

Supporting Information

Preparation of Carbon Nanodots from Single Chain Polymeric Nanoparticles and Theoretical Investigation of Photoluminescence Mechanism

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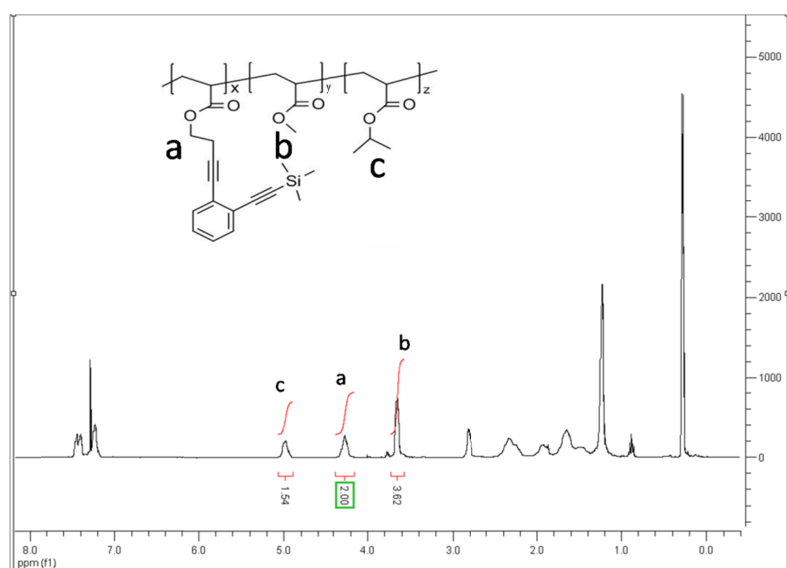


Figure S1. ^1H -NMR spectrum of linear PMA-EDY (LP 3). The molar fraction and quantity of EDY moieties in polymer chain were calculated according to the area integrals of the indicated peaks.

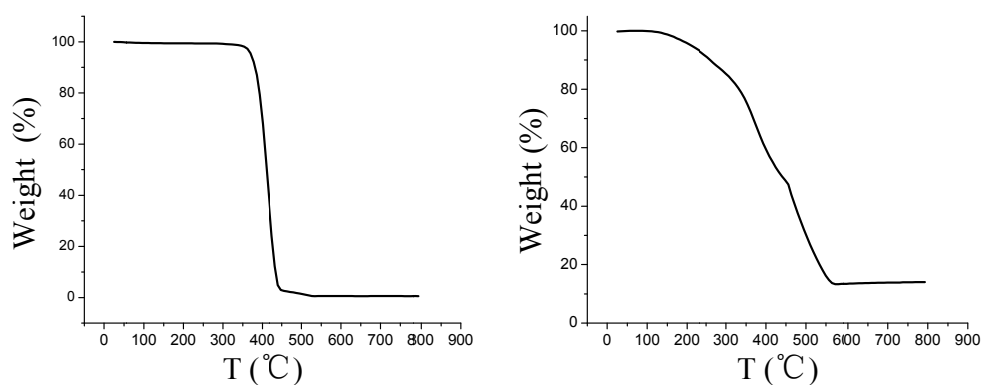


Figure S2. TGA curves of PMA (left) and polymeric nanoparticles (PN 1) (right). (in air, 20 °C/min)

