8.148843	2.678095	1.206886
57	6	0	10.111025	0.994207	-0.004640
58	16	0	10.229559	-1.631111	-0.192492
59	6	0	11.027156	-0.041677	-0.076067
60	1	0	10.401044	2.035736	0.073795
61	16	0	-5.879385	4.732334	-0.183364
62	16	0	5.871823	-4.732774	0.169462
63	-2	0	23.493383	0.011880	0.007164

Ρ2

Center	Atomic	Atomic	Coord	dinates (Ang	stroms)
Number	Number	Туре	Х	Y	Ζ
1	7	0	-4.674799	3.801954	-0.096462
2	7	0	-7.189412	3.778665	-0.400361
3	7	0	-4.271994	-0.922991	-0.006372
4	7	0	-7.577647	-0.919898	0.115652
5	6	0	-7.380924	-2.231994	0.716477
6	1	0	-7.304469	-3.027706	-0.032653
7	1	0	-6.480843	-2.227632	1.332758
8	1	0	-8.231892	-2.450305	1.367235
9	6	0	-4.462806	-2.299965	-0.441356
10	1	0	-4.541609	-2.997251	0.399934
11	1	0	-5.359681	-2.374386	-1.057909
12	1	0	-3.608029	-2.594206	-1.056068
13	6	0	-0.711950	0.101064	0.097274
14	6	0	-11.141087	0.072038	-0.110044
15	6	0	-1.691729	-0.871913	0.057399
16	1	0	-1.450072	-1.929536	0.022369
17	6	0	-10.158234	-0.885129	0.051539
18	1	0	-10.396671	-1.930160	0.222590
19	6	0	-8.719752	1.007262	-0.232457
20	6	0	-8.843690	-0.363713	-0.022390
21	6	0	-6.642400	0.107419	-0.022999
22	6	0	-7.348482	1.327196	-0.210375
23	6	0	-5.210367	0.110969	-0.002324
24	6	0	-4.508284	1.346826	0.028251
25	6	0	-3.136107	1.036726	0.093926
26	6	0	-3.007765	-0.349477	0.061433
27	6	0	-5.210703	2.586505	-0.083355
28	6	0	-6.649857	2.573120	-0.258490
29	6	0	0.711036	-0.083216	0.112181
30	6	0	1.691991	0.876268	-0.047115
31	1	0	1.451388	1.920848	-0.217886
32	6	0	3.007569	0.357785	0.028621
33	6	0	3.134210	-1.013037	0.238013
34	7	0	4.272622	0.916912	-0.106697
35	6	0	4.506231	-1.329848	0.218264
36	6	0	4.467420	2.229920	-0.706131

37	6	0	5.209954	-0.108393	0.032961
38	6	0	5.207431	-2.574287	0.267033
39	1	0	4.543061	3.024960	0.043773
40	1	0	5.367260	2.227466	-1.322815
41	1	0	3.615909	2.447760	-1.356300
42	6	0	6.642071	-0.108842	0.014763
43	7	0	4.670176	-3.781054	0.407239
44	6	0	6.646918	-2.584493	0.094668
45	7	0	7.578356	0.926959	0.021175
46	6	0	7.346849	-1.343247	-0.015024
47	7	0	7.185418	-3.798795	0.108190
48	6	0	7.383834	2.304004	0.454057
49	6	0	8.843873	0.356140	-0.044511
50	6	0	8.718492	-1.030299	-0.077870
51	1	0	7.302811	2.999830	-0.388223
52	1	0	6.487014	2.376916	1.070909
53	1	0	8.238038	2.601479	1.067963
54	6	0	10.158812	0.881367	-0.037920
55	6	0	11.140717	-0.089509	-0.076553
56	1	0	10.398132	1.939487	-0.001945
57	16	0	-5.933754	4.863347	-0.316955
58	34	0	-10.385890	1.815333	-0.389242
59	16	0	5.928305	-4.862986	0.325880
60	34	0	-1.472713	1.863268	0.150074
61	34	0	1.469645	-1.824969	0.391342
62	34	0	10.383734	-1.853347	-0.131325
63	-2	0	23.704474	0.025777	0.021076

