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Supplementary material

SUPPLEMENTARY MATERIAL TO

Study on charge mobility of hexathiapentacene and its selenium analogs

SU-QIN ZHOU[1], QI-YING XIA[2]*, MENG LIANG[3] and XUE-HAI JU[3]**

[1]Faculty of Chemical Engineering, Huaiyin Institute of Technology, Key Laboratory for Attapulgite Science and Applied Technology of Jiangsu Province, Huaian 223003, P. R. China, [2]School of Chemistry and Chemical Engineering, Linyi University, Linyi 276005, P. R. China and [3]School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China

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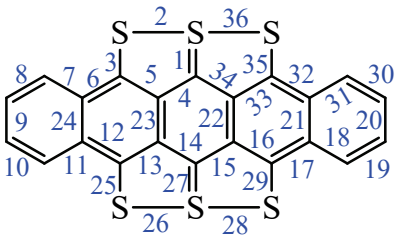

HTP

Fig. S-1. Bond labels of HTP. (Same labels for its selenium analogs).

*,** Corresponding authors. E-mail: (*)xiaqiying@163.com; (**)xhju@njust.edu.cn

TABLE S-I. Bond lengths and their variations in the ionic states of HTP

Bond labels	Bond length, Å					
	Crystal	Ground state	Anion state	Cation state	Δr_{A-G}	Δr_{C-G}
1	1.746	1.749	1.771	1.746	0.022	–0.003
2	2.385	2.380	2.403	2.384	0.023	0.004
3	1.693	1.716	1.736	1.693	0.020	–0.023
4	1.419	1.420	1.419	1.419	–0.001	–0.001
5	1.426	1.406	1.415	1.426	0.009	0.019
6	1.450	1.446	1.427	1.450	–0.019	0.004
7	1.408	1.413	1.421	1.408	0.008	–0.005
8	1.383	1.378	1.374	1.383	–0.004	0.004
9	1.401	1.406	1.414	1.401	0.008	–0.005
10	1.383	1.378	1.374	1.383	–0.004	0.005
11	1.408	1.413	1.421	1.408	0.008	–0.005
12	1.450	1.445	1.427	1.450	–0.018	0.005
13	1.426	1.406	1.415	1.426	0.009	0.020
14	1.419	1.420	1.419	1.419	–0.001	–0.001
15	1.419	1.420	1.419	1.419	–0.001	–0.001
16	1.426	1.406	1.415	1.426	0.009	0.020
17	1.450	1.446	1.427	1.450	–0.018	0.004
18	1.408	1.413	1.421	1.408	0.008	–0.005
19	1.383	1.378	1.374	1.383	–0.004	0.005
20	1.401	1.406	1.414	1.401	0.008	–0.005
21	1.423	1.423	1.433	1.423	0.010	0.000
22	1.430	1.448	1.452	1.430	0.004	–0.018
23	1.430	1.448	1.452	1.430	0.004	–0.018
24	1.423	1.423	1.433	1.423	0.010	0.000
25	1.693	1.716	1.736	1.692	0.020	–0.024
26	2.383	2.378	2.401	2.384	0.023	0.006
27	1.746	1.749	1.771	1.746	0.022	–0.003
28	2.385	2.380	2.403	2.384	0.023	0.004
29	1.69	1.716	1.736	1.693	0.020	–0.023
30	1.38	1.378	1.374	1.383	–0.005	0.005
31	1.408	1.413	1.421	1.408	0.008	–0.005
32	1.450	1.445	1.427	1.450	–0.018	0.005
33	1.426	1.406	1.415	1.426	0.009	0.020
34	1.419	1.420	1.419	1.419	–0.001	–0.001
35	1.693	1.716	1.736	1.693	0.020	–0.023
36	2.383	2.378	2.401	2.384	0.023	0.006