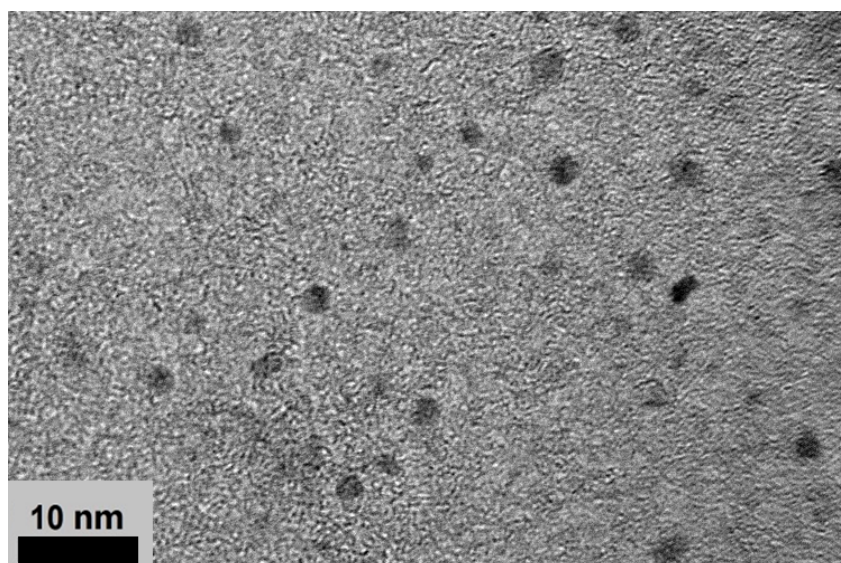


Figure S3. TEM image of CD3

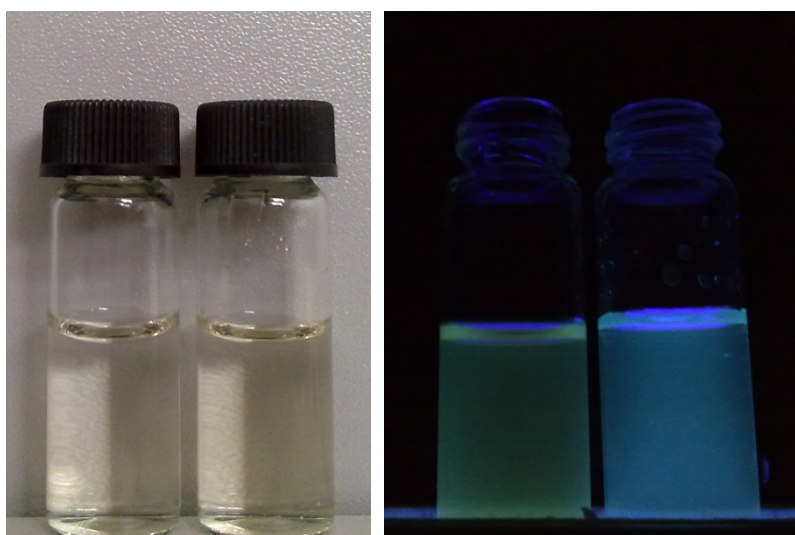


Figure S4. Optical images of carbon dots (CD2 & CD1) under natural light (left) and UV (right)

