Supporting Information

A Quantum-Chemical Insight into SOMO-HOMO Conversion in Phosphorus-Boron Cation Radicals

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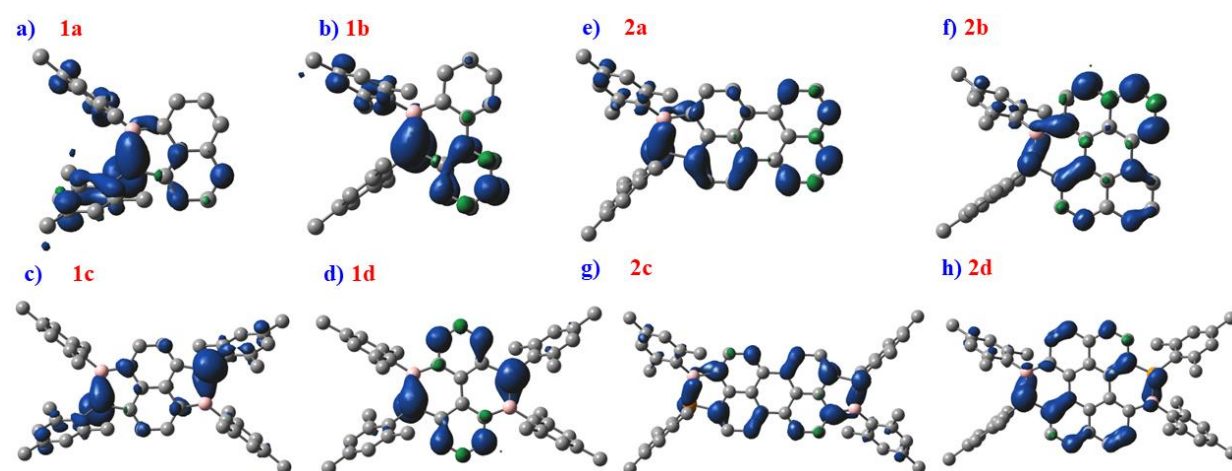*E-mail:* zhangli@gxust.edu.cn, zhangsf@ gxust.edu.cn

Fig. S1 Spin density plots (isosurface value=0.02 a.u.) of the studied **1a**-**1d** and **2a**-**2d** radicals calculated in UB3LYP-D3/6-31G* level.
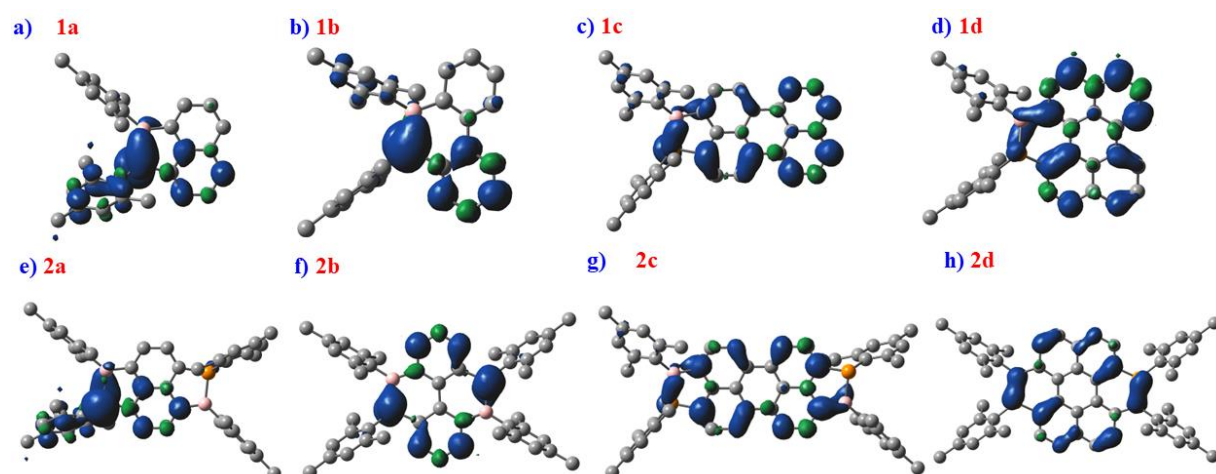

Fig. S2 Spin density plots (isosurface value=0.02 a.u.) of the studied **1a**-**1d** and **2a**-**2d** radicals calculated at UωB97XD/6-31G* level.
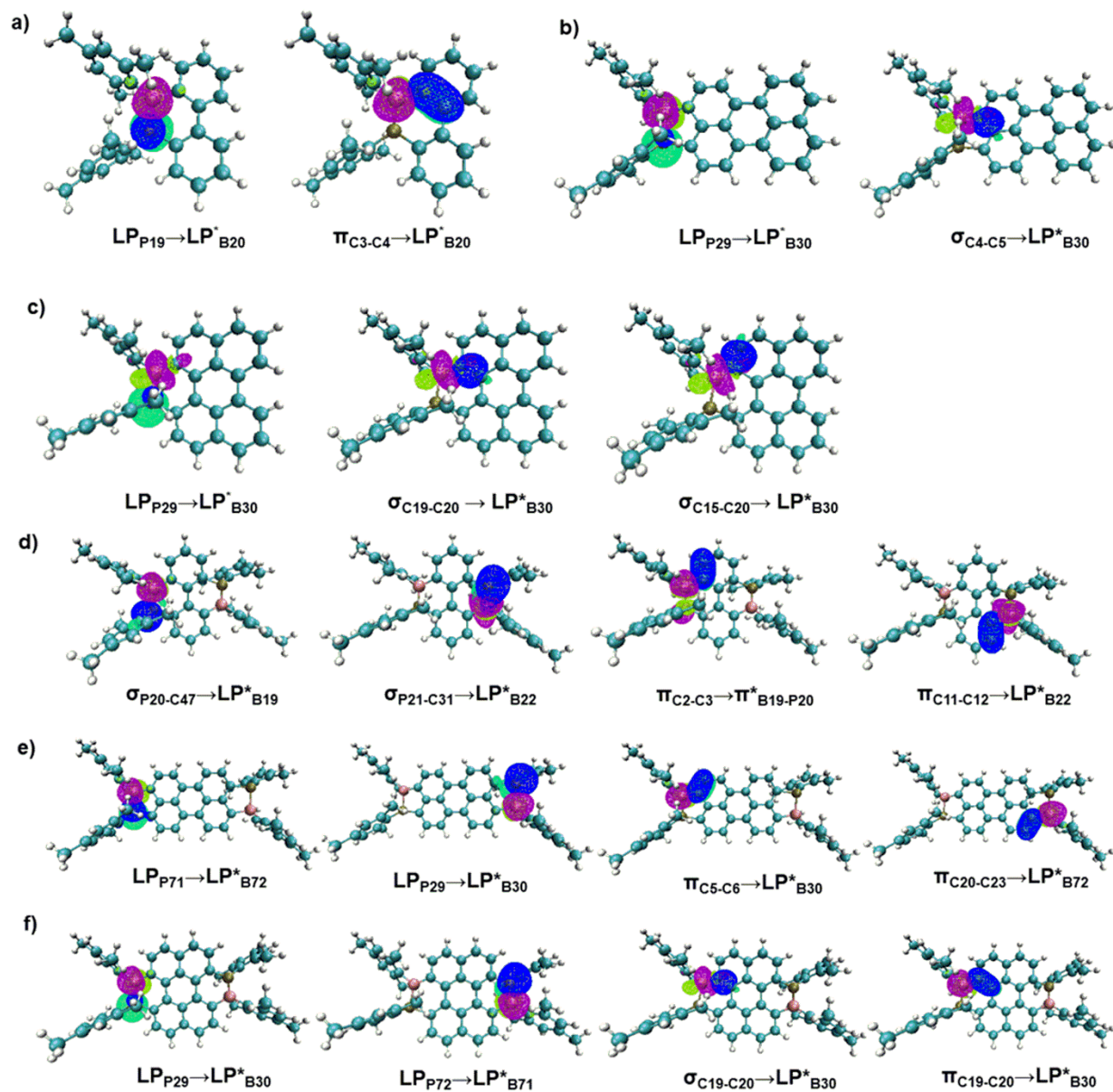
Fig. S3 NBO plots of principal donor-acceptor interactions in **1b** (a), **1c** (b), **1d** (c), **2b** (d), **2c** (e), and **2d** (f).