TABLE S-II. Bond lengths and their variations in the ionic states of 2Se-HTP

Bond labels	Bond length, Å				
	Ground state	Anion state	Cation state	Δr_{A-G}	Δr_{C-G}
1	1.892	1.915	1.889	0.023	–0.003
2	2.446	2.467	2.453	0.021	0.007
3	1.720	1.741	1.696	0.021	–0.024
4	1.419	1.418	1.419	–0.001	0.000
5	1.410	1.418	1.430	0.008	0.020
6	1.446	1.427	1.450	–0.019	0.004
7	1.414	1.422	1.409	0.001	–0.005
8	1.378	1.373	1.382	–0.005	0.004
9	1.406	1.414	1.401	0.008	–0.005
10	1.378	1.373	1.382	–0.005	0.004
11	1.414	1.422	1.409	0.008	–0.005
12	1.446	1.423	1.450	–0.023	0.004
13	1.410	1.418	1.430	0.008	0.020
14	1.419	1.418	1.419	–0.001	0.000
15	1.419	1.418	1.419	–0.001	0.000
16	1.410	1.418	1.430	0.008	0.020
17	1.446	1.427	1.450	–0.019	0.004
18	1.414	1.422	1.410	0.008	–0.004
19	1.378	1.373	1.382	–0.005	0.004
20	1.406	1.414	1.401	0.008	–0.005
21	1.422	1.432	1.421	0.010	–0.001
22	1.453	1.458	1.435	0.005	–0.018
23	1.453	1.458	1.435	0.005	–0.018
24	1.422	1.432	1.421	0.010	–0.001
25	1.720	1.741	1.696	0.021	–0.024
26	2.446	2.467	2.453	0.021	0.007
27	1.892	1.915	1.889	0.023	–0.003
28	2.446	2.467	2.453	0.021	0.0067
29	1.720	1.741	1.696	0.021	–0.024
30	1.378	1.372	1.382	–0.006	0.004
31	1.414	1.422	1.409	0.008	–0.005
32	1.446	1.427	1.450	–0.019	0.004
33	1.410	1.418	1.430	0.008	0.020
34	1.419	1.418	1.419	–0.001	0.000
35	1.720	1.741	1.696	0.021	–0.024
36	2.446	2.467	2.453	0.021	0.007

TABLE S-III. Bond lengths and their variations in the ionic states of 4Se-HTP

Bond labels	Bond length, Å				
	Ground state	Anion state	Cation state	Δr_{A-G}	Δr_{C-G}
1	1.760	1.784	1.758	0.024	–0.002
2	2.473	2.495	2.475	0.022	0.002
3	1.862	1.883	1.839	0.021	–0.023
4	1.432	1.429	1.431	–0.003	–0.001
5	1.410	1.418	1.428	0.008	0.018
6	1.441	1.424	1.445	–0.017	0.004
7	1.415	1.424	1.412	0.009	–0.003
8	1.376	1.371	1.379	–0.005	0.003
9	1.406	1.414	1.403	0.008	–0.003
10	1.376	1.371	1.379	–0.005	0.003
11	1.415	1.423	1.412	0.008	–0.003
12	1.441	1.424	1.445	–0.017	0.004
13	1.410	1.418	1.428	0.008	0.018
14	1.432	1.429	1.431	–0.003	–0.001
15	1.432	1.429	1.431	–0.003	–0.001
16	1.410	1.418	1.428	0.008	0.018
17	1.441	1.424	1.445	–0.017	0.004
18	1.416	1.423	1.412	0.007	–0.004
19	1.376	1.371	1.379	–0.005	0.003
20	1.406	1.414	1.403	0.008	–0.003
21	1.418	1.428	1.417	0.010	–0.001
22	1.461	1.466	1.444	0.005	–0.017
23	1.461	1.466	1.444	0.005	–0.017
24	1.418	1.428	1.417	0.010	–0.001
25	1.862	1.883	1.839	0.021	–0.023
26	2.473	2.495	2.475	0.022	0.002
27	1.760	1.784	1.758	0.024	–0.002
28	2.473	2.495	2.475	0.022	0.002
29	1.862	1.883	1.839	0.021	–0.023
30	1.376	1.371	1.379	–0.005	0.003
31	1.415	1.424	1.412	0.008	–0.003
32	1.441	1.424	1.445	–0.017	0.004
33	1.410	1.418	1.428	0.008	0.018
34	1.432	1.429	1.431	–0.003	–0.001
35	1.862	1.883	1.839	0.021	–0.023
36	2.473	2.495	2.475	0.022	0.002

TABLE S-IV. Bond lengths and their variations in the ionic states of 6Se-HTP

Bond labels	Bond length, Å				
	Ground state	Anion state	Cation state	Δr_{A-G}	Δr_{C-G}
1	1.908	1.932	1.906	0.024	–0.002
2	2.537	2.559	2.541	0.022	0.004
3	1.867	1.889	1.843	0.022	–0.024
4	1.431	1.428	1.431	–0.003	0.000
5	1.414	1.422	1.433	0.008	0.019
6	1.441	1.425	1.446	–0.017	0.005
7	1.417	1.425	1.413	0.008	–0.004
8	1.375	1.371	1.378	–0.004	0.003
9	1.406	1.414	1.403	0.008	–0.003
10	1.375	1.371	1.378	–0.004	0.003
11	1.417	1.425	1.413	0.008	–0.004
12	1.441	1.425	1.446	–0.016	0.005
13	1.415	1.422	1.433	0.007	0.018
14	1.431	1.428	1.431	–0.003	0.000
15	1.431	1.428	1.431	–0.003	0.000
16	1.415	1.422	1.433	0.007	0.018
17	1.441	1.425	1.446	–0.016	0.005
18	1.417	1.425	1.413	0.008	–0.004
19	1.375	1.371	1.378	–0.004	0.003
20	1.406	1.414	1.403	0.008	–0.003
21	1.417	1.427	1.416	0.010	–0.001
22	1.467	1.472	1.449	0.005	–0.018
23	1.467	1.472	1.449	0.005	–0.018
24	1.417	1.427	1.416	0.010	–0.001
25	1.867	1.889	1.843	0.022	–0.024
26	2.537	2.559	2.541	0.022	0.004
27	1.908	1.932	1.906	0.024	–0.002
28	2.537	2.559	2.541	0.022	0.004
29	1.867	1.889	1.843	0.022	–0.024
30	1.375	1.371	1.378	–0.004	0.003
31	1.417	1.425	1.413	0.008	–0.004
32	1.441	1.425	1.446	–0.016	0.005
33	1.415	1.422	1.432	0.007	0.017
34	1.431	1.428	1.431	–0.003	0.000
35	1.867	1.889	1.843	0.022	–0.024
36	2.537	2.559	2.541	0.022	0.004