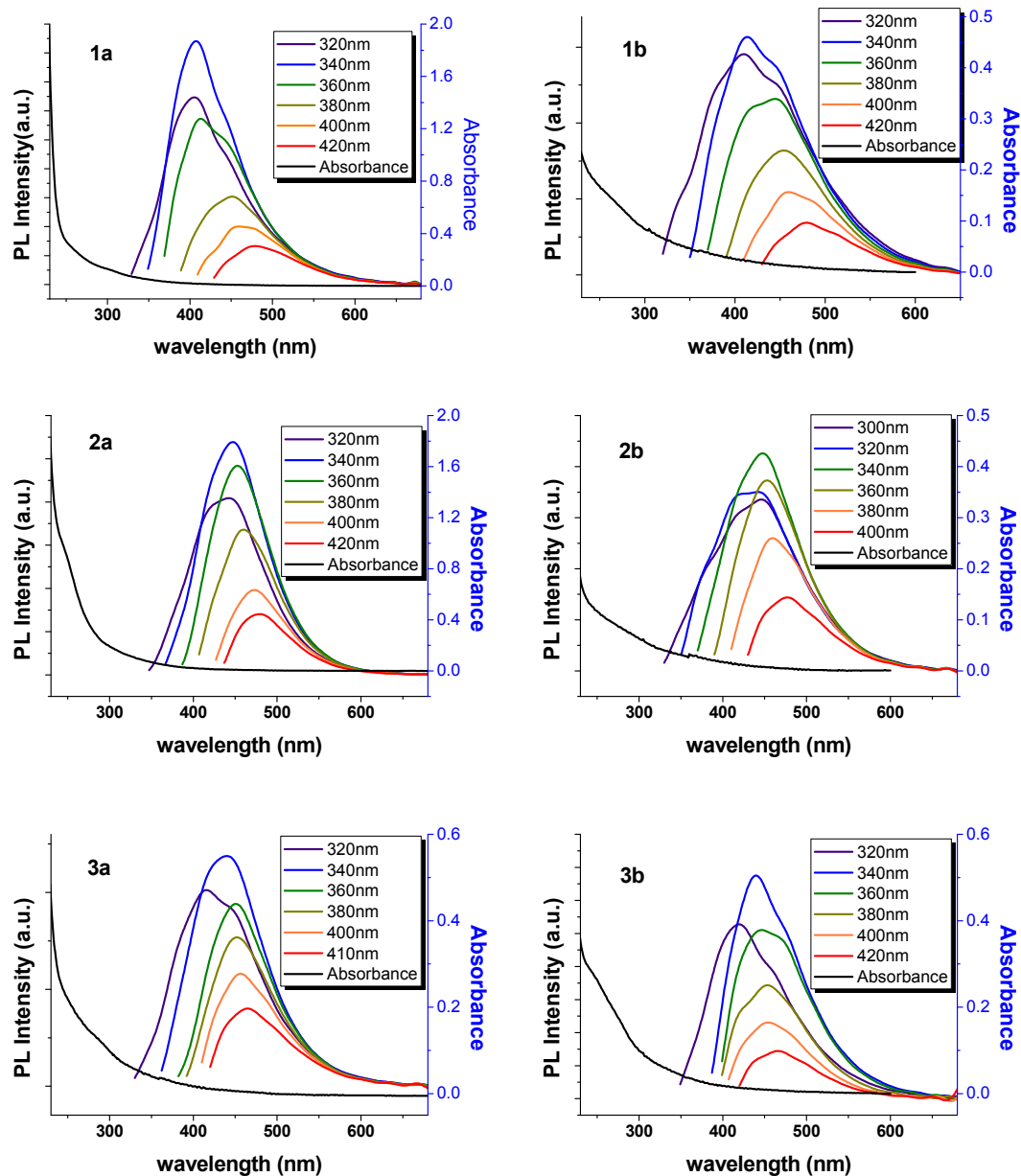


Figure S5. PL & UV-vis spectra of CD1-3(1a, 2a, and 3a) and corresponding surface reduced samples (1b, 2b, and 3b).

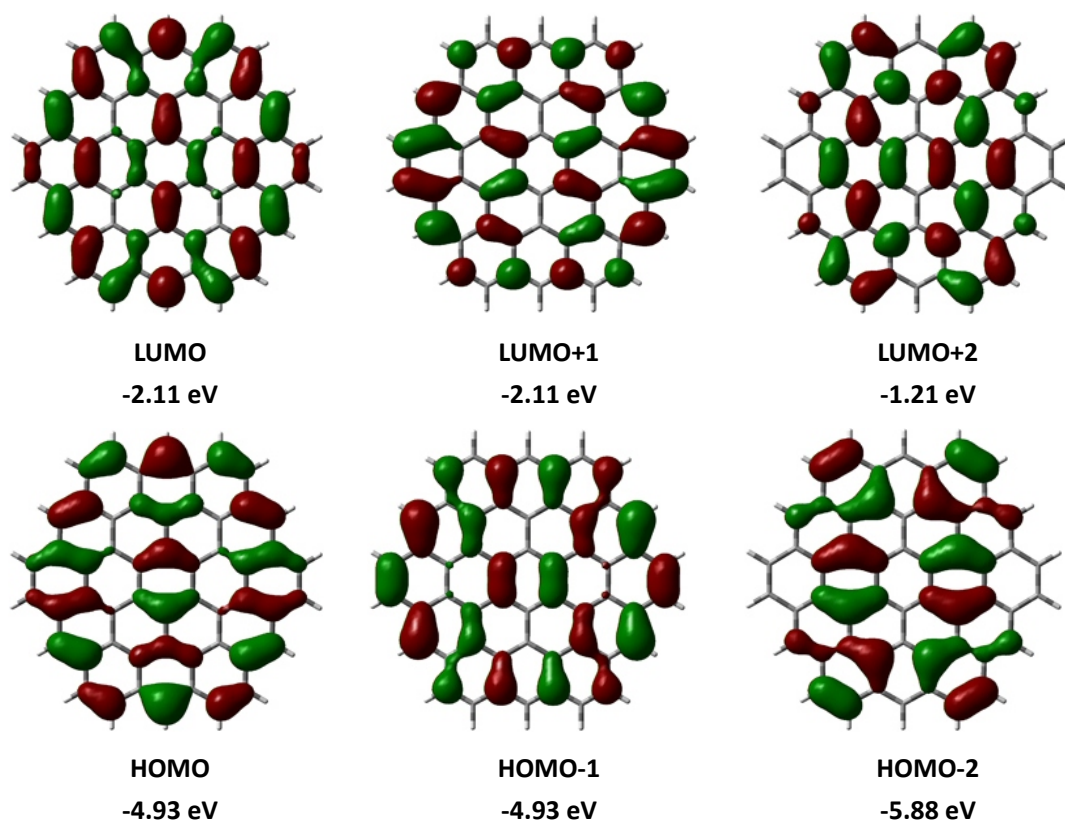


Figure S6. Frontier molecular orbitals of FAR-19.

