New WOLEDs based on π-extended azatrioxa[8]circulenes

K. B. Ivaniuk,[a] G. V. Baryshnikov[b,c,*], P. Y. Stakhiraa, , S. K. Pedersen,[d] M. Pittelkow[d], A. Lazauskas,[e] D. Volyniuk,[e] J. V. Grazulevicius,[e] B. F. Minaev[b,c] and H. Ågren[b]

[a]*Lviv Polytechnic National University, S. Bandera 12, 79013 Lviv, Ukraine.*
[b]*Division of Theoretical Chemistry and Biology, School of Biotechnology, KTH Royal Institute of Technology, 10691 Stockholm, Sweden*
[c]*Department of Chemistry and Nanomaterials Science, Bohdan Khmelnytsky National University, Shevchenko 81, 18031 Cherkassy, Ukraine*
[d]*Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark.*
[e]*Institute of Materials Science, Kaunas University of Technology, K. Baršausko St. 59, LT51423 Kaunas, Lithuania*

Electronic Supplementary Information

List of Content

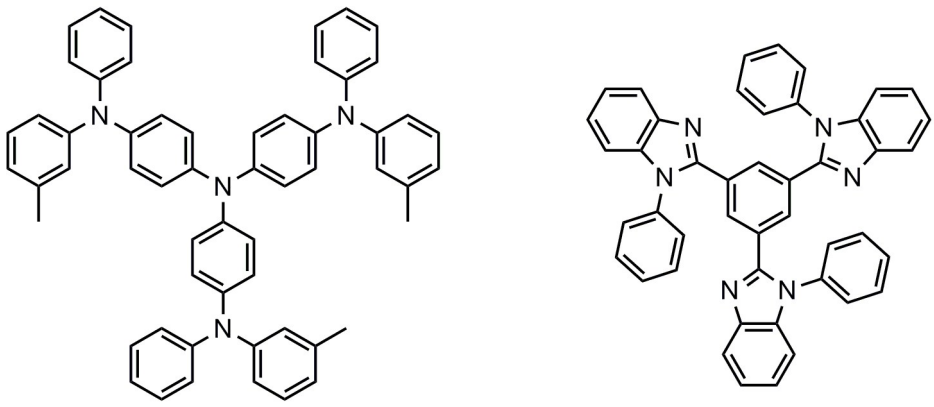

Figure S1. Structures for the exciplex-forming m-MTDATA and electron-transporting TPBi materials.

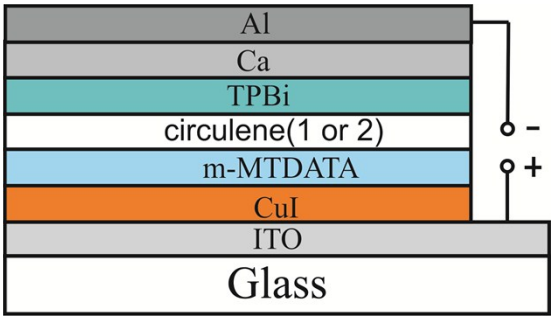

Figure S2. Layer-by-layer scheme of the fabricated devices.