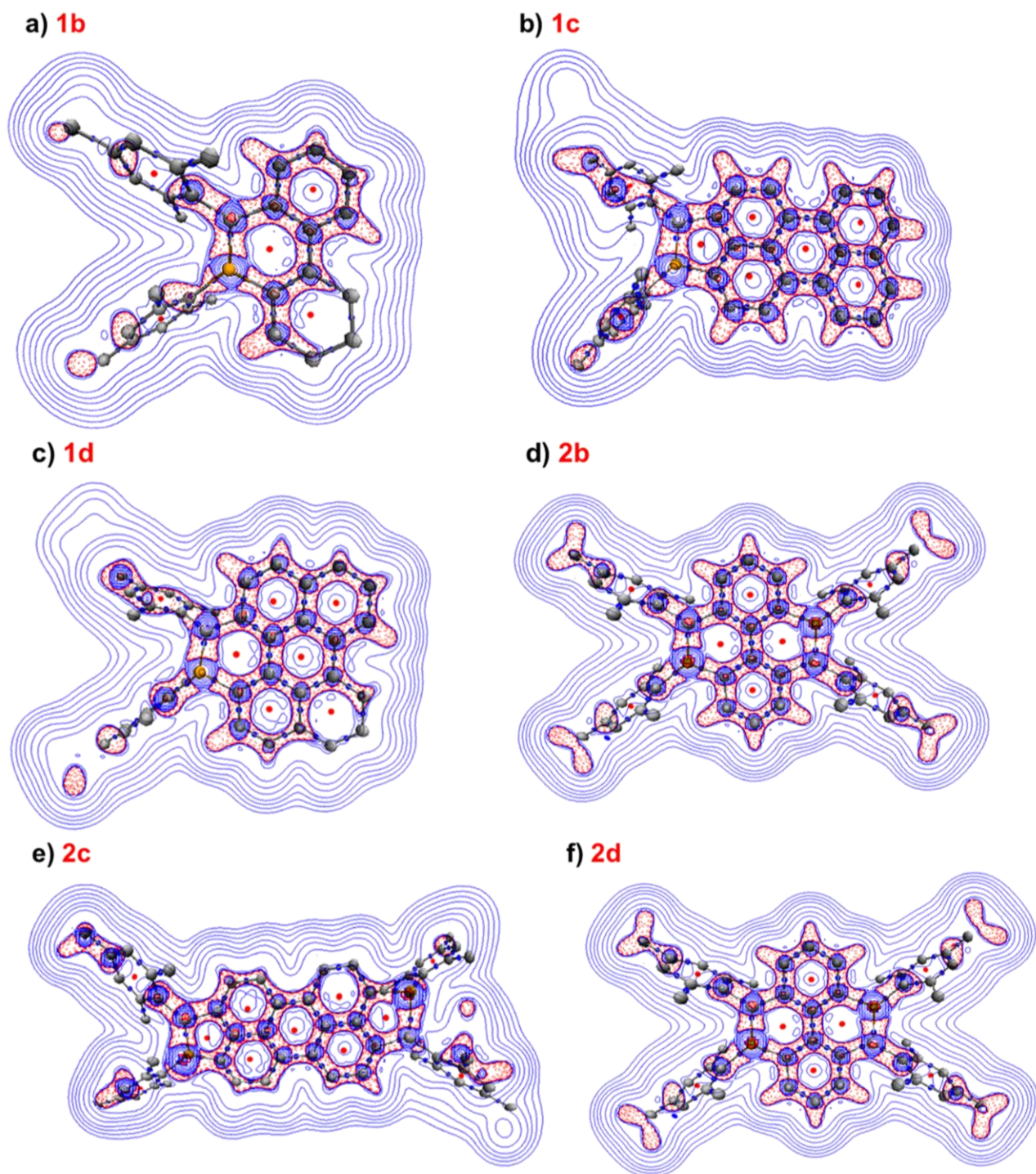**Fig. S4** Plots of the Laplacian $\nabla^2\rho(r)$ and critical points of studied compounds. Solid blue lines demonstrate areas of charge depletion ($\nabla^2\rho(r) > 0$), red dashed lines show areas of charge concentration ($\nabla^2\rho(r) < 0$). Blue dots are bond critical points, red dots are ring critical points.
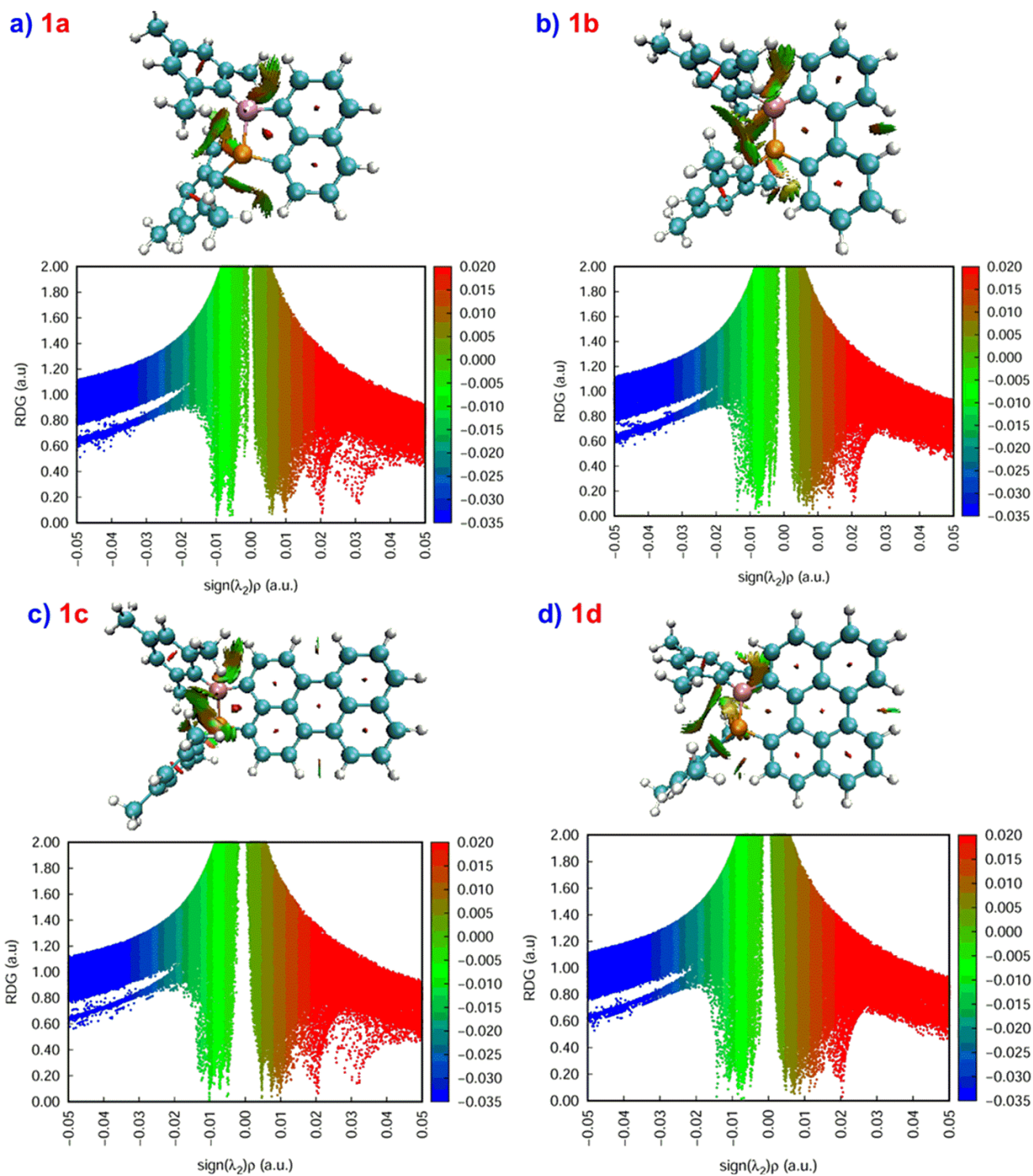
Fig. S5 3D color filled RDG isosurfaces and NCI-RDG 2D scatter maps of complexes **1a-1d**, respectively.
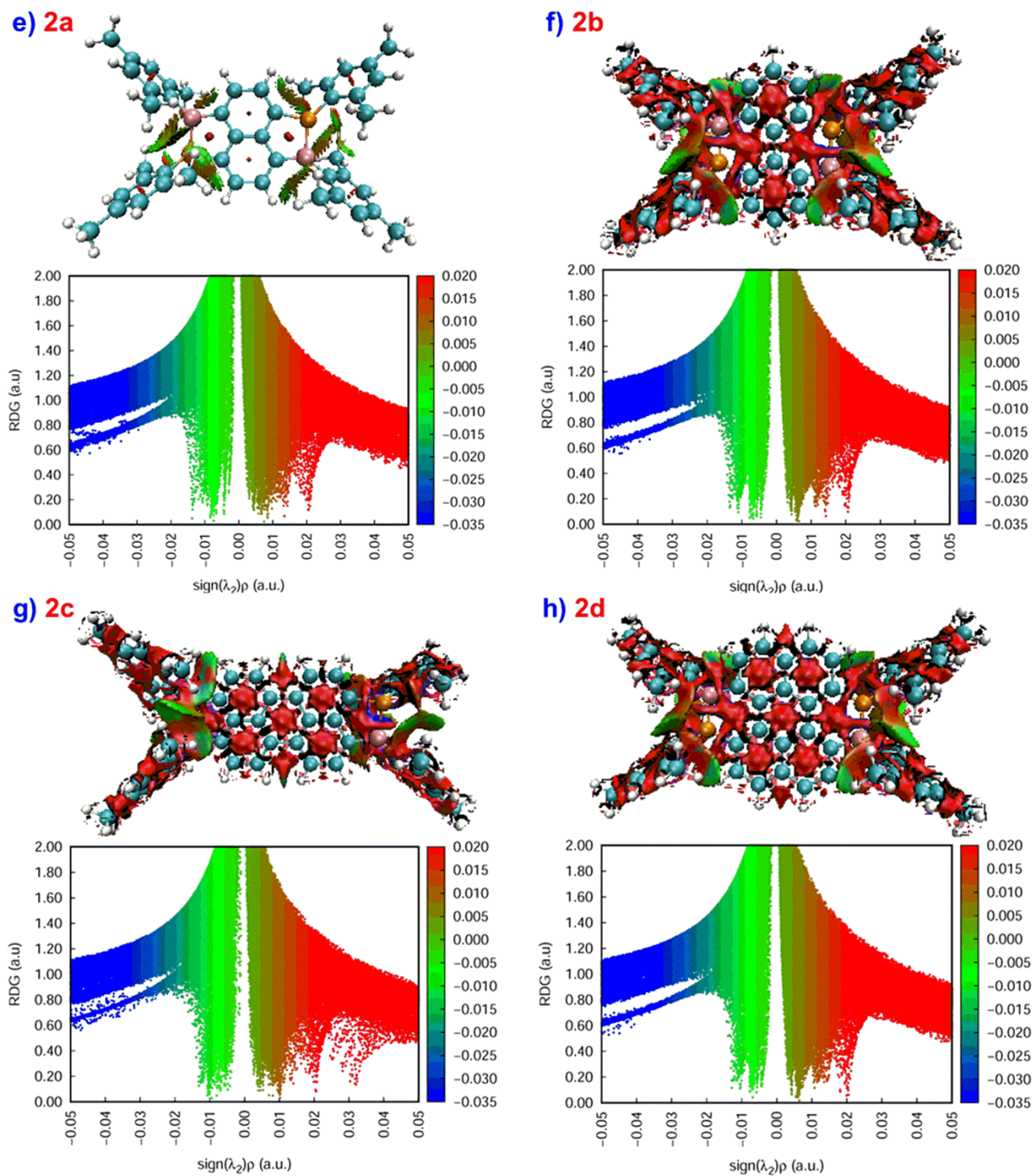
Fig. S6 3D color filled RDG isosurfaces and NCI-RDG 2D scatter maps of complexes **2a-2d**, respectively.

Table S1 Calculated excited wavelengths (λ), oscillator strengths (*f*) and the transition nature of the selected transitions of studied compounds at TD-DFT//UM06-2X-D3/6-31G* level.

Compounds	Excited state	Wavelength/nm	*f*	Dominant Excitations	
1a	D_1	739.3	0.02	HOMO(β)→SOMO(β)	79%