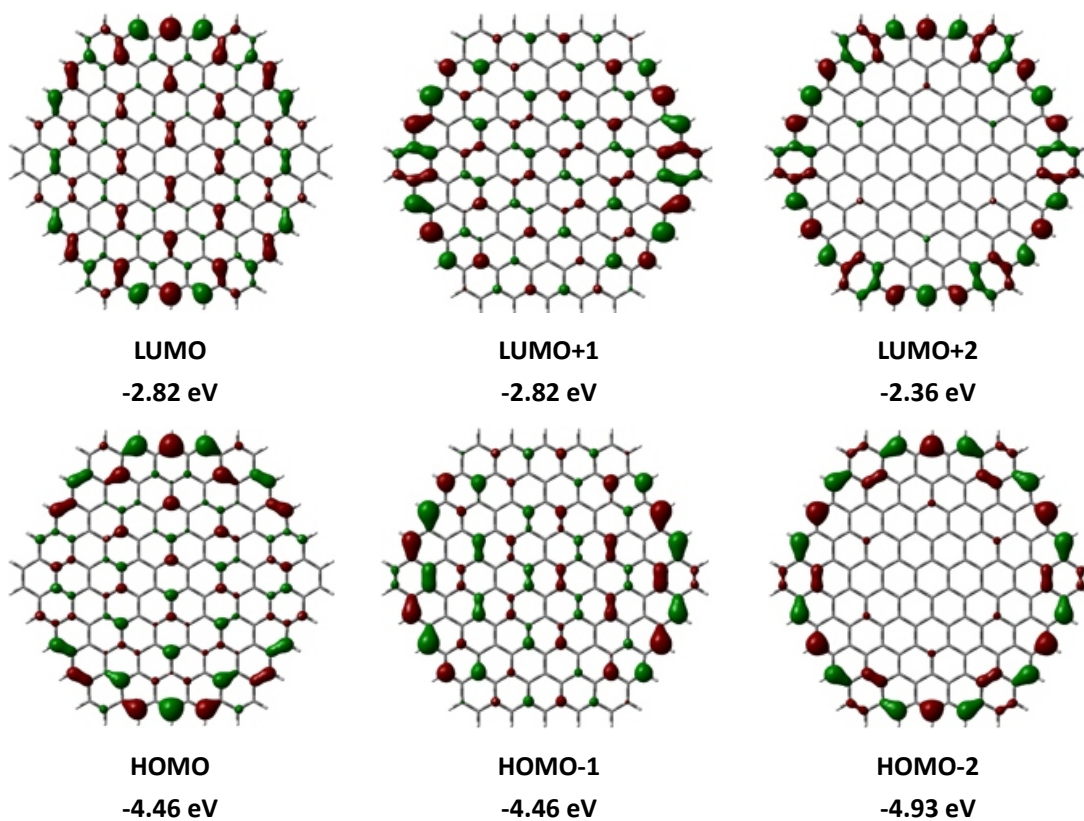


Figure S7. Frontier molecular orbitals of FAR-61.