Ρ3

Center Number	Atomic Number	Atomic Type	Coord X	dinates (Ang: Y	stroms) Z
1	7	0	-4.538140	3.622448	0.360582
2	7	0	-7.169521	3.654028	0.026017
3	7	0	-4.232175	-1.061654	-0.142991
4	7	0	-7.523215	-1.053785	0.005881
5	6	0	-7.328695	-2.418865	0.476861
6	1	0	-7.268609	-3.139801	-0.345734
7	1	0	-6.419662	-2.478542	1.076992
8	1	0	-8.172551	-2.692243	1.116345
9	6	0	-4.442384	-2.366039	-0.757100
10	1	0	-4.508366	-3.170350	-0.016312
11	1	0	-5.353251	-2.351570	-1.357263
12	1	0	-3.602873	-2.578311	-1.424913
13	6	0	-0.718846	0.033256	0.064547
14	6	0	-11.025041	0.092543	-0.086206
15	6	0	-1.635052	-0.992712	-0.096663
16	1	0	-1.344599	-2.022705	-0.269439
17	6	0	-10.119109	-0.953879	-0.038664
18	1	0	-10.419678	-1.993962	0.015835
19	6	0	-8.659141	0.904287	-0.119934
20	6	0	-8.786200	-0.481623	-0.066210
21	6	0	-6.588470	-0.015682	-0.015167
22	6	0	-7.283987	1.221058	-0.063185

23	6	0	-5.156452	-0.023617	-0.002397
24	6	0	-4.448320	1.193158	0.181768
25	6	0	-3.076350	0.858494	0.197951
26	6	0	-2.963340	-0.513802	-0.011521
27	6	0	-5.132599	2.453463	0.219900
28	6	0	-6.586972	2.470755	0.037930
29	34	0	-5.847822	4.872195	0.260224
30	16	0	-1.516770	1.605968	0.325740
31	16	0	-10.211292	1.676788	-0.166505
32	6	0	0.719491	-0.047957	0.055966
33	6	0	1.633957	0.990768	0.003447
34	16	0	1.520181	-1.638707	0.138271
35	1	0	1.341872	2.033147	-0.053244
36	6	0	2.962954	0.507460	0.028703
37	6	0	3.078605	-0.879317	0.085546
38	7	0	4.230461	1.068884	-0.047873
39	6	0	4.450942	-1.207653	0.026411
40	6	0	4.435092	2.431499	-0.521591
41	6	0	5.156652	0.023170	-0.026361
42	6	0	5.137225	-2.463408	-0.073133
43	1	0	4.504141	3.153141	0.299682
44	1	0	5.342529	2.482491	-1.124936
45	1	0	3.591407	2.711106	-1.158592
46	6	0	6.588690	0.019147	-0.042626
47	7	0	4.544912	-3.641782	-0.056912
48	6	0	6.591285	-2.458660	-0.258289
49	7	0	7.522084	1.049732	0.092869
50	6	0	7.286128	-1.204036	-0.225054
51	34	0	5.856011	-4.871440	-0.290826
52	7	0	7.175736	-3.632879	-0.397205
53	6	0	7.324389	2.357671	0.703596
54	6	0	8.785922	0.490781	-0.039964
55	6	0	8.660826	-0.881068	-0.245323
56	1	0	7.262303	3.160207	-0.039446
57	1	0	6.415499	2.352392	1.306913
58	1	0	8.167878	2.565281	1.367841
59	6	0	10.118401	0.958727	0.040344
60	16	0	10.213709	-1.642072	-0.374817
61	6	0	11.025561	-0.075340	-0.120350
62	1	0	10.417829	1.986812	0.209111
63	-2	0	23.489578	-0.098794	-0.029258

1

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Туре	Х	Y	Z
1	 16	0	-2.035741	-4.344519	0.197560
2	16	0	-2.033861	4.345291	-0.197802
3	16	0	-5.101456	0.001052	0.000319
4	7	0	-4.027906	1.256260	-0.162248
5	7	0	0.701856	-1.660105	-0.072854
6	7	0	0.702608	1.659697	0.072532
7	6	0	1.995781	-1.491399	-0.745186
8	1	0	2.093945	-0.444805	-1.034621