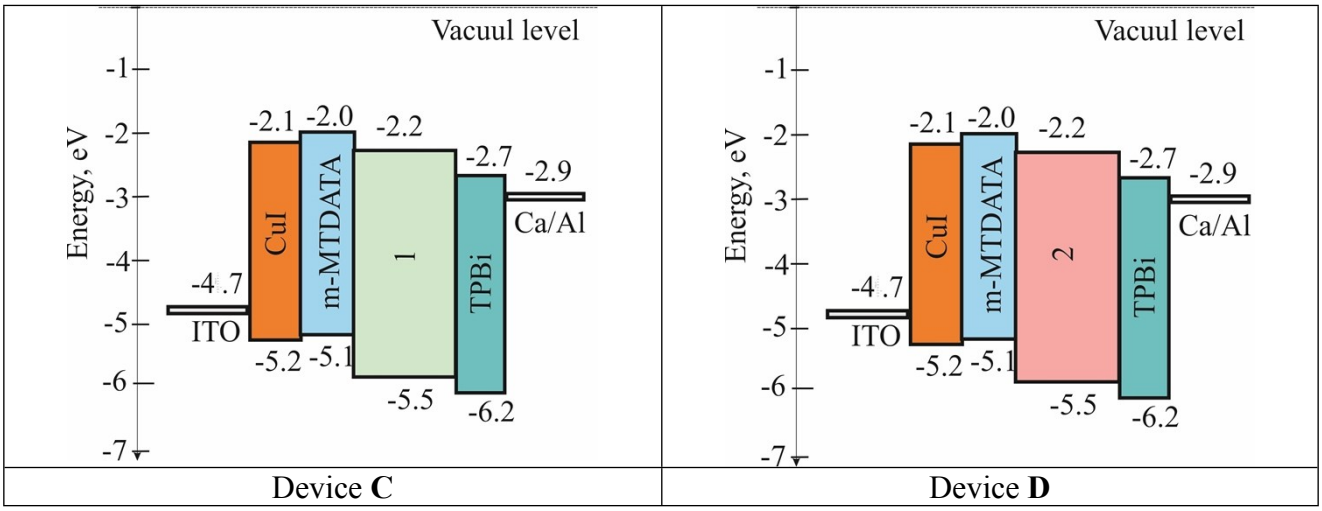

Figure S3. Energy diagram for the devices **C** and **D**

Table S1. Selected electronic transitions for AOC **1** calculated by the parameterized B3LYP/6-31G(d) method (a_X^{HF}=0.14, a_X^{Slater}=0.86) using the PCM model (solvent – dichloromethane).

State	$\lambda_{theor.}$, nm	$\lambda_{exp.}$, nm	*F*	Assignment
S_1	405*	406 386 (0-1) 369 (0-2)	0.265	HOMO → LUMO (+91%)
S_2	403*		0.277	HOMO-1 → LUMO (+88%)
S_9	327	325	0.287	HOMO-4 → LUMO (+50%) HOMO-2 → LUMO+1 (+42%)
S_{12}	304	298	0.253	HOMO-2 → LUMO+2 (+54%) HOMO-3 → LUMO+1 (+31%)
S_{13}	301		0.366	HOMO-3 → LUMO+2 (+66%) HOMO-4 → LUMO+1 (16%) HOMO-2 → LUMO+1 (12%)

* Singlet excited states S1 and S2 are strictly degenerate for the symmetrical (C_{2v}) model of compound 1 without side substituents. This is due to the fact that frontier HOMO and HOMO-1 orbitals are strictly degenerate within the C_{2v} symmetry point group. In the case of substituted AOC **1** these orbitals are quasidegenerate and therefore S1 and S2 electronic states are slightly split (only by 2 nm) with the different oscillator strength values. The same conclusion is also valid for the S_{12} and S_{13} states.

Table S2. Selected electronic transitions for the AOC **2** calculated by the parameterized B3LYP/6-31G(d) method (a_X^{HF}=0.14, a_X^{Slater}=0.86) using PCM model (solvent – dichloromethane).

State	$\lambda_{theor.}$, nm	$\lambda_{exp.}$, nm	*f*	Assignment
S_1	409*	404, 382 (0-1) 366 (0-2)	0.298	HOMO → LUMO (96%)
S_2	403*		0.332	HOMO-1 → LUMO (92%)
S_9	331	325	0.304	HOMO-2 → LUMO+1 (48%) HOMO-4 → LUMO+0 (42%)
S_{12}	309	299	0.415	HOMO-3 → LUMO+2 (52%) HOMO-2 → LUMO+2 (15%)
S_{13}	308		0.347	HOMO-2 → LUMO+2 (44%) HOMO-3 → LUMO+1 (19%) HOMO-3 → LUMO+2 (18%)

* See footnotes below Table S1.