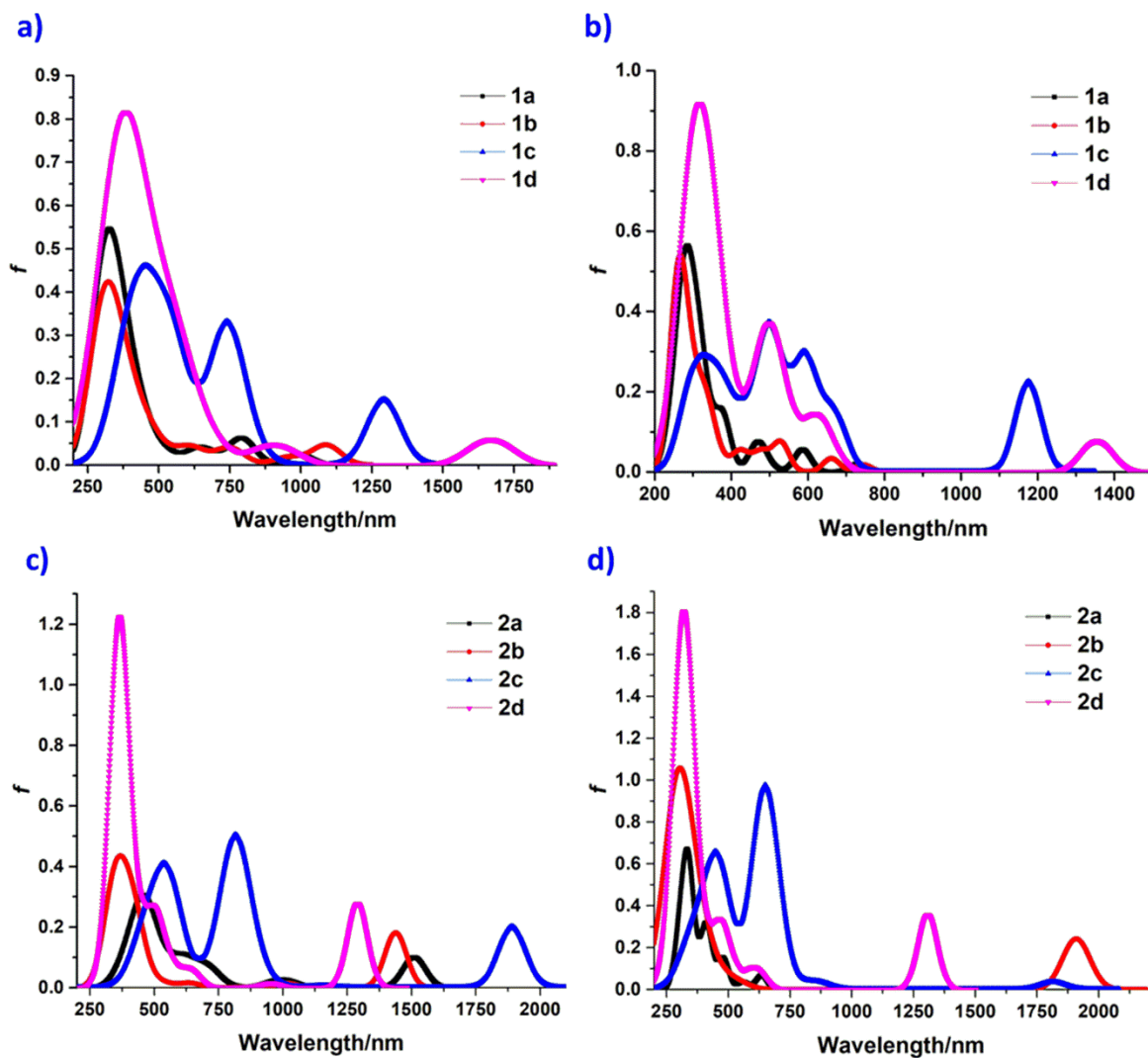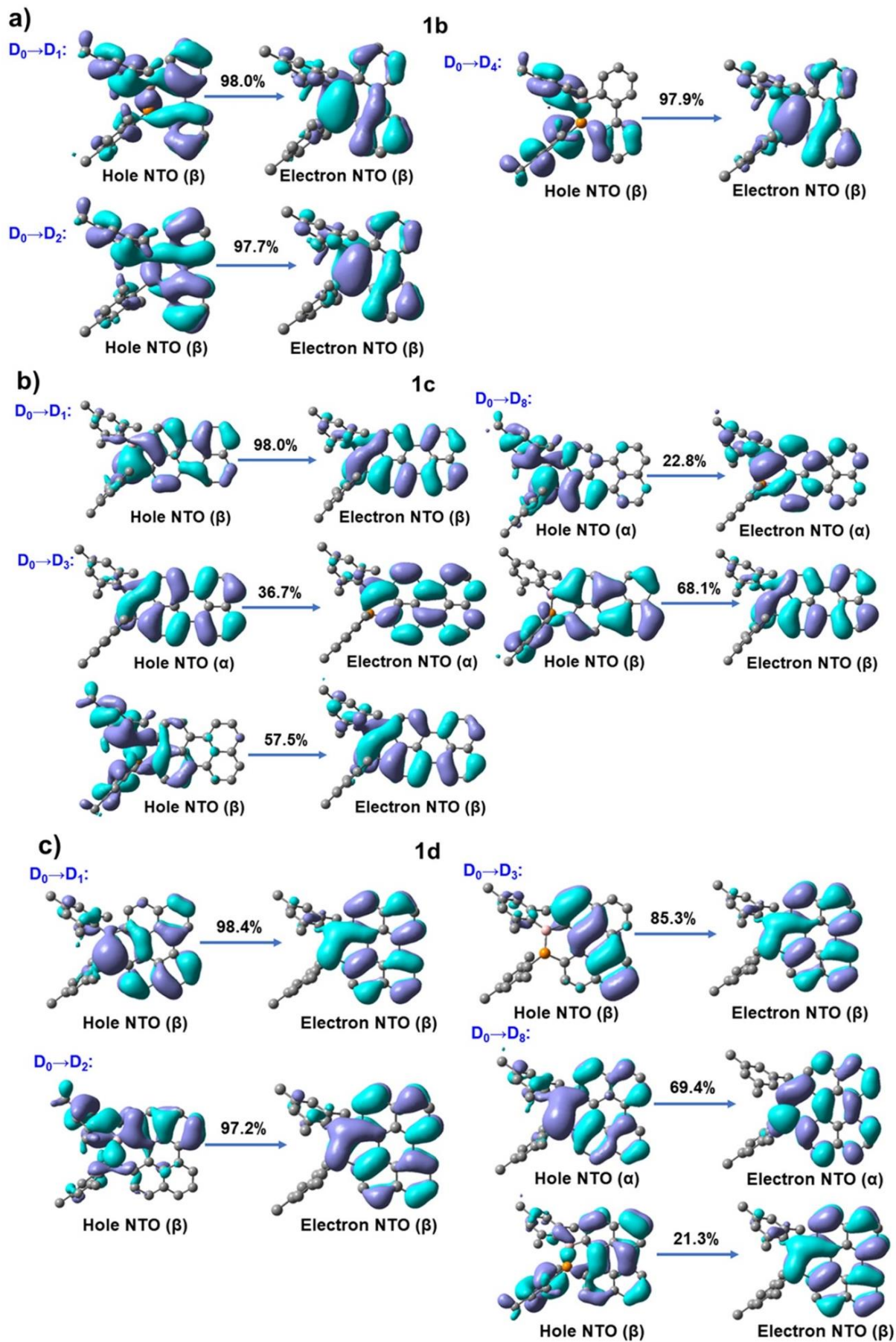|					
	D_2	601.9	0.06	HOMO-2(β)→SOMO(β)	63%
1b	D_1	758.0	0.02	HOMO(β)→SOMO(β)	67%
				HOMO-2(β)→SOMO(β)	21%
	D_2	670.0	0.03	HOMO-2(β)→SOMO(β)	66%
				HOMO(β)→SOMO(β)	22%
	D_4	535.6	0.06	HOMO-4(β)→SOMO(β)	87%
1c	D_1	1254.9	0.20	HOMO(β)→SOMO(β)	93%
	D_3	629.2	0.30	HOMO-1(β)→SOMO(β)	47%
				SOMO(α)→LUMO(α)	34%
	D_8	497.2	0.37	HOMO-6(β)→SOMO(β)	33%
				SOMO(α)→LUMO(α)	12%
1d	D_1	1534.4	0.07	HOMO(β)→SOMO(β)	92%
	D_2	674.8	0.07	HOMO-1(β)→SOMO(β)	38%
				HOMO-2(β)→SOMO(β)	30%
	D_3	601.9	0.07	HOMO-5(β)→SOMO(β)	73%
	D_8	487.4	0.23	SOMO(α)→LUMO(α)	56%
2a	D_1	850.0	0.03	HOMO(β)→SOMO(β)	78%
	D_2	675.4	0.05	HOMO-3(β)→SOMO(β)	68%
	D_5	511.3	0.06	HOMO(α)→LUMO(α)	36%
				HOMO-7(B)→SOMO(B)	14%
	D_{11}	434.3	0.23	HOMO(β)→LUMO(β)	34%
				HOMO-1(α)→LUMO(α)	24%
2b	D_1	1664.9	0.23	HOMO(β)→SOMO(β)	99%
	D_7	510.1	0.03	HOMO-10(β)→SOMO(β)	41%
				HOMO-9(β)→SOMO(β)	40%
	D_{12}	396.6	0.17	HOMO(α)→LUMO(α)	70%
2c	D_1	1483.6	0.24	HOMO(β)→SOMO(β)	88%
	D_3	706.7	0.21	HOMO(α)→LUMO(α)	73%
	D_4	658.3	0.39	HOMO-2(β)→SOMO(β)	50%
	D_{12}	501.4	0.17	SOMO(α)→LUMO(α)	19%
				HOMO-10(β)→SOMO(β)	16%
				HOMO-12(β)→SOMO(β)	16%
2d	D_2	1320.8	0.36	HOMO(β)→SOMO(β)	95%
	D_5	564.3	0.09	HOMO-10(β)→SOMO(β)	77%
	D_9	491.9	0.06	HOMO-11(β)→SOMO(β)	58%
	D_{13}	445.8	0.27	HOMO(α)→LUMO(α)	74%

Fig. S7 Calculated UV-vis absorption spectra of the studied compounds performed at UB3LYP-D3/6-31G(d)+SMD (a, b) and UωB97XD/6-31G(d)+SMD (c, d), respectively.

a)

$D_0 \rightarrow D_1$:

98.0%

Hole NTO (β)   Electron NTO (β)

$D_0 \rightarrow D_2$:

97.7%

Hole NTO (β)   Electron NTO (β)

1b

$D_0 \rightarrow D_4$:

97.9%

Hole NTO (β)   Electron NTO (β)

b)

$D_0 \rightarrow D_1$:

98.0%

Hole NTO (β)   Electron NTO (β)

$D_0 \rightarrow D_3$:

36.7%

Hole NTO (α)   Electron NTO (α)

57.5%

Hole NTO (β)   Electron NTO (β)

1c

$D_0 \rightarrow D_8$:

22.8%

Hole NTO (α)   Electron NTO (α)

68.1%

Hole NTO (β)   Electron NTO (β)

c)

$D_0 \rightarrow D_1$:

98.4%

Hole NTO (β)   Electron NTO (β)

$D_0 \rightarrow D_2$:

97.2%

Hole NTO (β)   Electron NTO (β)

1d

$D_0 \rightarrow D_3$:

85.3%

Hole NTO (β)   Electron NTO (β)

$D_0 \rightarrow D_8$:

69.4%

Hole NTO (α)   Electron NTO (α)

21.3%

Hole NTO (β)   Electron NTO (β)
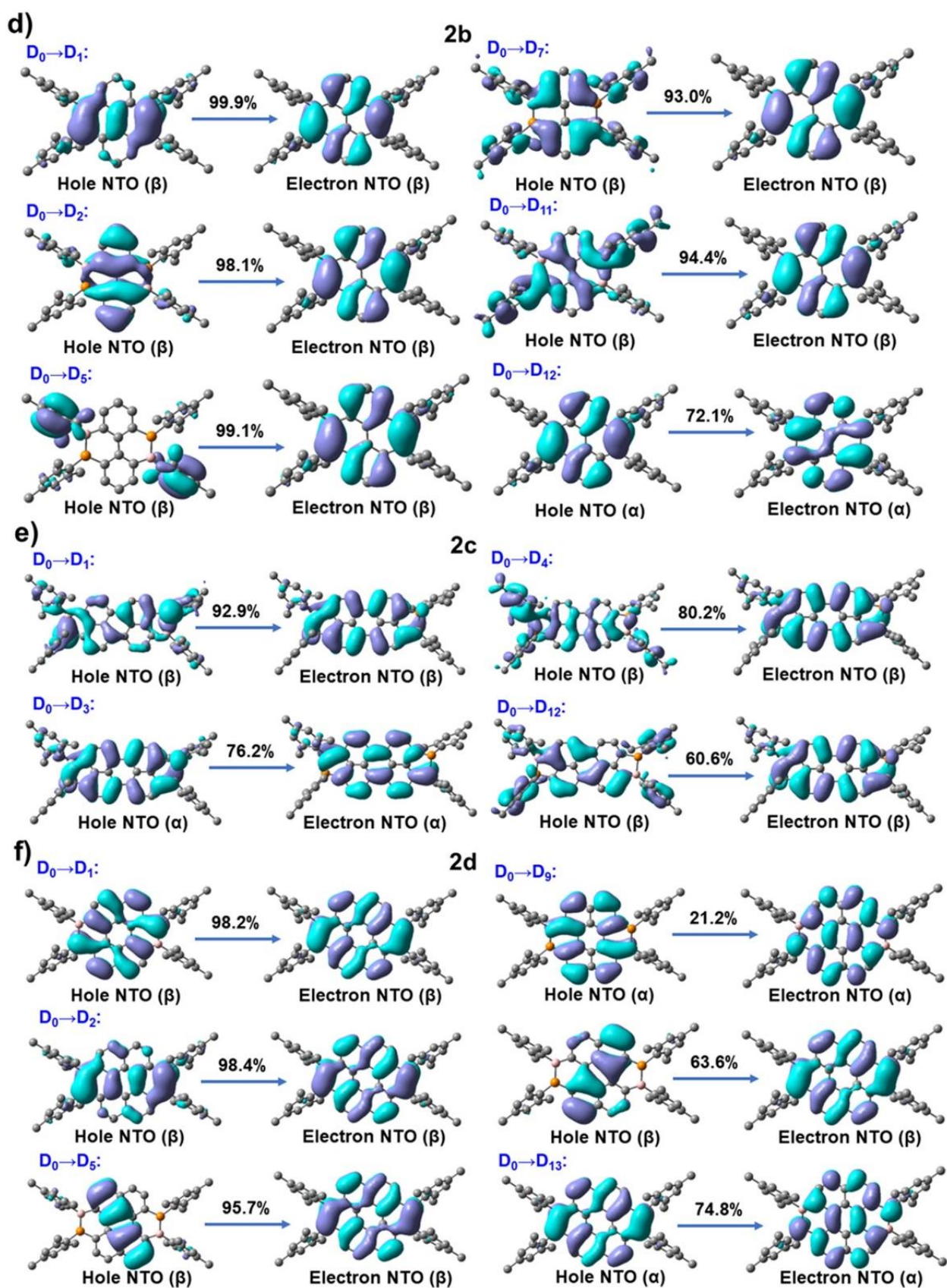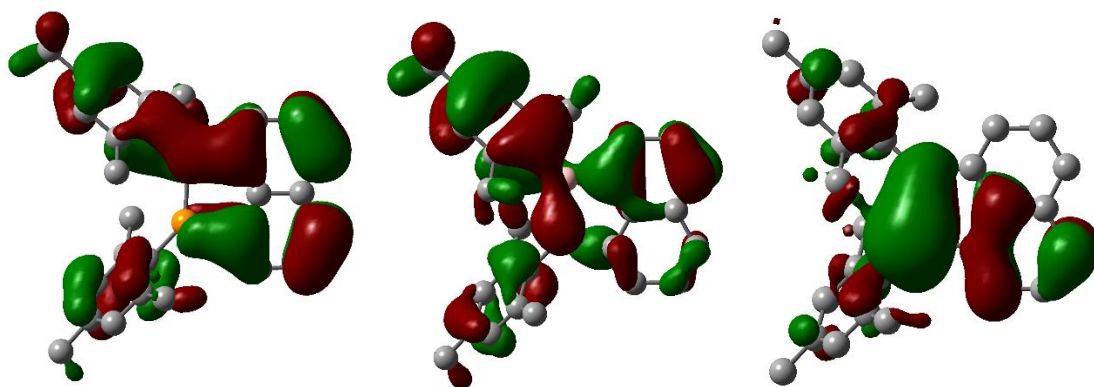
Fig. S8 Natural transition orbitals (NTOs) of the studied radicals.
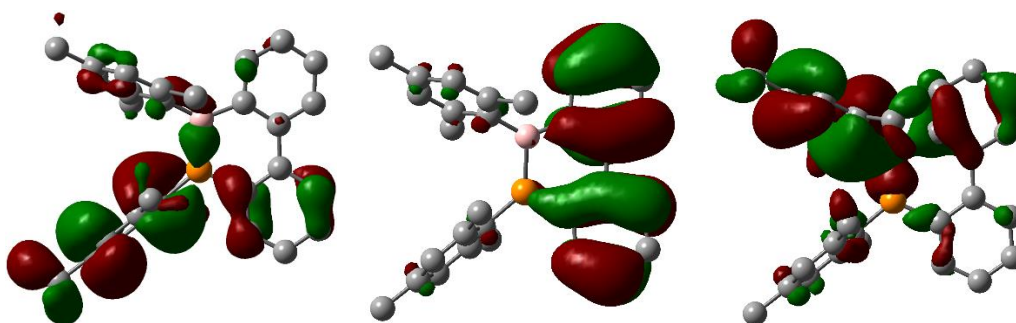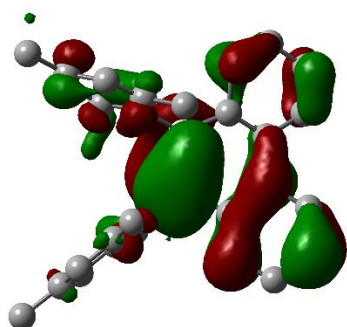
1a