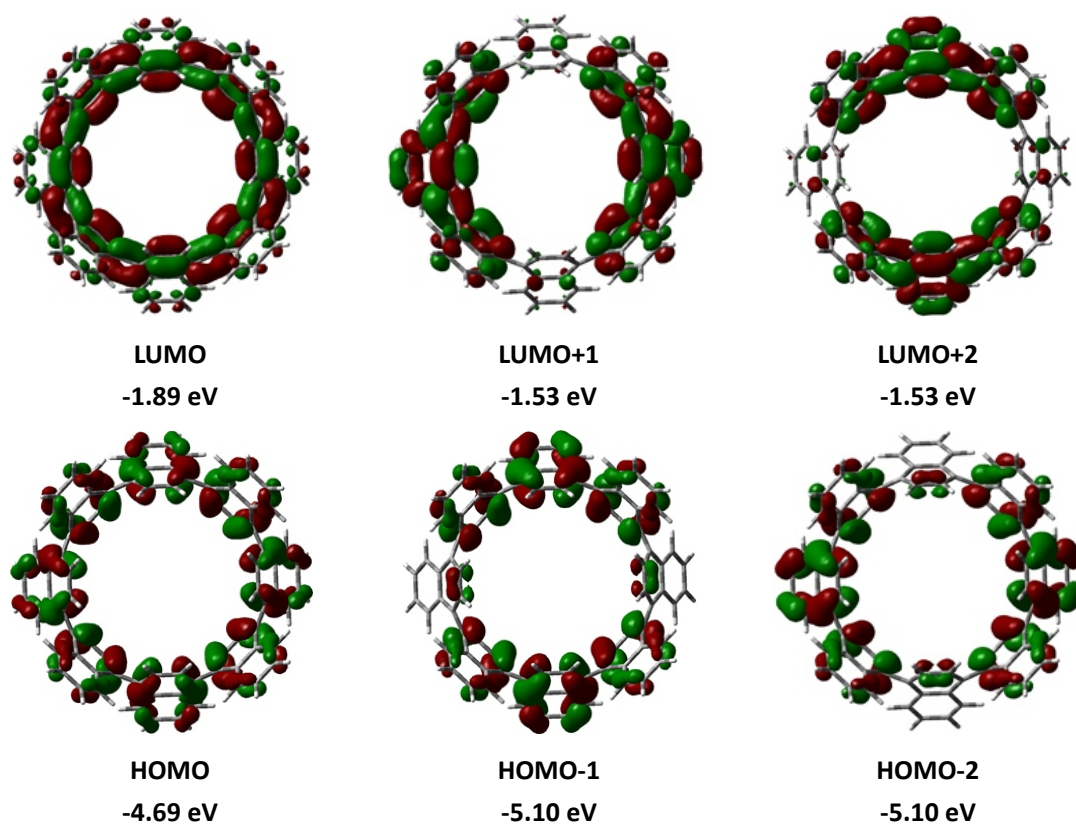


Figure S8. Frontier molecular orbitals of CN-8.

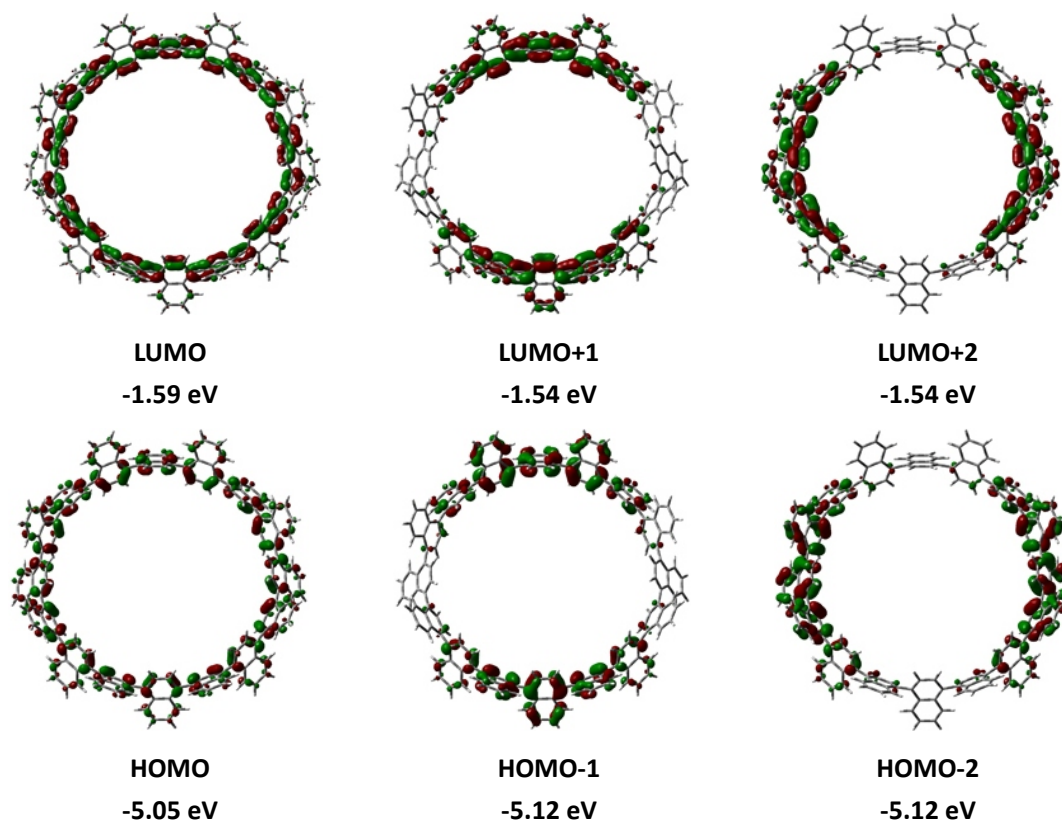


Figure S9. Frontier molecular orbitals of CN-16.