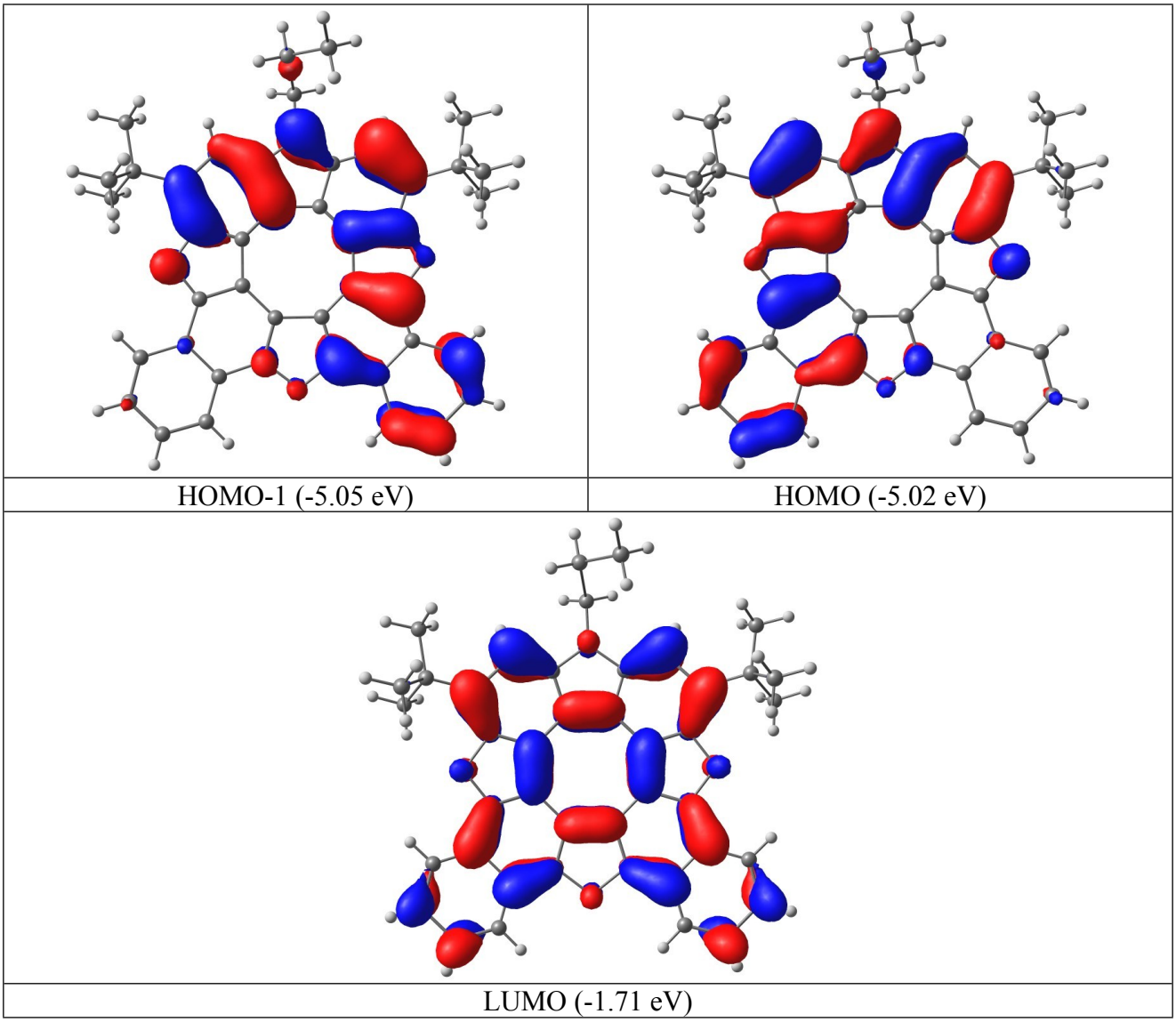

Figure S4. Shapes of frontier molecular orbitals of AOC **1** calculated by the parameterized B3LYP/6-31G(d) method (a_X^{HF}=0.14, a_X^{Slater}=0.86)