HOMO-2(β)   HOMO(β)   SOMO(β)
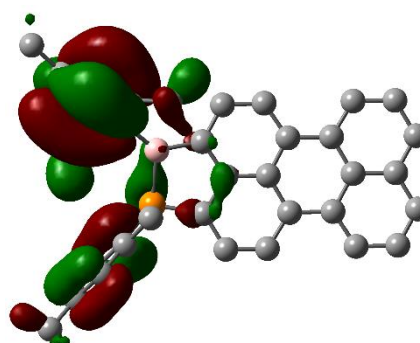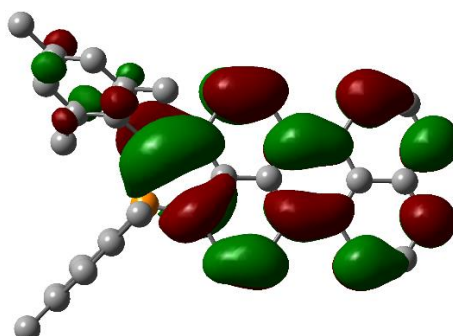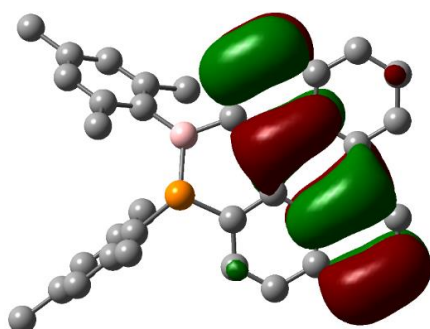
1b

HOMO-4(β)   HOMO-2(β)   HOMO(β)

SOMO(β)

1c

HOMO-6(β)   HOMO-1(β)

HOMO(β)

SOMO(β)

SOMO(α)

LUMO(α)

1d

HOMO-5(β)

HOMO-2(β)

HOMO-1(β)

HOMO(β)

SOMO(β)

SOMO(α)

LUMO(α)

2a

HOMO-3(β)

HOMO(β)

SOMO(β)

LUMO(β)

HOMO-1(α)

HOMO(α)

LUMO(α)

2b

HOMO-10(β)

HOMO-9(β)

HOMO(β)

SOMO(β)

HOMO(α)   LUMO(α)

2c

HOMO-12(β)   HOMO-10(β)

HOMO-2(β)   HOMO(β)

SOMO(β)   SOMO(α)

HOMO(α)   LUMO(α)

2d

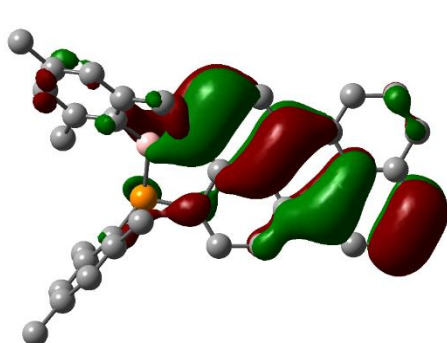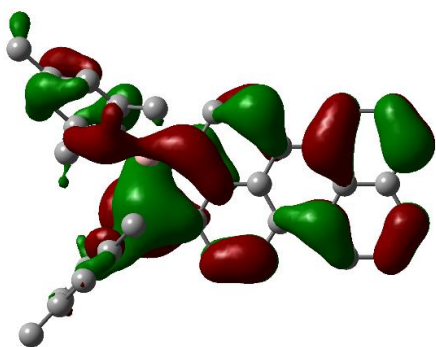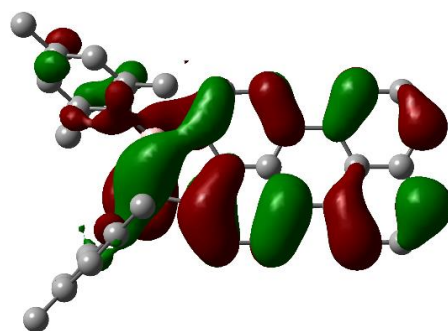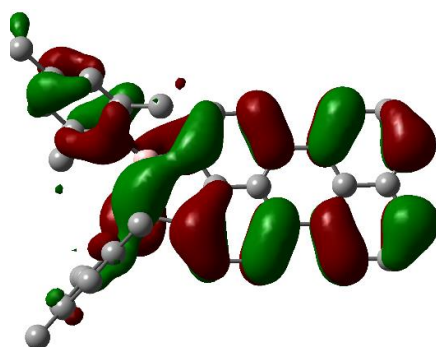HOMO-11(β)   HOMO-10(β)

HOMO(β)   SOMO(β)