9	1	0	1.967494	-2.069634	-1.679109
10	6	0	0.122267	-2.925660	0.007859
11	7	0	-4.028424	-1.254638	0.162642
12	6	0	-2.814116	-0.718165	0.093183
13	6	0	-2.813821	0.719275	-0.092915
14	6	0	1.996403	1.490448	0.745007
15	1	0	2.094205	0.443763	1.034258
16	1	0	1.968170	2.068512	1.679030
17	6	0	0.571068	-4.276016	-0.088263
18	1	0	1.596228	-4.602626	-0.212662
19	6	0	-0.338229	-0.720336	0.003121
20	6	0	-0.337925	0.720386	-0.003186
21	6	0	-1.253360	-2.797173	0.148044
22	6	0	-0.485819	-5.142539	0.005272
23	1	0	-0.447978	-6.223542	-0.010342
24	6	0	-1.568621	-1.416351	0.121609
25	6	0	-1.568025	1.416920	-0.121488
26	6	0	3.196124	1.945109	-0.097146
27	1	0	3.277574	1.322519	-0.997465
28	1	0	3.021955	2.965934	-0.457806
29	6	0	-1.252172	2.797612	-0.148052
30	6	0	-0.483563	5.142657	-0.005823
31	1	0	-0.445267	6.223644	0.009715
32	6	0	4.511447	-1.905482	-0.690919
33	1	0	4.420155	-2.543362	-1.581147
34	1	0	4.686401	-0.886887	-1.064732
35	6	0	4.512202	1.903696	0.691164
36	1	0	4.420922	2.541267	1.581616
37	1	0	4.686855	0.884920	1.064620
38	6	0	0.123535	2.925507	-0.008121
39	6	0	0.572959	4.275680	0.087639
40	1	0	1.598279	4.601859	0.211843
41	6	0	3.195241	-1.946321	0.097206
42	1	0	3.020660	-2.967040	0.457962
43	1	0	3.276760	-1.323643	0.997465
44	6	0	5.716591	-2.357382	0.140230
45	1	0	5.857258	-1.715056	1.018060
46	1	0	6.639894	-2.324430	-0.448281
47	1	0	5.586488	-3.384979	0.500374
48	6	0	5.717571	2.355642	-0.139635
49	1	0	5.588034	3.383621	-0.498881
50	1	0	5.857840	1.713993	-1.018026
51	1	0	6.640878	2.321652	0.448811

2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Туре	Х	Y	Z
1	1	0	6.297388	0.105535	-0.087064
2	1	0	4.549416	1.997544	-0.345289
3	1	0	-6.261043	-0.042437	-0.030248
4	1	0	-4.559643	1.905398	0.070955
5	1	0	-0.493027	2.484961	0.834960
6	1	0	-2.131302	2.387188	1.444195

7	1	0	-2.976896	3.251973	-0.804235
8	1	0	-1.319585	3.453086	-1.318859
9	1	0	-0.955388	5.057757	0.640145
10	1	0	-2.070551	5.607450	-0.595506
11	1	0	-2.910368	4.437244	2.132191
12	1	0	-4.029095	4.932910	0.852895
13	1	0	-2.990861	6.129541	1.639568
14	1	0	0.479325	2.410566	-1.172921
15	1	0	2.125488	2.305023	-1.760516
16	1	0	2.929916	3.364950	0.417689
17	1	0	1.262958	3.626178	0.874340
18	1	0	2.609856	4.743795	-1.651098
19	1	0	0.926351	5.007596	-1.229238
20	1	0	3.330140	5.938196	0.460629
21	1	0	1.632806	6.208046	0.880416
22	1	0	2.320521	6.975318	-0.559109
23	6	0	-1.530175	2.349531	0.527572
24	6	0	-1.967252	3.465479	-0.433598
25	6	0	-1.945919	4.866101	0.203943
26	6	0	-3.027130	5.099803	1.267298
27	6	0	1.516056	2.326569	-0.846759
28	6	0	1.928053	3.535094	0.005917
29	6	0	1.923654	4.842372	-0.798320
30	6	0	2.323925	6.059421	0.041796
31	6	0	2.950160	0.461976	-0.074227
32	6	0	4.285321	0.958663	-0.183328
33	6	0	5.224073	-0.026151	-0.058146
34	6	0	2.821727	-0.906381	0.113108
35	6	0	1.445390	-1.219231	0.102904
36	6	0	0.765448	-2.473502	0.127478
37	6	0	-0.669857	-2.497451	-0.047908
38	6	0	-1.379218	-1.261773	-0.124287
39	6	0	-2.762391	-0.983493	-0.156260
40	6	0	-5.184893	-0.150360	-0.051383
41	6	0	-4.270375	0.863750	-0.008298
42	6	0	-2.923487	0.392295	-0.079852
43	6	0	-0.703011	-0.015502	-0.066169
44	6	0	0.740036	0.001719	-0.056840
45	7	0	-1.668769	1.000813	-0.032865
46	7	0	1.681675	1.034875	-0.172256
47	7	0	1.319863	-3.676243	0.241135
48	7	0	-1.195889	-3.718113	-0.062761
49	16	0	0.074562	-4.770944	0.132968
50	34	0	-4.398096	-1.863394	-0.180958
51	34	0	4.478144	-1.741771	0.208546

3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Туре	Х	Y	Z
1	 34	0	4.808783	-0.011061	0.101122
2	16	0	1.598216	-4.318716	-0.340024
3	16	0	1.631822	4.338487	0.328093
4	7	0	3.575826	1.306008	0.275220