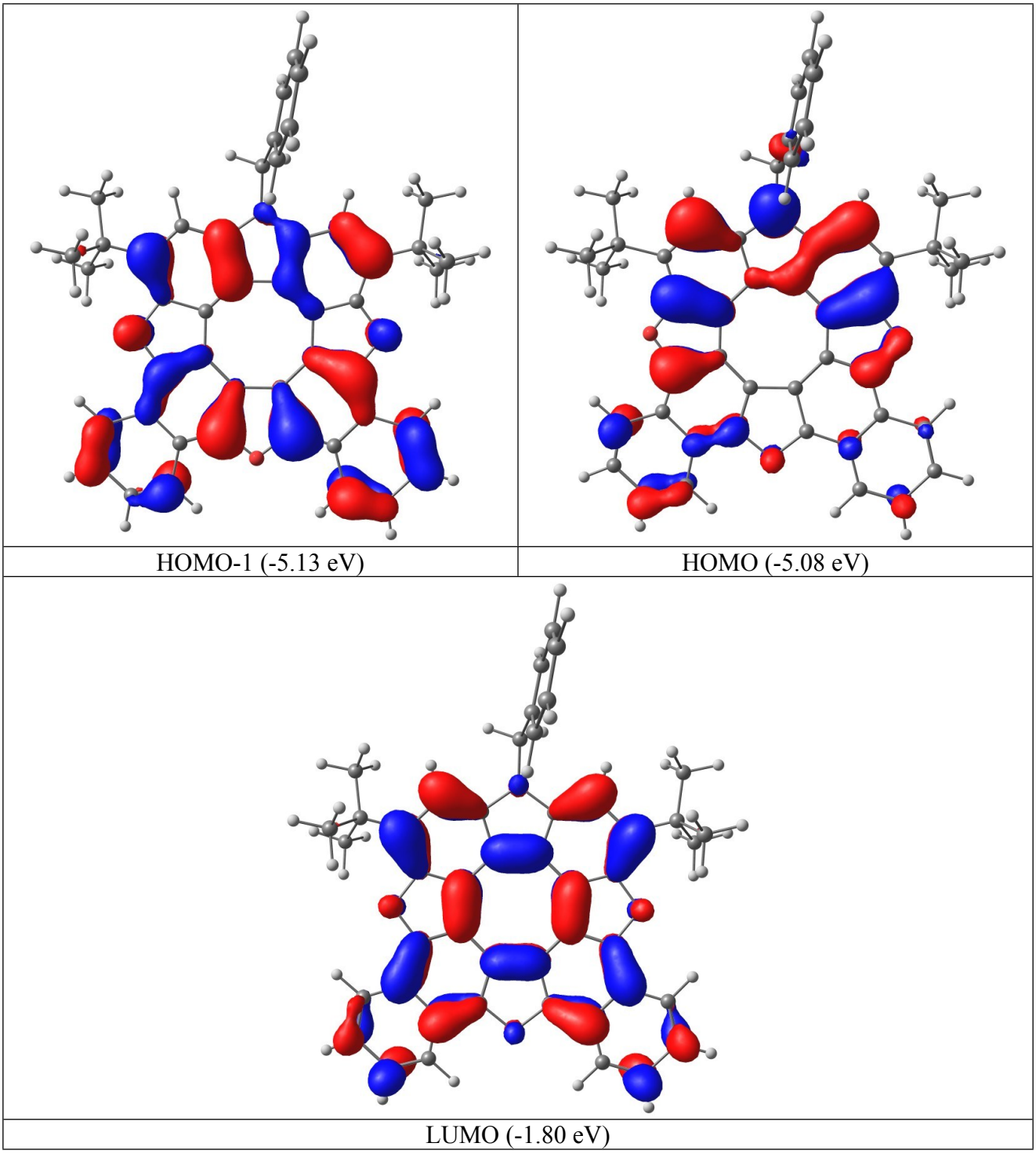

Figure S5. Shapes of frontier molecular orbitals of AOC **2** calculated by the parameterized B3LYP/6-31G(d) method (a_X^{HF}=0.14, a_X^{Slater}=0.86)

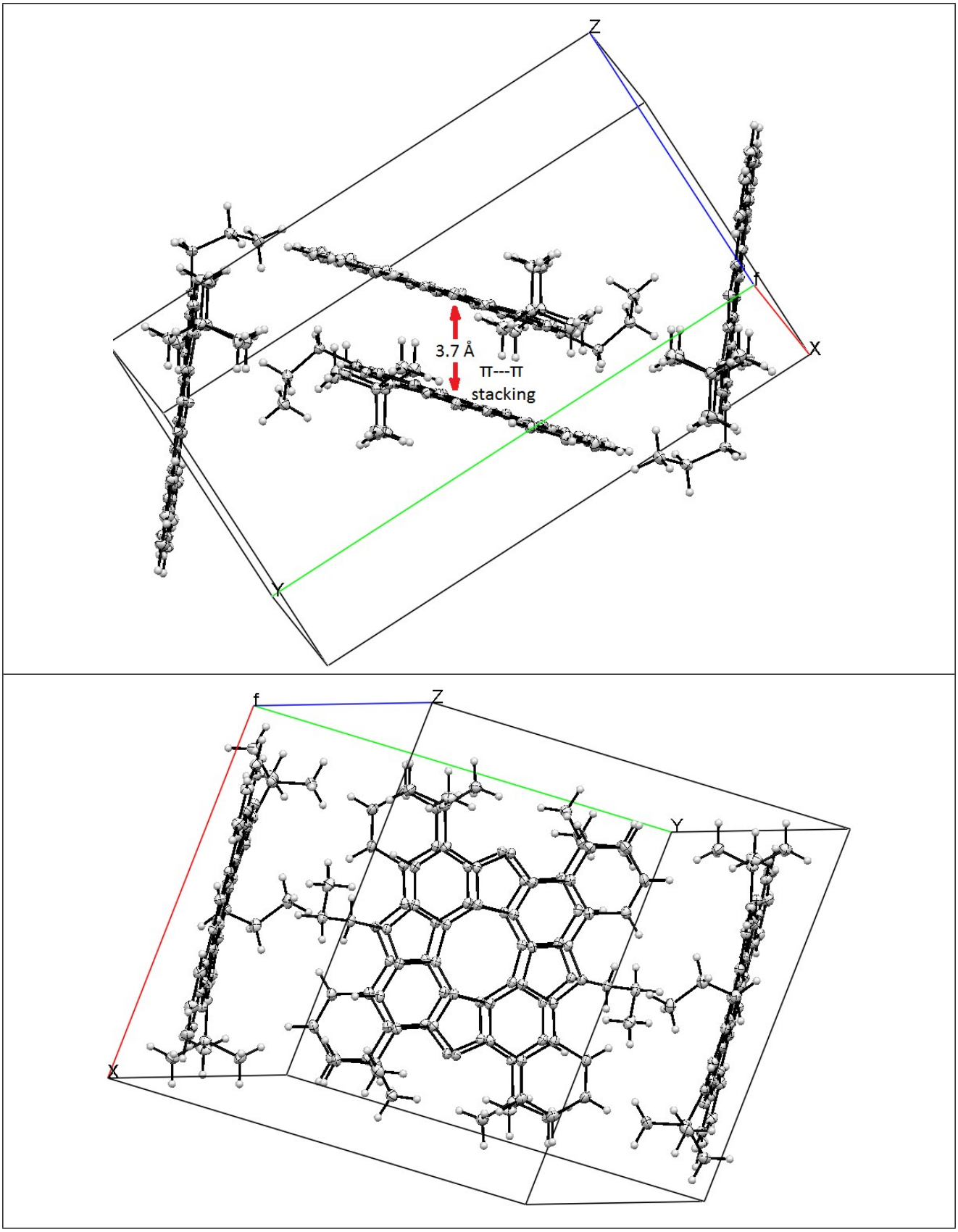

Figure S6. X-ray data for crystal packing of AOC **1** (side and top view)