HOMO(α)   LUMO(α)
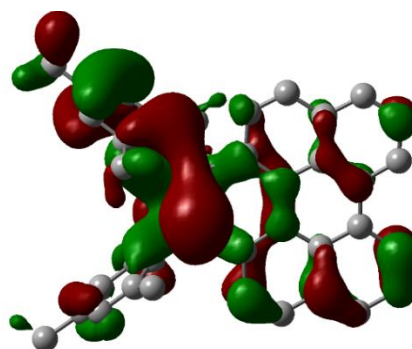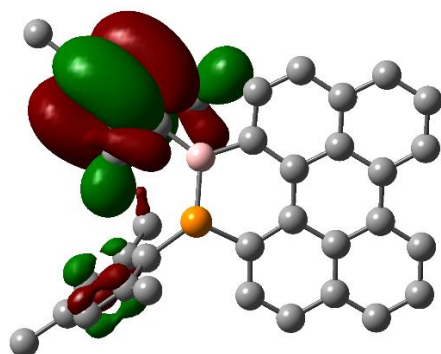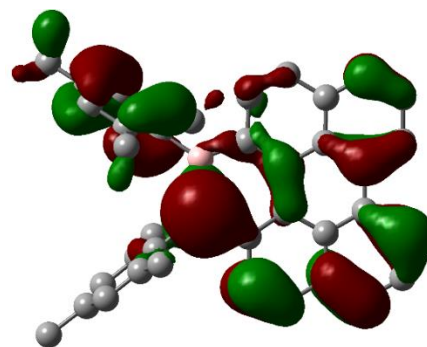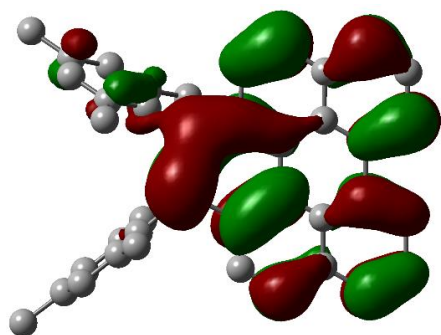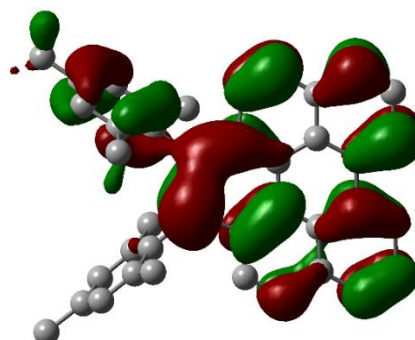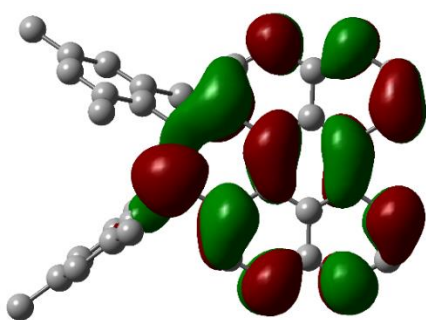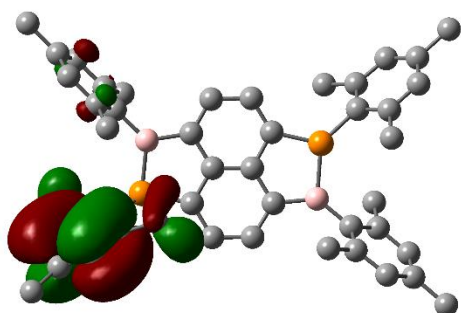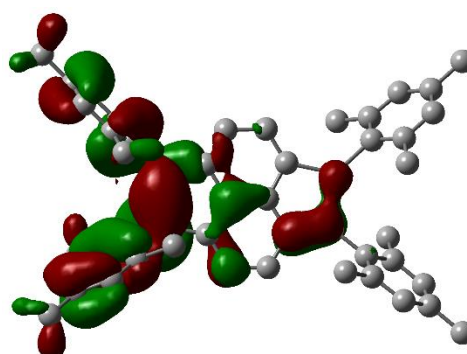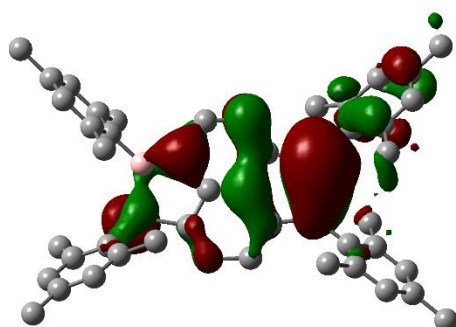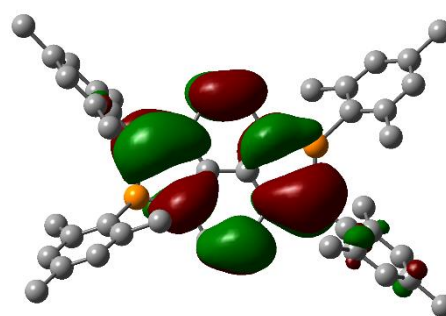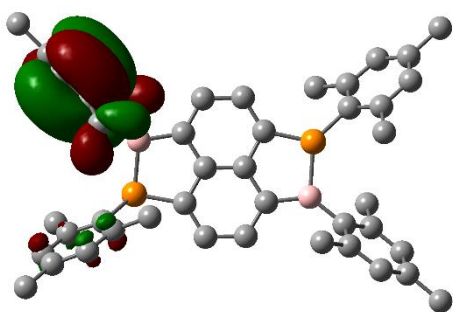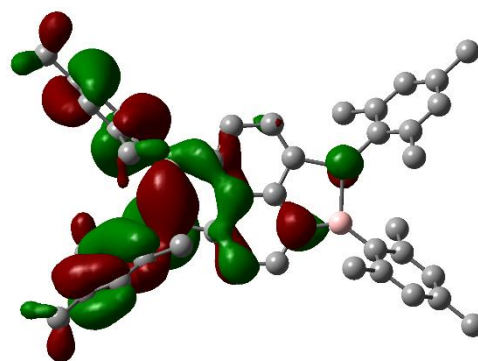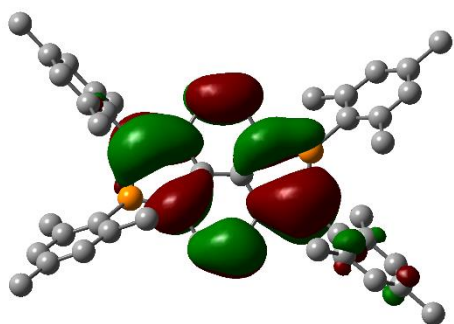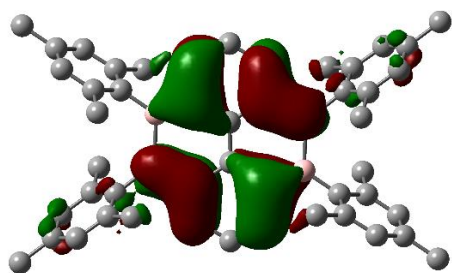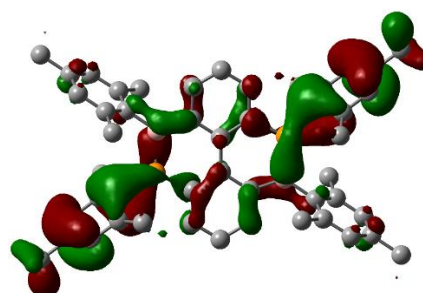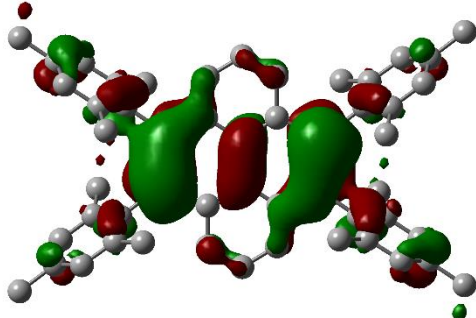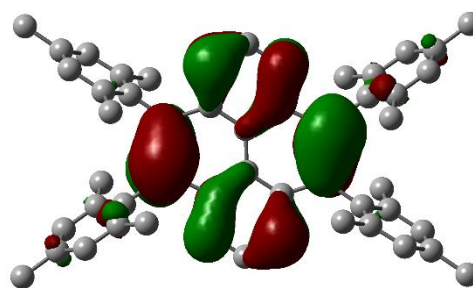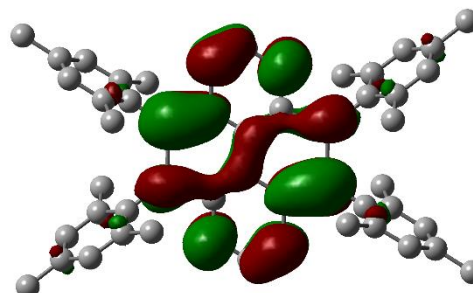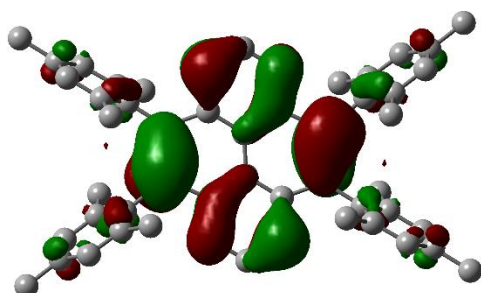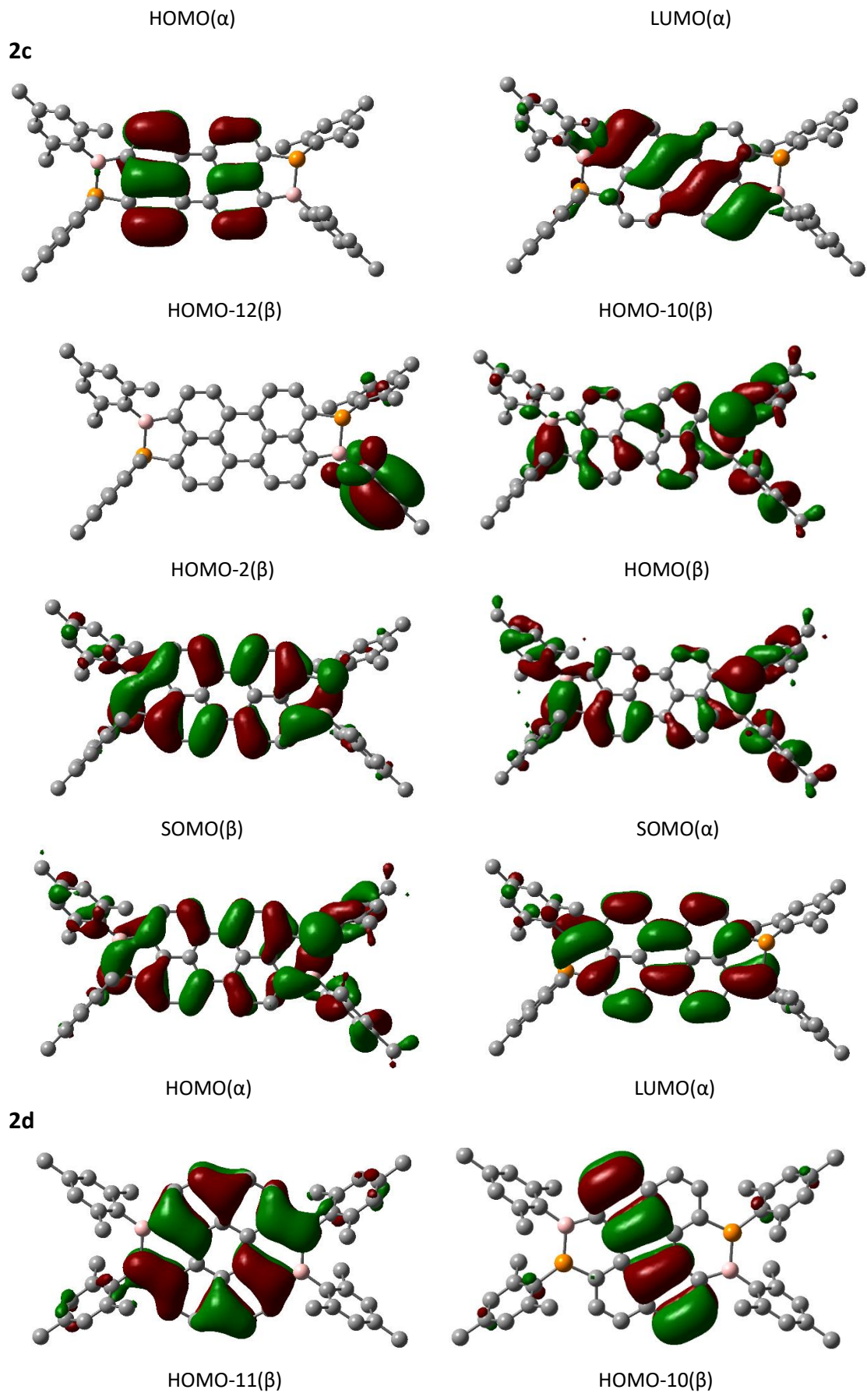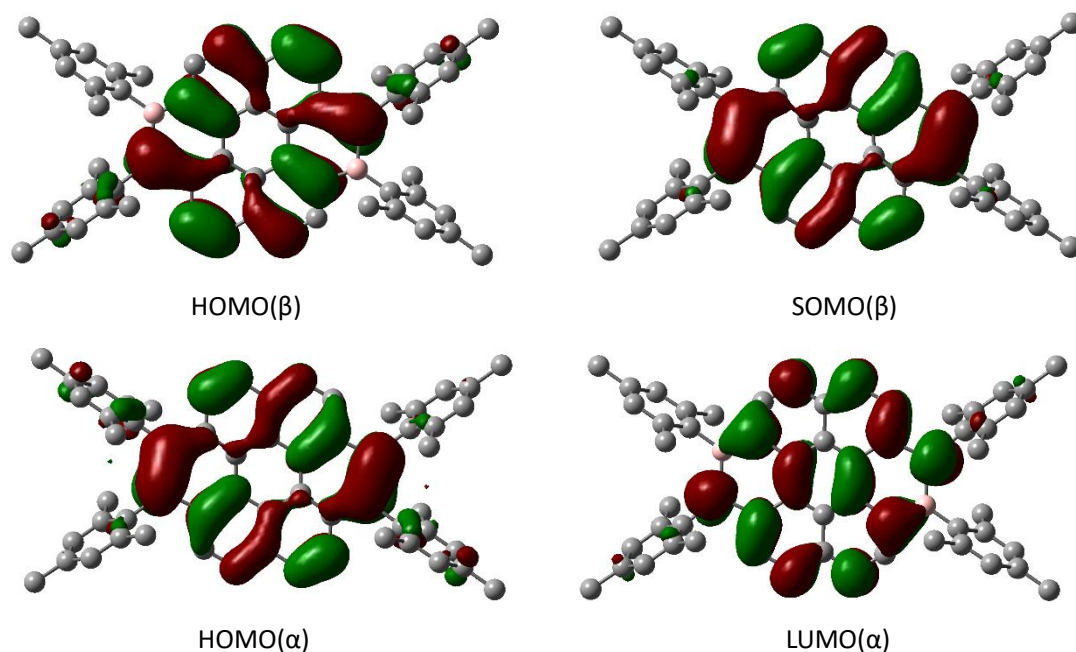
Fig. S9 The mainly frontier molecular orbitals (isosurface value=0.02 a.u.) related to absorption peaks.