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5	7	0	-1.114502	1.689572	-0.130231
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6	7	0	3.573498	-1.311997	-0.156666
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	7	6	0	-0.529849	2.947910	0.012424
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8	6	0	2.398155	0.726720	0.136469
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	9	7	0	-1.138652	-1.633023	-0.080686
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	10	6	0	0.838542	2.802051	0.200042
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	11	6	0	0.818085	-2.771772	-0.269987
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	12	6	0	-0.963372	4 304754	-0.057110
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	13	1	0	-1.980412	4 644947	-0.209126
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	14	-	0	0 096720	5 157624	0 103766
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	15	1	0	0 068425	6 238903	0 121449
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	16	± 6	0	-0 562022	-2 899358	-0 179032
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	17	6	0	-0 083894	0 741382	-0 043399
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1.8	6	0	-1 985555	-1 8/186/	0.0400313
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	10	1	0	5 777102	1 062756	0.400313
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	19	1	0	-J.///IUJ	-1.902730	-0.330097
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20		0	-5.132577	-0.842677	0.834284
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	21	0	0	-2.3/5/89	1.54/693	-0.868092
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	22	1	0	-2.299318	2.150489	-1./83604
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	23	l	0	-2.464532	0.509656	-1.190309
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	24	6	0	2.396/56	-0./1/269	-0.099094
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	25	6	0	1.137498	-1.394183	-0.192192
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	26	6	0	-4.885735	1.980825	-0.933918
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	27	1	0	-5.046144	0.975773	-1.348453
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	28	1	0	-4.741338	2.645604	-1.796997
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	29	6	0	1.144525	1.420262	0.142223
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	30	6	0	-0.091921	-0.698838	-0.094623
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	31	6	0	-3.627585	-1.894845	-0.322346
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32	1	0	-3.657377	-1.252245	-1.210827
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	33	1	0	-3.456903	-2.911265	-0.697200
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	34	6	0	-2.448060	-1.471650	0.565061
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	35	1	0	-2.437897	-2.066228	1.487028
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	36	1	0	-2.548198	-0.429507	0.870559
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37	6	0	0.040437	-5.117257	-0.223184
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	38	1	0	-0.000784	-6.198124	-0.240996
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	39	6	0	-3.613881	1.986581	-0.074757
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	40	1	0	-3.451948	2.994233	0.326448
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	41	1	0	-3.747898	1.336502	0.799422
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42	6	0	-1.017045	-4.250403	-0.138451
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	43	1	0	-2.046549	-4.576702	-0.056850
45 1 0 -5.048003 -3.915460 1.079528 46 1 0 -4.451578 -2.790965 2.309308 47 1 0 -6.173320 -2.845575 1.926961 48 6 0 -6.131870 2.416236 -0.156203 49 1 0 -7.021023 2.411209 -0.796034 50 1 0 -6.326306 1.746395 0.690200 51 1 0 -6.014621 3.430203 0.244775	44	6	0	-5.170311	-2.905700	1.490393
46 1 0 -4.451578 -2.790965 2.309308 47 1 0 -6.173320 -2.845575 1.926961 48 6 0 -6.131870 2.416236 -0.156203 49 1 0 -7.021023 2.411209 -0.796034 50 1 0 -6.326306 1.746395 0.690200 51 1 0 -6.014621 3.430203 0.244775	45	1	0	-5.048003	-3.915460	1 079528
47 1 0 -6.173320 -2.845575 1.926961 48 6 0 -6.131870 2.416236 -0.156203 49 1 0 -7.021023 2.411209 -0.796034 50 1 0 -6.326306 1.746395 0.690200 51 1 0 -6.014621 3.430203 0.244775	46	1	0	-4.451578	-2 790965	2 309308
48 6 0 -6.131870 2.416236 -0.156203 49 1 0 -7.021023 2.411209 -0.796034 50 1 0 -6.326306 1.746395 0.690200 51 1 0 -6.014621 3.430203 0.244775	47	1	0	-6 173320	-2 845575	1 926961
49 1 0 -7.021023 2.411209 -0.796034 50 1 0 -6.326306 1.746395 0.690200 51 1 0 -6.014621 3.430203 0.244775	4.8	÷	0	-6 131870	2 416236	-0 156203
10 1 0 7.021025 2.411205 0.790034 50 1 0 -6.326306 1.746395 0.690200 51 1 0 -6.014621 3.430203 0.244775	49	1	0	-7 021023	2 411209	-0 796034
50 1 0 -6.014621 3.430203 0.244775	50	⊥ 1	0	-6 326306	1 746395	0 690200
	51	⊥ 1	0	-6 014621	3 430203	0 244775
	J± 	ـــــــــــــــــــــــــــــــــــــ		0.014021		