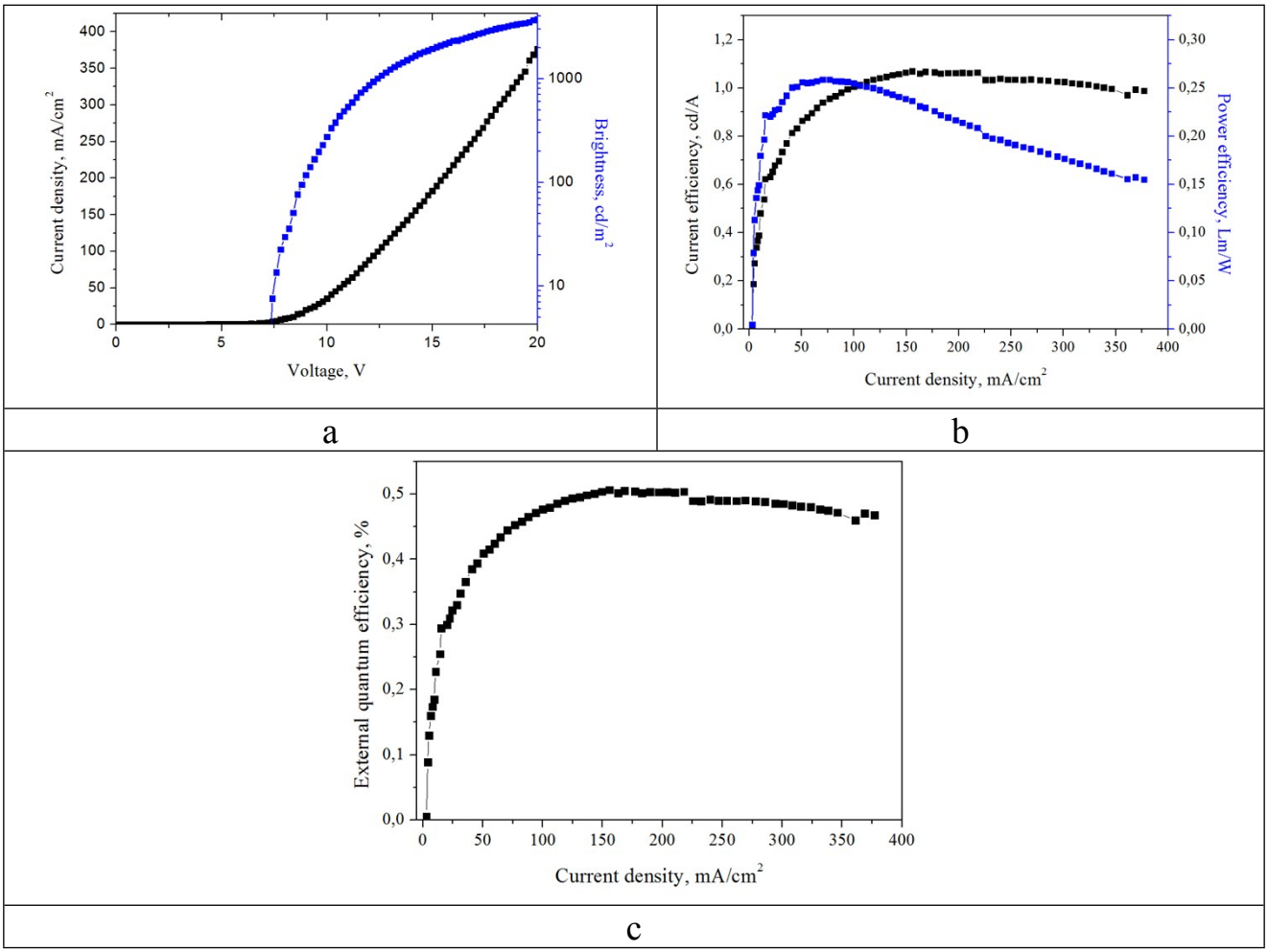

Figure S7. Current density and brightness vs. voltage (a), current and power efficiency vs. current density (b), external quantum efficiency vs. current density (c) characteristics of the device **A**.