Cartesian coordinates of the optimized geometries by DFT calculations at UM06-2X-D3/6-31G* level

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.280680	4.593410	0.269774
2	6	0	0.043482	4.986968	0.241839
3	6	0	1.090386	4.040461	0.087076
4	6	0	0.746937	2.678320	-0.032481
5	6	0	-0.634924	2.294144	-0.041398
6	6	0	-1.635078	3.239409	0.116372
7	1	0	2.756770	5.424912	0.146769
8	1	0	-2.060981	5.335098	0.399598
9	1	0	0.297356	6.038421	0.343957
10	6	0	2.470151	4.380777	0.055984
11	6	0	1.741243	1.655217	-0.138812
12	1	0	-2.680639	2.943700	0.123645
13	6	0	3.069881	2.043586	-0.184043
14	6	0	3.431805	3.407044	-0.090224
15	1	0	3.846276	1.290299	-0.289651
16	1	0	4.479777	3.684337	-0.124062
17	5	0	1.207434	0.204391	-0.221314
18	15	0	-0.705583	0.561013	-0.339140

19	6	0	1.874509	-1.173799	-0.215192
20	6	0	1.530638	-2.145355	-1.196090
21	6	0	2.835308	-1.505335	0.771366
22	6	0	2.175113	-3.372905	-1.199730
23	6	0	3.437592	-2.762451	0.744813
24	6	0	3.137158	-3.702278	-0.237692
25	1	0	1.925970	-4.101555	-1.967825
26	1	0	4.158664	-3.016458	1.518703
27	6	0	-2.198342	-0.351644	0.012566
28	6	0	-2.242874	-1.187788	1.149391
29	6	0	-3.288120	-0.241838	-0.877117
30	6	0	-3.420881	-1.886452	1.389550
31	6	0	-4.440003	-0.964114	-0.584393
32	6	0	-4.527794	-1.784794	0.542710
33	1	0	-3.479373	-2.529194	2.264267
34	1	0	-5.289417	-0.894709	-1.259022
35	6	0	-1.068465	-1.330150	2.085333
36	1	0	-0.213763	-1.800338	1.585134
37	1	0	-0.739563	-0.357251	2.469983
38	1	0	-1.334909	-1.950635	2.942866
39	6	0	-3.206645	0.583887	-2.137698
40	1	0	-2.900761	1.616949	-1.940639
41	1	0	-2.480820	0.154621	-2.838814
42	1	0	-4.174216	0.615973	-2.641683
43	6	0	-5.796414	-2.531316	0.851072
44	1	0	-5.587165	-3.477754	1.355144
45	1	0	-6.432924	-1.936291	1.515273
46	1	0	-6.366965	-2.738646	-0.056973
47	6	0	3.207789	-0.576503	1.906331
48	1	0	4.174003	-0.093624	1.723371
49	1	0	2.470129	0.210750	2.075404
50	1	0	3.307711	-1.144550	2.835279
51	6	0	0.489549	-1.870474	-2.257743
52	1	0	-0.522696	-1.861525	-1.830464
53	1	0	0.653082	-0.914214	-2.765476
54	1	0	0.503412	-2.652283	-3.020247
55	6	0	3.827012	-5.037869	-0.277759
56	1	0	4.341358	-5.250845	0.661712
57	1	0	3.114453	-5.843759	-0.474583
58	1	0	4.571806	-5.057513	-1.080837

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1b

Center   Atomic   Atomic   Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-4.231424	2.409762	0.948378
2	6	0	-2.886025	2.234772	0.654698
3	6	0	-2.356264	0.980148	0.292574
4	6	0	-3.238975	-0.134441	0.195061
5	6	0	-4.584182	0.057192	0.529528
6	6	0	-5.076186	1.306443	0.899153
7	6	0	-2.813873	-1.493529	-0.246464
8	6	0	-1.471270	-1.966963	-0.172666
9	6	0	-1.133332	-3.283972	-0.553982
10	1	0	-0.098124	-3.607003	-0.481212
11	6	0	-2.101988	-4.139806	-1.039507
12	6	0	-3.413063	-3.673483	-1.168215
13	6	0	-3.753350	-2.379292	-0.786585
14	1	0	-4.610984	3.385480	1.231692
15	1	0	-2.206239	3.080084	0.725435
16	1	0	-6.125736	1.409023	1.155548
17	1	0	-1.842943	-5.149075	-1.339188
18	1	0	-4.179302	-4.321481	-1.581028
19	15	0	-0.202926	-0.863588	0.319144
20	5	0	-0.820661	0.931496	0.206228
21	1	0	-5.267921	-0.783521	0.536678
22	1	0	-4.773207	-2.049047	-0.942653
23	6	0	0.193984	2.089891	0.097144
24	6	0	1.194884	2.292485	1.074466
25	6	0	0.152845	2.934198	-1.040622
26	6	0	2.112130	3.326642	0.912233
27	6	0	1.105546	3.938188	-1.177445
28	6	0	2.088387	4.157756	-0.208151
29	1	0	2.866265	3.491219	1.678511
30	1	0	1.084432	4.570338	-2.062440
31	6	0	1.463169	-1.491110	0.135733
32	6	0	2.214308	-1.170716	-1.012778
33	6	0	1.993530	-2.286866	1.174941
34	6	0	3.514284	-1.665392	-1.093287
35	6	0	3.296271	-2.751772	1.039654
36	6	0	4.073442	-2.446935	-0.081948
37	1	0	4.106067	-1.436774	-1.975926
38	1	0	3.719931	-3.367716	1.828997
39	6	0	-0.876937	2.740280	-2.131353
40	1	0	-0.976840	1.687586	-2.419908
41	1	0	-1.868076	3.081262	-1.815093
42	1	0	-0.601636	3.304027	-3.025346

43	6	0	1.280765	1.425233	2.309930
44	1	0	0.293449	1.191808	2.722489
45	1	0	1.796799	0.479888	2.094377
46	1	0	1.852301	1.925849	3.095117
47	6	0	3.077833	5.280818	-0.360383
48	1	0	3.355658	5.424752	-1.407700
49	1	0	2.644916	6.221842	-0.003397
50	1	0	3.985808	5.093343	0.217474
51	6	0	1.184514	-2.627249	2.402957
52	1	0	0.889895	-1.723986	2.951107
53	1	0	0.268408	-3.172484	2.147607
54	1	0	1.762262	-3.253766	3.084855
55	6	0	1.656875	-0.331363	-2.134769
56	1	0	0.653337	-0.661385	-2.428687
57	1	0	1.596239	0.723957	-1.844655
58	1	0	2.296533	-0.398801	-3.016873
59	6	0	5.490843	-2.940785	-0.182143
60	1	0	5.582769	-3.958546	0.205573
61	1	0	5.845627	-2.928870	-1.214830
62	1	0	6.157066	-2.302477	0.408281

1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.334832	2.425685	0.456629
2	6	0	-3.060706	1.237170	0.284554
3	6	0	-2.347391	0.005976	0.274885
4	6	0	-0.944458	0.039362	0.428020
5	6	0	-0.216865	1.245866	0.505799
6	6	0	-0.944718	2.434989	0.559474
7	6	0	-2.991231	-1.254883	0.090063
8	6	0	-0.177706	-1.169343	0.513555
9	1	0	-0.425373	3.383940	0.663279
10	6	0	-0.823578	-2.393855	0.297231
11	6	0	-2.190246	-2.423435	0.078261
12	1	0	-0.257999	-3.320805	0.324406
13	6	0	-6.675152	2.326079	-0.036697
14	6	0	-7.313203	1.118329	-0.210360
15	6	0	-6.573138	-0.086414	-0.227093
16	6	0	-5.159241	-0.052889	-0.062433
17	6	0	-4.511551	1.203693	0.116060
18	6	0	-5.285302	2.363675	0.123452

19	1	0	-7.241496	3.250597	-0.023515
20	6	0	-7.230635	-1.326816	-0.406372
21	6	0	-4.427861	-1.284141	-0.081578
22	6	0	-5.130184	-2.482162	-0.261952
23	6	0	-6.517108	-2.506724	-0.423244
24	1	0	-7.025425	-3.454631	-0.559395
25	1	0	-4.600902	-3.427211	-0.276841
26	1	0	-2.653558	-3.389581	-0.079794
27	1	0	-4.815104	3.330801	0.256575
28	1	0	-2.852839	3.376686	0.487255
29	15	0	1.471716	-0.837911	1.075028
30	5	0	1.334881	1.038041	0.547025
31	1	0	-8.390998	1.074080	-0.336869
32	1	0	-8.309815	-1.333322	-0.529973
33	6	0	2.654182	-1.928254	0.227086
34	6	0	3.418384	-2.807897	1.021484
35	6	0	2.816915	-1.897494	-1.175697
36	6	0	4.336244	-3.648410	0.393748
37	6	0	3.745124	-2.760564	-1.752325
38	6	0	4.515399	-3.638766	-0.988225
39	1	0	4.924585	-4.331820	1.000977
40	1	0	3.876575	-2.744143	-2.831772
41	6	0	2.471962	2.014960	0.226844
42	6	0	3.658184	2.042657	1.014713
43	6	0	2.363977	2.916237	-0.867009
44	6	0	4.638547	2.988699	0.750516
45	6	0	3.388254	3.826782	-1.113282
46	6	0	4.521754	3.896701	-0.305743
47	1	0	5.529108	3.017485	1.374034
48	1	0	3.304030	4.497332	-1.965724
49	6	0	3.259858	-2.879471	2.522346
50	1	0	3.423756	-1.905631	2.996455
51	1	0	2.255225	-3.210338	2.805565
52	1	0	3.976884	-3.583956	2.948641
53	6	0	5.533775	-4.533249	-1.642785
54	1	0	6.476470	-3.994828	-1.789467
55	1	0	5.745479	-5.411385	-1.028372
56	1	0	5.191955	-4.871150	-2.624438
57	6	0	2.051829	-0.948103	-2.063888
58	1	0	0.970058	-1.016422	-1.906997
59	1	0	2.354983	0.088658	-1.874897
60	1	0	2.251575	-1.163211	-3.115646
61	6	0	1.204197	2.907911	-1.841002
62	1	0	0.455494	3.663765	-1.579832

63	1	0	1.564106	3.149336	-2.844795
64	1	0	0.694895	1.943602	-1.894373
65	6	0	3.896525	1.069719	2.145613
66	1	0	3.060769	1.027037	2.849969
67	1	0	4.062498	0.057451	1.754185
68	1	0	4.791044	1.348418	2.706767
69	6	0	5.595598	4.918520	-0.557874
70	1	0	5.490500	5.759569	0.136524
71	1	0	6.590592	4.491781	-0.405237
72	1	0	5.539188	5.315523	-1.573876

1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.704151	1.501973	0.127934
2	6	0	-1.945350	0.776234	0.047480
3	6	0	-3.133711	1.528363	-0.234373
4	6	0	-3.052539	2.924583	-0.520392
5	6	0	-1.784586	3.580916	-0.484888
6	6	0	-0.658043	2.899037	-0.156923
7	6	0	-4.416390	0.910710	-0.245702
8	6	0	-4.200249	3.652273	-0.836714
9	1	0	-1.741061	4.641794	-0.714188
10	1	0	0.300865	3.406172	-0.114797
11	6	0	-5.443680	3.029930	-0.873646
12	6	0	-5.544886	1.681405	-0.580027
13	1	0	-4.108693	4.711298	-1.059274
14	1	0	-6.331919	3.596201	-1.131098
15	6	0	-1.069934	-2.880676	0.592201
16	6	0	-2.320202	-3.444346	0.719223
17	6	0	-3.473266	-2.648816	0.562946
18	6	0	-3.339531	-1.254709	0.290039
19	6	0	-2.032931	-0.656241	0.229389
20	6	0	-0.888104	-1.504251	0.349888
21	1	0	-4.817035	-4.303509	0.890116
22	1	0	-0.187782	-3.507104	0.686815
23	1	0	-2.432148	-4.505691	0.921906
24	6	0	-4.750979	-3.241686	0.672197
25	6	0	-4.523138	-0.494765	0.090148
26	6	0	-5.772549	-1.124998	0.220110
27	6	0	-5.890972	-2.481393	0.511051
28	1	0	-6.873360	-2.930104	0.606015

29	15	0	0.777748	0.740521	0.653399
30	5	0	0.608495	-1.065793	0.293300
31	1	0	-6.683012	-0.550746	0.104826
32	1	0	-6.523601	1.221522	-0.627074
33	6	0	2.238444	1.735781	0.285687
34	6	0	2.820492	1.718308	-0.998845
35	6	0	2.786215	2.517253	1.324615
36	6	0	3.964133	2.486021	-1.210331
37	6	0	3.929833	3.265396	1.058397
38	6	0	4.536885	3.256484	-0.198236
39	1	0	4.421093	2.483211	-2.196919
40	1	0	4.357520	3.873918	1.851339
41	6	0	1.814635	-2.010711	0.045633
42	6	0	1.856776	-2.760519	-1.155127
43	6	0	2.890980	-2.115414	0.956746
44	6	0	2.946750	-3.588172	-1.411701
45	6	0	3.948203	-2.976194	0.675561
46	6	0	3.997204	-3.721522	-0.502915
47	1	0	2.980669	-4.143387	-2.346757
48	1	0	4.762463	-3.064485	1.391472
49	6	0	2.928146	-1.316916	2.239259
50	1	0	3.662343	-1.733217	2.933028
51	1	0	3.222680	-0.277695	2.042595
52	1	0	1.959249	-1.301791	2.748621
53	6	0	5.143658	-4.657023	-0.778013
54	1	0	4.934118	-5.651608	-0.368773
55	1	0	5.314135	-4.771701	-1.851363
56	1	0	6.067660	-4.299532	-0.316712
57	6	0	0.760327	-2.665389	-2.194983
58	1	0	-0.079392	-3.328006	-1.957493
59	1	0	0.356749	-1.650814	-2.283134
60	1	0	1.139525	-2.957388	-3.177370
61	6	0	2.252274	0.905974	-2.134371
62	1	0	1.176539	1.075991	-2.254012
63	1	0	2.741326	1.168760	-3.074523
64	1	0	2.406563	-0.165514	-1.962996
65	6	0	2.156380	2.574092	2.695759
66	1	0	2.105679	1.581999	3.158328
67	1	0	2.733579	3.223582	3.356804
68	1	0	1.133589	2.965345	2.652262
69	6	0	5.793268	4.045973	-0.450017
70	1	0	6.675758	3.442576	-0.210918
71	1	0	5.871478	4.345243	-1.497916
72	1	0	5.829269	4.944049	0.171350