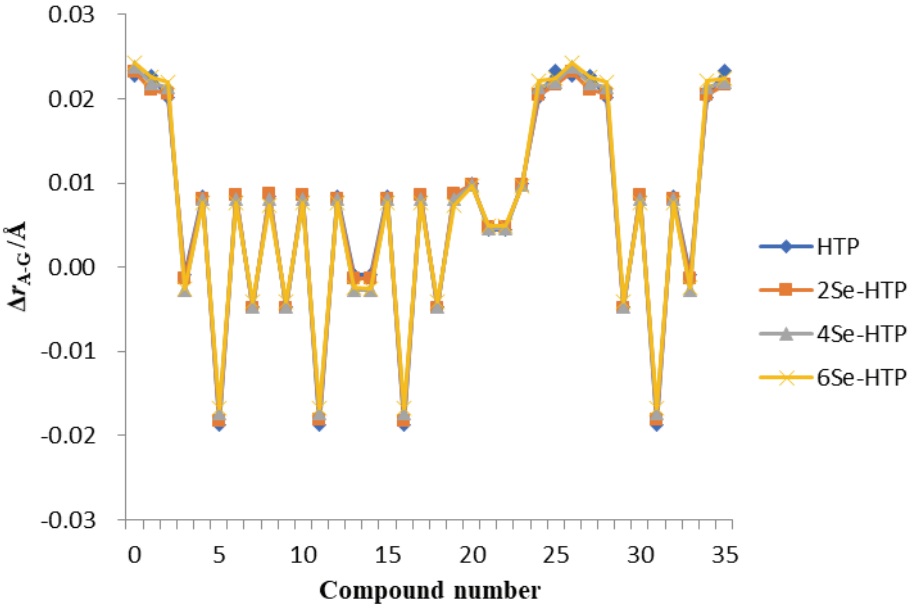

Fig. S-2. Variations of bond lengths ($\Delta r_{A\text{-}G}$) from molecule to anion.

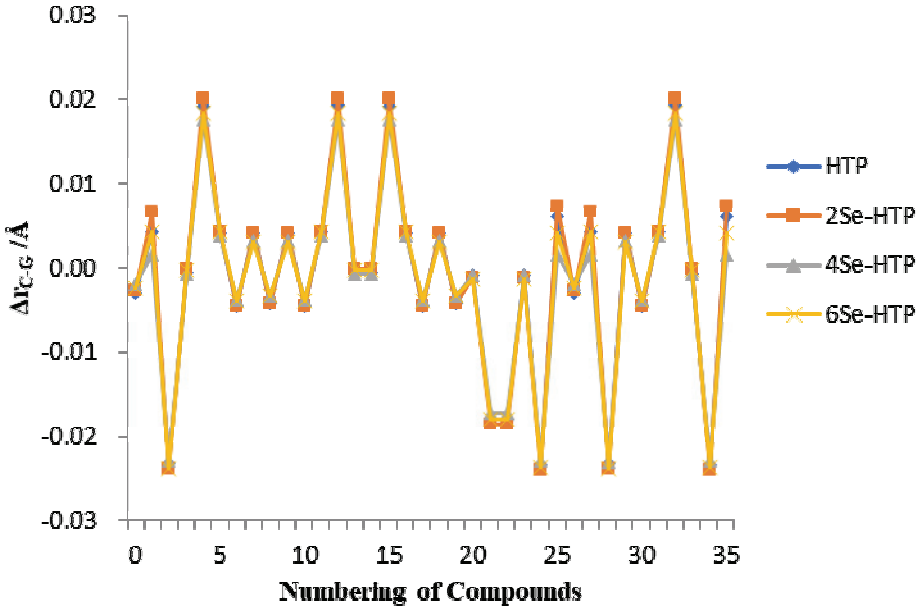

Fig. S-3. Variations of bond lengths ($\Delta r_{C\text{-}G}$) from molecule to cation.