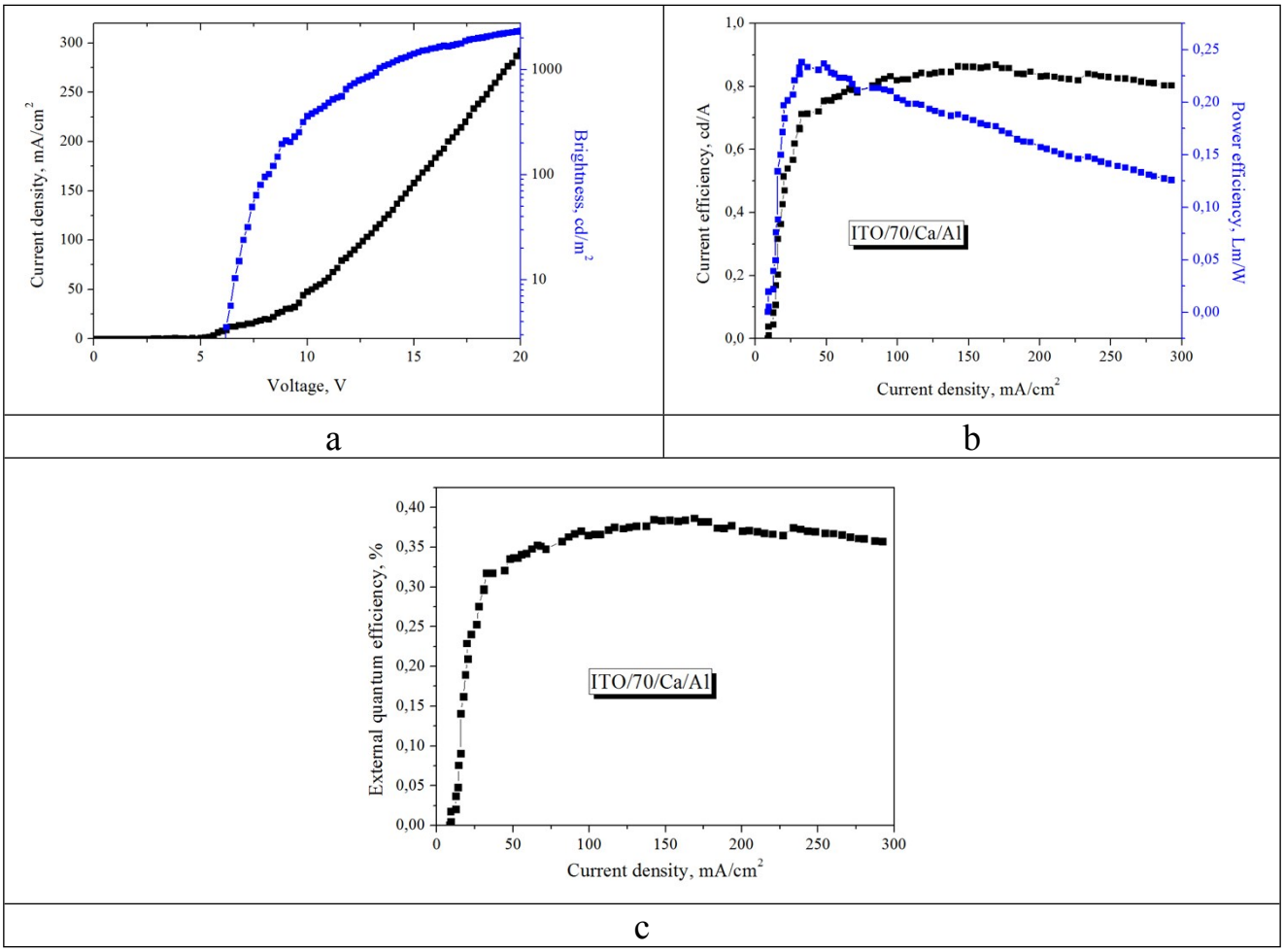

Figure S8. Current density and brightness *vs.* voltage (a), current and power efficiency *vs.* current density (b), current efficiency *vs.* quantum density (c) characteristics of the device **B**.

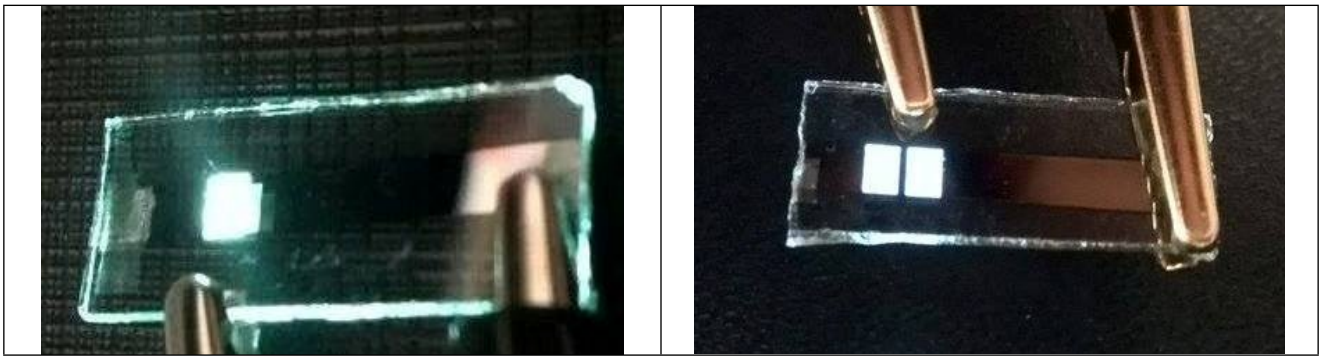

Figure S9. Photos of devices C (left) and D (right) at 10 V.