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-0.734908	-2.335154	-0.963948
2	6	0	-1.441278	-1.161075	-0.769258
3	6	0	-0.728293	0.021932	-0.394394
4	6	0	0.651516	-0.012806	-0.251126
5	6	0	1.391486	-1.232581	-0.424448
6	6	0	0.668505	-2.366095	-0.782238
7	1	0	-1.253481	-3.242078	-1.261881
8	6	0	-1.476092	1.211693	-0.152567
9	6	0	1.331990	1.196744	0.108416
10	1	0	1.197171	-3.303423	-0.940412
11	6	0	0.615574	2.359295	0.357773
12	6	0	-0.792472	2.356926	0.231817
13	1	0	1.129076	3.264781	0.668867
14	1	0	-1.347328	3.266726	0.447221
15	5	0	-3.032200	0.992276	-0.289411
16	15	0	-3.176387	-0.733418	-1.069803
17	6	0	-4.154156	2.027310	-0.005229
18	6	0	-4.905696	1.961778	1.183963
19	6	0	-4.424766	3.044174	-0.939915
20	6	0	-5.895965	2.909355	1.423046
21	6	0	-5.431718	3.971643	-0.673193
22	6	0	-6.174875	3.923877	0.504683
23	1	0	-6.468993	2.856071	2.346736
24	1	0	-5.642434	4.749102	-1.404585
25	6	0	-4.356926	-1.935022	-0.379407
26	6	0	-5.545105	-2.140933	-1.113783
27	6	0	-4.144886	-2.609733	0.840998
28	6	0	-6.487037	-3.042360	-0.626737
29	6	0	-5.117958	-3.509704	1.278744
30	6	0	-6.286864	-3.747673	0.559863
31	1	0	-7.406221	-3.195683	-1.187251
32	1	0	-4.960238	-4.031013	2.220242
33	6	0	-7.308605	-4.742039	1.043697
34	1	0	-8.325301	-4.377767	0.873583
35	1	0	-7.206028	-5.691265	0.506674
36	1	0	-7.190117	-4.948095	2.110074
37	6	0	-2.931863	-2.391607	1.710708
38	1	0	-2.069496	-2.967599	1.358377

39	1	0	-2.631767	-1.338981	1.733548
40	1	0	-3.144066	-2.705442	2.735409
41	6	0	-5.835922	-1.386510	-2.389074
42	1	0	-5.889594	-0.306518	-2.209799
43	1	0	-5.059018	-1.553758	-3.141893
44	1	0	-6.793125	-1.701799	-2.809481
45	6	0	-4.634837	0.871207	2.192907
46	1	0	-4.870593	-0.116978	1.778588
47	1	0	-3.580417	0.861445	2.496948
48	1	0	-5.236259	1.005771	3.095263
49	6	0	-3.662536	3.106413	-2.242787
50	1	0	-2.578615	3.119042	-2.077273
51	1	0	-3.880912	2.234276	-2.871029
52	1	0	-3.923962	4.000742	-2.813319
53	6	0	-7.240860	4.948160	0.795581
54	1	0	-7.530263	5.488800	-0.108773
55	1	0	-8.135231	4.478736	1.215068
56	1	0	-6.885152	5.683781	1.525187
57	5	0	2.905327	-1.119535	-0.211712
58	15	0	3.039953	0.772997	0.230965
59	6	0	4.085226	-2.109175	-0.251341
60	6	0	5.121756	-1.944290	-1.194738
61	6	0	4.151133	-3.169261	0.678778
62	6	0	6.178402	-2.849575	-1.215336
63	6	0	5.235825	-4.041620	0.639863
64	6	0	6.252344	-3.907152	-0.307211
65	1	0	6.966484	-2.728692	-1.955361
66	1	0	5.292655	-4.847792	1.367918
67	6	0	5.095235	-0.800271	-2.182609
68	1	0	4.117028	-0.701281	-2.667099
69	1	0	5.325532	0.155196	-1.692203
70	1	0	5.838462	-0.944742	-2.970086
71	6	0	3.089153	-3.343187	1.740794
72	1	0	2.899888	-2.407284	2.279960
73	1	0	2.134672	-3.665984	1.312716
74	1	0	3.392594	-4.092464	2.475241
75	6	0	7.390635	-4.890906	-0.361303
76	1	0	7.145455	-5.723944	-1.029246
77	1	0	8.302941	-4.422998	-0.739634
78	1	0	7.600359	-5.310657	0.625652
79	6	0	4.343741	1.974281	0.342633
80	6	0	5.368760	1.733506	1.288669
81	6	0	4.388700	3.082748	-0.535458
82	6	0	6.408644	2.651161	1.369199

83	6	0	5.455503	3.964633	-0.406270
84	6	0	6.463728	3.777116	0.543385
85	1	0	7.200905	2.484732	2.094396
86	1	0	5.514064	4.816371	-1.079123
87	6	0	3.368939	3.298793	-1.625357
88	1	0	3.176924	2.376834	-2.185866
89	1	0	2.410101	3.647742	-1.231182
90	1	0	3.726650	4.049286	-2.332571
91	6	0	5.350489	0.522632	2.188743
92	1	0	4.470733	0.521903	2.842238
93	1	0	5.342014	-0.409268	1.609061
94	1	0	6.236994	0.505826	2.825260
95	6	0	7.583464	4.771067	0.678190
96	1	0	7.319830	5.537754	1.415327
97	1	0	8.503545	4.289509	1.017424
98	1	0	7.782606	5.277389	-0.269057

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-0.003674	-0.722368	-0.147794
2	6	0	-1.206334	-1.509793	-0.289478
3	6	0	-1.120809	-2.876338	-0.625512
4	6	0	0.082987	-3.548625	-0.816583
5	6	0	1.243579	-2.835934	-0.646262
6	6	0	1.222925	-1.458515	-0.307069
7	6	0	0.003661	0.722359	0.147753
8	6	0	-1.222933	1.458494	0.307077
9	6	0	-1.243583	2.835909	0.646294
10	6	0	-0.082993	3.548613	0.816555
11	6	0	1.120805	2.876340	0.625426
12	6	0	1.206323	1.509794	0.289406
13	1	0	-2.051696	-3.423814	-0.743965
14	1	0	0.102581	-4.597936	-1.089147
15	1	0	2.206692	-3.320825	-0.783730
16	1	0	-2.206695	3.320783	0.783831
17	1	0	-0.102588	4.597922	1.089128
18	1	0	2.051691	3.423825	0.743838
19	5	0	-2.681213	-1.070380	-0.151421
20	15	0	-2.791428	0.718409	0.138575
21	15	0	2.791418	-0.718428	-0.138563
22	5	0	2.681192	1.070378	0.151364

23	6	0	3.963024	1.964937	0.199426
24	6	0	4.249020	2.831942	-0.877699
25	6	0	4.870511	1.880200	1.272903
26	6	0	5.417060	3.591201	-0.858271
27	6	0	6.021724	2.666771	1.265693
28	6	0	6.312972	3.529498	0.210111
29	1	0	5.635947	4.247933	-1.697830
30	1	0	6.712298	2.601658	2.103966
31	6	0	4.222103	-1.798736	-0.169806
32	6	0	5.176308	-1.638416	-1.196530
33	6	0	4.414175	-2.732839	0.872966
34	6	0	6.308994	-2.447694	-1.170662
35	6	0	5.563907	-3.517043	0.845321
36	6	0	6.517277	-3.394633	-0.167301
37	1	0	7.052174	-2.333981	-1.955900
38	1	0	5.727085	-4.236770	1.643677
39	6	0	-3.963028	-1.964957	-0.199526
40	6	0	-4.870496	-1.880194	-1.273018
41	6	0	-4.249043	-2.831986	0.877576
42	6	0	-6.021711	-2.666762	-1.265848
43	6	0	-5.417092	-3.591231	0.858113
44	6	0	-6.312984	-3.529503	-0.210284
45	1	0	-6.712268	-2.601623	-2.104133
46	1	0	-5.636009	-4.247969	1.697658
47	6	0	-4.222108	1.798721	0.169893
48	6	0	-5.176310	1.638364	1.196625
49	6	0	-4.414166	2.732894	-0.872810
50	6	0	-6.308964	2.447681	1.170825
51	6	0	-5.563876	3.517138	-0.845099
52	6	0	-6.517229	3.394699	0.167529
53	1	0	-7.052140	2.333943	1.956064
54	1	0	-5.727039	4.236915	-1.643413
55	6	0	-4.622936	-0.938182	-2.428598
56	1	0	-4.861881	0.096560	-2.148863
57	1	0	-3.578258	-0.961417	-2.757856
58	1	0	-5.249824	-1.195657	-3.285795
59	6	0	-7.549381	-4.389650	-0.230958
60	1	0	-7.330342	-5.371230	-0.665419
61	1	0	-7.933959	-4.555919	0.778711
62	1	0	-8.341074	-3.933024	-0.830225
63	6	0	-3.316334	-2.929184	2.063644
64	1	0	-2.380173	-3.435754	1.802520
65	1	0	-3.045449	-1.937538	2.446449
66	1	0	-3.779353	-3.488483	2.879910

67	6	0	-3.432813	2.888829	-2.008377
68	1	0	-2.499308	3.359065	-1.680087
69	1	0	-3.170903	1.919942	-2.448316
70	1	0	-3.858844	3.512796	-2.796383
71	6	0	-5.009746	0.614712	2.291344
72	1	0	-4.039407	0.711823	2.790512
73	1	0	-5.789876	0.730531	3.046399
74	1	0	-5.080696	-0.403094	1.888830
75	6	0	-7.736334	4.276645	0.185876
76	1	0	-8.589499	3.764247	0.636878
77	1	0	-7.543886	5.180077	0.774968
78	1	0	-8.014043	4.591926	-0.822644
79	6	0	5.009715	-0.614862	-2.291335
80	1	0	4.039383	-0.712056	-2.790501
81	1	0	5.080624	0.402982	-1.888911
82	1	0	5.789854	-0.730716	-3.046375
83	6	0	3.432803	-2.888718	2.008523
84	1	0	3.171022	-1.919818	2.448512
85	1	0	2.499237	-3.358816	1.680211
86	1	0	3.858754	-3.512777	2.796500
87	6	0	7.736403	-4.276553	-0.185561
88	1	0	7.543879	-5.180185	-0.774321
89	1	0	8.589485	-3.764287	-0.636871
90	1	0	8.014284	-4.591498	0.823018
91	6	0	3.316282	2.929142	-2.063746
92	1	0	3.045220	1.937500	-2.446430
93	1	0	2.380214	3.435902	-1.802649
94	1	0	3.779364	3.488274	-2.880091
95	6	0	4.622979	0.938213	2.428508
96	1	0	3.578296	0.961410	2.757752
97	1	0	4.861983	-0.096524	2.148811
98	1	0	5.249841	1.195747	3.285706
99	6	0	7.549375	4.389640	0.230727
100	1	0	7.934154	4.555542	-0.778925
101	1	0	7.330264	5.371379	0.664797
102	1	0	8.340940	3.933212	0.830311

2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-1.526675	-2.548880	0.007651
2	6	0	-0.750077	-1.373479	0.004811