Table S3. Cartesian coordinates for the compound **1** optimized by the DFT/B3LYP/6-31G(d) method.

7	-0.280246000	-3.509765000	-0.520357000
8	3.901581000	0.001219000	-0.049206000
8	0.375638000	4.168869000	0.057043000
8	-3.810080000	0.659920000	-0.059333000
6	3.305102000	-2.412733000	-0.180653000
6	0.609060000	-1.427748000	-0.338132000
6	3.698621000	2.461577000	0.021026000
6	1.398930000	3.241233000	-0.015705000
6	-2.872589000	1.672743000	-0.043610000
6	-0.520277000	2.075915000	-0.093302000
6	-3.193319000	3.054575000	0.028104000
6	-1.721062000	-0.247938000	-0.246157000
6	3.149681000	1.158705000	-0.057337000
6	-2.094100000	3.973736000	0.047059000
6	2.777283000	3.560767000	0.025304000
6	-0.808098000	-1.305191000	-0.356519000
6	1.807361000	0.884212000	-0.145640000
6	1.683820000	-0.538132000	-0.227766000
6	-0.789896000	3.424032000	0.008063000
6	-1.596635000	1.170440000	-0.133693000
6	0.901039000	1.960578000	-0.110190000
6	0.910958000	-2.796086000	-0.423311000
6	-3.079852000	-0.524069000	-0.193083000
6	-2.714884000	-2.855089000	-0.385858000
1	-3.030153000	-3.748380000	-0.453985000
6	-1.332489000	-2.605390000	-0.452343000
6	-3.630761000	-1.820416000	-0.222528000
6	5.074697000	2.729135000	0.109412000
1	5.693481000	2.007819000	0.120009000
6	4.637104000	5.098332000	0.166481000
1	4.966013000	5.988663000	0.206048000
6	2.223153000	-3.280008000	-0.346331000
1	2.379664000	-4.214168000	-0.408388000
6	2.979065000	-1.042316000	-0.165491000
6	-0.364870000	-4.938827000	-0.789125000
1	0.353902000	-5.185249000	-1.423023000
1	-1.230178000	-5.128791000	-1.230184000
6	4.720160000	-2.902169000	0.094478000
6	-5.110384000	-2.083960000	0.061135000
6	5.535917000	4.021614000	0.181725000
1	6.469323000	4.187771000	0.242109000
6	-4.726439000	4.916301000	0.119317000
1	-5.616401000	5.247945000	0.139043000
6	-5.352932000	-1.746120000	1.544976000
1	-6.295351000	-1.901088000	1.765388000
1	-5.130849000	-0.805685000	1.706218000
1	-4.787747000	-2.316858000	2.107001000
6	3.286868000	4.874865000	0.095790000
1	2.688264000	5.611927000	0.094768000

6	4.833556000	-4.421812000	-0.054897000
1	5.756529000	-4.700157000	0.124222000
1	4.586508000	-4.680285000	-0.966919000
1	4.230435000	-4.858074000	0.582234000
6	-2.359853000	5.356227000	0.099653000
1	-1.638694000	5.974389000	0.113455000
6	-4.506486000	3.561702000	0.079914000
1	-5.243470000	2.962993000	0.087177000
6	-3.650459000	5.814734000	0.130759000
1	-3.818190000	6.750463000	0.160040000
6	5.731661000	-2.251291000	-0.854055000
1	6.629935000	-2.586737000	-0.653784000
1	5.712336000	-1.278827000	-0.735228000
1	5.499418000	-2.471088000	-1.780193000
6	5.068964000	-2.534450000	1.550285000
1	5.979159000	-2.836644000	1.753989000
1	4.434782000	-2.969937000	2.158597000
1	5.014956000	-1.561543000	1.663413000
6	-5.478759000	-3.551828000	-0.169501000
1	-6.432555000	-3.681520000	0.016456000
1	-4.947704000	-4.119649000	0.427376000
1	-5.291550000	-3.792410000	-1.101193000
6	-1.409116000	-5.643944000	1.409892000
1	-1.274626000	-6.222282000	2.189106000
1	-2.243090000	-5.891199000	0.959277000
1	-1.460130000	-4.709410000	1.700915000
6	-0.246098000	-5.812006000	0.447968000
1	-0.194328000	-6.760631000	0.168827000
1	0.595075000	-5.590164000	0.919789000
6	-6.021094000	-1.218474000	-0.814813000
1	-6.957821000	-1.416317000	-0.607847000
1	-5.846986000	-1.413217000	-1.759791000
1	-5.840632000	-0.271923000	-0.638268000

Table S4. Cartesian coordinates for the compound **2** optimized by the DFT/B3LYP/6-31G(d) method.

1	0.783504000	-7.006458000	-1.479190000
1	1.002385000	-5.405072000	1.237843000
1	0.172243000	-6.955858000	0.959991000
1	-0.736556000	-5.572351000	1.639592000
1	-3.524910000	5.927225000	-1.624262000
1	-1.861613000	5.332968000	-1.420597000
1	-2.932376000	4.595451000	-2.660220000
1	-1.494504000	-7.190116000	-0.904884000
1	-1.914134000	-5.787933000	-1.922317000
1	-2.434122000	-5.846002000	-0.200959000
1	-2.569821000	-3.836836000	-0.828332000
1	-4.264065000	1.411404000	-0.902545000
1	-4.986716000	3.291177000	-1.921453000
1	-5.311217000	3.069499000	-0.165005000
1	-5.438105000	4.687790000	-0.906596000
6	-2.892522000	5.028919000	-1.650786000
6	-3.311280000	4.637885000	0.782691000
6	-4.878354000	3.744008000	-0.922631000
6	-3.404095000	4.023826000	-0.617438000
6	0.051197000	-5.864412000	0.930189000
6	0.775374000	-5.907737000	-1.457802000
6	-0.313344000	-5.428196000	-0.492806000
6	-1.625666000	-6.099781000	-0.905663000
6	-0.430833000	-3.918269000	-0.521146000
6	4.745501000	-1.117484000	0.455469000
6	2.578102000	-0.016211000	0.034322000
1	-4.234266000	-2.514207000	-1.216056000
1	-3.397390000	-0.832123000	1.685387000
6	-4.493795000	-0.993372000	1.575799000
1	-4.873632000	-0.677102000	3.682630000
6	-5.316183000	-0.908377000	2.703935000
6	-6.687948000	-1.120492000	2.587552000
6	-7.246721000	-1.396445000	1.340327000
6	-6.430444000	-1.464817000	0.210395000
6	-5.049197000	-1.279396000	0.327511000
1	-6.885608000	-1.673667000	-0.782234000
1	-8.327851000	-1.562718000	1.248199000
1	-7.330458000	-1.068328000	3.486285000
6	-4.230572000	-1.438150000	-0.928453000
1	-4.699040000	-0.839742000	-1.742529000
7	-2.837064000	-1.015379000	-0.840891000
6	-1.708020000	-1.861262000	-0.674978000
6	-0.571374000	-1.037701000	-0.531242000
6	-1.011117000	0.319186000	-0.579416000
6	-2.409766000	0.331729000	-0.740375000
6	-3.180671000	1.495660000	-0.788507000
6	-2.588171000	2.751175000	-0.657053000
6	-1.191023000	2.740312000	-0.505695000
6	-0.415231000	1.556891000	-0.468693000

6	0.932321000	1.974984000	-0.227071000
6	0.898155000	3.371302000	-0.125961000
8	-0.397529000	3.868396000	-0.316010000
6	2.041882000	4.155821000	0.138578000
6	3.279645000	3.513772000	0.283671000
6	3.298262000	2.108010000	0.216167000
6	2.147624000	1.339460000	-0.035929000
6	3.947421000	0.022637000	0.334604000
8	4.428828000	1.327079000	0.421457000
6	4.145685000	-2.389361000	0.339668000
6	2.750941000	-2.405336000	0.089966000
6	1.970091000	-1.253436000	-0.090718000
8	1.983516000	-3.552826000	-0.073891000
6	0.691629000	-3.093645000	-0.332550000
6	0.635744000	-1.681258000	-0.351917000
6	-1.649504000	-3.258348000	-0.689965000
6	1.969944000	5.574237000	0.224429000
6	4.983139000	-3.531758000	0.337017000
6	6.141968000	-0.952550000	0.533883000
6	6.357309000	-3.347832000	0.366645000
6	6.931028000	-2.070291000	0.453535000
6	4.462498000	4.278396000	0.442636000
6	3.137920000	6.290516000	0.367969000
6	4.397649000	5.644941000	0.453789000
1	0.969864000	6.000935000	0.253396000
1	3.077951000	7.386113000	0.366312000
1	5.351728000	6.126765000	0.546138000
1	5.459529000	3.813282000	0.423736000
1	6.588066000	0.049846000	0.570694000
1	8.010013000	-1.942149000	0.452787000
1	7.086405000	-4.157912000	0.312756000
1	4.571962000	-4.549928000	0.262302000
1	-3.908239000	5.559885000	0.812095000
1	-3.701894000	3.939225000	1.537248000
1	-2.268683000	4.890761000	1.023577000
1	0.584504000	-5.532077000	-2.472804000
1	1.766799000	-5.571785000	-1.120899000