3	6	0	-1.408157	-0.126100	0.217761
4	6	0	-2.807915	-0.132733	0.411099
5	6	0	-3.584074	-1.307056	0.309665
6	6	0	-2.910482	-2.520813	0.148564
7	6	0	-0.722486	1.121387	0.221814
8	6	0	-3.523329	1.063479	0.726629
9	1	0	-3.471737	-3.450385	0.107581
10	6	0	-2.839331	2.280600	0.693940
11	6	0	-1.475104	2.298660	0.434506
12	1	0	-3.364414	3.209422	0.896571
13	6	0	2.805858	-2.529309	-0.633638
14	6	0	3.493529	-1.319295	-0.663796
15	6	0	2.767678	-0.114053	-0.415936
16	6	0	1.368817	-0.121538	-0.213435
17	6	0	0.682971	-1.369011	-0.205233
18	6	0	1.433372	-2.545481	-0.400919
19	1	0	3.332133	-3.463216	-0.808295
20	6	0	3.529141	1.078171	-0.364222
21	6	0	0.708471	1.127479	0.002915
22	6	0	1.478018	2.306030	0.005948
23	6	0	2.860143	2.285791	-0.171543
24	1	0	3.423210	3.214780	-0.136497
25	1	0	0.997430	3.262693	0.174474
26	1	0	-0.975893	3.260719	0.424874
27	1	0	0.933704	-3.507500	-0.391789
28	1	0	-1.046742	-3.510101	-0.135281
29	15	0	-5.189727	0.699800	1.296615
30	5	0	-5.130635	-1.034496	0.420181
31	6	0	-6.319174	1.932909	0.558712
32	6	0	-7.063951	2.736591	1.447913
33	6	0	-6.456536	2.100979	-0.836842
34	6	0	-7.930530	3.695398	0.924421
35	6	0	-7.330701	3.077361	-1.309088
36	6	0	-8.078933	3.880672	-0.448269
37	1	0	-8.502168	4.317511	1.608888
38	1	0	-7.436610	3.211842	-2.383188
39	6	0	-6.287907	-1.936530	-0.040223
40	6	0	-7.465820	-2.072261	0.748873
41	6	0	-6.200848	-2.670936	-1.252251
42	6	0	-8.451430	-2.972311	0.367696
43	6	0	-7.229556	-3.540204	-1.610611
44	6	0	-8.350298	-3.725035	-0.805883
45	1	0	-9.335445	-3.084983	0.991242
46	1	0	-7.157908	-4.081707	-2.551634

47	6	0	-6.944632	2.603089	2.948760
48	1	0	-7.180412	1.588810	3.287689
49	1	0	-5.930425	2.827285	3.294526
50	1	0	-7.630082	3.291792	3.447096
51	6	0	-9.041927	4.902024	-0.992370
52	1	0	-10.014841	4.441079	-1.195168
53	1	0	-9.203038	5.715286	-0.280676
54	1	0	-8.678606	5.329643	-1.930375
55	6	0	-5.722762	1.245077	-1.839240
56	1	0	-4.645746	1.206353	-1.644840
57	1	0	-6.106008	0.218135	-1.822151
58	1	0	-5.865300	1.632335	-2.850507
59	6	0	-5.066986	-2.517227	-2.245528
60	1	0	-4.364719	-3.356060	-2.186547
61	1	0	-5.470061	-2.510689	-3.262449
62	1	0	-4.497074	-1.596161	-2.111910
63	6	0	-7.692373	-1.260921	2.002930
64	1	0	-6.865011	-1.341169	2.713955
65	1	0	-7.821719	-0.199336	1.755994
66	1	0	-8.602263	-1.588873	2.510304
67	6	0	-9.433263	-4.697932	-1.184010
68	1	0	-9.379888	-5.593106	-0.554759
69	1	0	-10.424502	-4.258402	-1.040880
70	1	0	-9.341541	-5.013807	-2.225552
71	15	0	5.206478	-0.992038	-1.159176
72	5	0	5.068324	0.843884	-0.577244
73	6	0	6.216800	1.872129	-0.447758
74	6	0	6.653601	2.303776	0.818777
75	6	0	6.832854	2.390870	-1.607564
76	6	0	7.682327	3.239625	0.910843
77	6	0	7.848436	3.332516	-1.477875
78	6	0	8.292865	3.765716	-0.226016
79	1	0	8.016454	3.564718	1.893898
80	1	0	8.304476	3.746108	-2.375233
81	6	0	6.364118	-1.901538	-0.062642
82	6	0	7.595898	-2.270939	-0.649098
83	6	0	6.113568	-2.199471	1.294162
84	6	0	8.533167	-2.958618	0.116367
85	6	0	7.085288	-2.896115	2.015530
86	6	0	8.292688	-3.293938	1.448068
87	1	0	9.481524	-3.235411	-0.338394
88	1	0	6.892584	-3.125124	3.061302
89	6	0	4.855776	-1.800876	2.028689
90	1	0	4.513167	-0.799498	1.752932

Center Number	Atomic Number	Atomic Type	X	Y	Z
91	1	0	4.030402	-2.493016	1.830451
92	1	0	5.037359	-1.804838	3.106258
93	6	0	9.311288	-4.066427	2.243208
94	1	0	9.272983	-5.130966	1.987776
95	1	0	10.325222	-3.715724	2.032210
96	1	0	9.131477	-3.974574	3.316954
97	6	0	7.948629	-1.899758	-2.069852
98	1	0	7.194176	-2.245852	-2.782971
99	1	0	8.031603	-0.812013	-2.181619
100	1	0	8.910532	-2.333805	-2.350778
101	6	0	6.058919	1.709763	2.072154
102	1	0	4.965011	1.647098	2.010379
103	1	0	6.437954	0.692948	2.234780
104	1	0	6.310713	2.302971	2.954670
105	6	0	6.372926	1.959692	-2.981127
106	1	0	6.586680	0.900165	-3.164377
107	1	0	5.291623	2.093955	-3.104958
108	1	0	6.869676	2.539655	-3.762446
109	6	0	9.417375	4.761656	-0.115470
110	1	0	10.384478	4.272821	-0.276174
111	1	0	9.321877	5.551294	-0.866044
112	1	0	9.440396	5.227601	0.872612

2d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.477194	-1.452625	-0.233830
2	6	0	-1.262673	-0.686176	-0.123682
3	6	0	-0.021067	-1.390827	-0.266279
4	6	0	-0.051319	-2.797521	-0.545258
5	6	0	-1.286874	-3.498303	-0.684058
6	6	0	-2.460513	-2.851114	-0.527586
7	6	0	1.257209	-0.738612	-0.133343
8	6	0	1.127413	-3.527599	-0.692836
9	1	0	-1.256917	-4.558480	-0.916124
10	1	0	-3.405626	-3.375228	-0.634704
11	6	0	2.343712	-2.902528	-0.543035
12	6	0	2.449968	-1.528691	-0.253866
13	1	0	1.069775	-4.588430	-0.917641
14	1	0	3.258465	-3.478176	-0.651269
15	6	0	-2.343814	2.903204	0.539738
16	6	0	-1.127542	3.528403	0.689254

17	6	0	0.051234	2.798062	0.543314
18	6	0	0.021104	1.391130	0.265568
19	6	0	-1.257147	0.738851	0.132878
20	6	0	-2.449971	1.528966	0.252556
21	1	0	1.256690	4.559238	0.913549
22	1	0	-3.258589	3.479010	0.646953
23	1	0	-1.069953	4.589504	0.912791
24	6	0	1.286741	3.498813	0.682629
25	6	0	1.262768	0.686273	0.124054
26	6	0	2.477295	1.452495	0.235661
27	6	0	2.460426	2.851197	0.528401
28	1	0	3.405508	3.375177	0.636337
29	15	0	-4.031422	-0.730264	-0.034979
30	5	0	-3.922818	1.077152	0.143688
31	6	0	-5.458447	-1.816557	-0.091671
32	6	0	-6.380807	-1.687428	-1.150541
33	6	0	-5.671190	-2.734899	0.959980
34	6	0	-7.504952	-2.509495	-1.144344
35	6	0	-6.809705	-3.534637	0.911756
36	6	0	-7.736440	-3.436168	-0.127471
37	1	0	-8.221013	-2.424274	-1.957958
38	1	0	-6.983661	-4.249182	1.712532
39	6	0	-5.200899	1.976875	0.152928
40	6	0	-5.469616	2.815998	-0.950627
41	6	0	-6.121748	1.927332	1.217735
42	6	0	-6.632523	3.583370	-0.964803
43	6	0	-7.266383	2.722152	1.176948
44	6	0	-7.539752	3.558079	0.095240
45	1	0	-6.838339	4.217060	-1.825178
46	1	0	-7.966345	2.685154	2.009175
47	6	0	-5.895523	1.015894	2.402012
48	1	0	-6.535571	1.298421	3.241470
49	1	0	-6.133683	-0.025304	2.146425
50	1	0	-4.856319	1.044461	2.747305
51	6	0	-8.769744	4.427490	0.079135
52	1	0	-8.549001	5.417835	0.492435
53	1	0	-9.140250	4.571854	-0.939156
54	1	0	-9.572501	3.991391	0.679068
55	6	0	-4.525509	2.874222	-2.130398
56	1	0	-3.600924	3.407994	-1.883085
57	1	0	-4.234362	1.871242	-2.465088
58	1	0	-4.989192	3.388131	-2.975766
59	6	0	-6.186418	-0.689246	-2.263877
60	1	0	-5.199654	-0.791557	-2.728546

61	1	0	-6.941503	-0.828726	-3.040150
62	1	0	-6.275611	0.337413	-1.888684
63	6	0	-4.716020	-2.862504	2.120984
64	1	0	-4.530800	-1.890984	2.593020
65	1	0	-5.124310	-3.533551	2.879171
66	1	0	-3.744690	-3.262242	1.809030
67	6	0	-8.977129	-4.288167	-0.133561
68	1	0	-9.797297	-3.769488	0.374803
69	1	0	-9.305052	-4.504003	-1.153300
70	1	0	-8.812001	-5.235108	0.385855
71	5	0	3.922830	-1.077361	-0.143610
72	15	0	4.031745	0.729455	0.041088
73	6	0	5.458641	1.816106	0.095538
74	6	0	6.385732	1.682617	1.149909
75	6	0	5.671118	2.732733	-0.957581
76	6	0	7.513680	2.499157	1.138064
77	6	0	6.813616	3.527330	-0.914786
78	6	0	7.741804	3.428824	0.122971
79	1	0	8.236815	2.405534	1.944490
80	1	0	6.990695	4.235804	-1.720207
81	6	0	5.200793	-1.977289	-0.154663
82	6	0	5.469634	-2.818467	0.947308
83	6	0	6.121587	-1.925648	-1.219384
84	6	0	6.632556	-3.585825	0.959947
85	6	0	7.266321	-2.720430	-1.180149
86	6	0	7.539768	-3.558419	-0.100076
87	1	0	6.838460	-4.221132	1.819106
88	1	0	7.966312	-2.681647	-2.012266
89	6	0	4.525914	-2.878369	2.127280
90	1	0	4.237556	-1.875721	2.465414
91	1	0	3.599823	-3.408892	1.878649
92	1	0	4.988680	-3.396243	2.970722
93	6	0	8.769855	-4.427724	-0.085698
94	1	0	9.139789	-4.574914	0.932394
95	1	0	8.549475	-5.416919	-0.501937
96	1	0	9.572895	-3.989822	-0.683937
97	6	0	5.895348	-1.011812	-2.401801
98	1	0	6.134828	0.028644	-2.144440
99	1	0	6.534472	-1.293388	-3.242278
100	1	0	4.855842	-1.038749	-2.746337
101	6	0	4.715410	2.859117	-2.118261
102	1	0	5.124105	3.528082	-2.878069
103	1	0	4.528170	1.886974	-2.588210
104	1	0	3.745013	3.261090	-1.806315

105	6	0	6.195656	0.680813	2.260770
106	1	0	6.952815	0.818893	3.035275
107	1	0	5.210199	0.781167	2.728612
108	1	0	6.284533	-0.344783	1.882627
109	6	0	8.955143	4.318693	0.156993
110	1	0	8.751722	5.218830	0.747400
111	1	0	9.806771	3.809712	0.615020
112	1	0	9.241712	4.638800	-0.847503