Table S2. Cartesian coordinates of optimized species.

FAR-19

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H	-2.971737	6.483124	2.063164	H	2.971737	6.483124	2.063164
H	-2.971737	-6.483124	2.063164	H	2.971737	-6.483124	2.063164
H	-2.482926	6.685596	-2.063164	H	2.482926	6.685596	-2.063164
H	-2.482926	-6.685596	-2.063164	H	2.482926	-6.685596	-2.063164
H	-2.363843	4.082307	-2.034260	H	2.363843	4.082307	-2.034260
H	-2.363843	-4.082307	-2.034260	H	2.363843	-4.082307	-2.034260
H	-1.248233	7.784300	-3.892348	H	1.248233	7.784300	-3.892348
H	-1.248233	-7.784300	-3.892348	H	1.248233	-7.784300	-3.892348
H	-1.215137	4.558116	2.034260	H	1.215137	4.558116	2.034260
H	-1.215137	-4.558116	2.034260	H	1.215137	-4.558116	2.034260
CN-16							
C	-13.020704	0.706629	-3.059391	C	13.020704	0.706629	-3.059391
C	-13.020704	-0.706629	-3.059391	C	13.020704	-0.706629	-3.059391
C	-12.368664	1.397941	-2.063563	C	12.368664	1.397941	-2.063563
C	-12.368664	-1.397941	-2.063563	C	12.368664	-1.397941	-2.063563
C	-12.299977	4.329968	3.059391	C	12.299977	4.329968	3.059391
C	-12.299977	-4.329968	3.059391	C	12.299977	-4.329968	3.059391
C	-11.962125	3.441754	2.063563	C	11.962125	3.441754	2.063563
C	-11.962125	-3.441754	2.063563	C	11.962125	-3.441754	2.063563
C	-11.759146	5.635648	3.059391	C	11.759146	5.635648	3.059391
C	-11.759146	-5.635648	3.059391	C	11.759146	-5.635648	3.059391
C	-11.682557	0.720049	-1.017765	C	11.682557	0.720049	-1.017765
C	-11.682557	-0.720049	-1.017765	C	11.682557	-0.720049	-1.017765
C	-11.068826	3.805482	1.017765	C	11.068826	3.805482	1.017765
C	-11.068826	-3.805482	1.017765	C	11.068826	-3.805482	1.017765
C	-11.013784	1.430520	0.035074	C	11.013784	1.430520	0.035074
C	-11.013784	-1.430520	0.035074	C	11.013784	-1.430520	0.035074
C	-10.892187	6.024812	2.063563	C	10.892187	6.024812	2.063563
C	-10.892187	-6.024812	2.063563	C	10.892187	-6.024812	2.063563
C	-10.722846	2.893164	-0.035074	C	10.722846	2.893164	-0.035074
C	-10.722846	-2.893164	-0.035074	C	10.722846	-2.893164	-0.035074
C	-10.517725	5.135960	1.017765	C	10.517725	5.135960	1.017765
C	-10.517725	-5.135960	1.017765	C	10.517725	-5.135960	1.017765

C	-10.483406	0.703504	1.088020	C	10.483406	0.703504	1.088020
C	-10.483406	-0.703504	1.088020	C	10.483406	-0.703504	1.088020
C	-9.954624	3.361873	-1.088020	C	9.954624	3.361873	-1.088020
C	-9.954624	-3.361873	-1.088020	C	9.954624	-3.361873	-1.088020
C	-9.734460	7.757473	-2.063563	C	9.734460	7.757473	-2.063563
C	-9.734460	-7.757473	-2.063563	C	9.734460	-7.757473	-2.063563
C	-9.706690	8.707366	-3.059391	C	9.706690	8.707366	-3.059391
C	-9.706690	-8.707366	-3.059391	C	9.706690	-8.707366	-3.059391
C	-9.627973	5.536421	-0.035074	C	9.627973	5.536421	-0.035074
C	-9.627973	-5.536421	-0.035074	C	9.627973	-5.536421	-0.035074
C	-9.416185	4.661779	-1.088020	C	9.416185	4.661779	-1.088020
C	-9.416185	-4.661779	-1.088020	C	9.416185	-4.661779	-1.088020
C	-8.799452	6.776391	0.035074	C	8.799452	6.776391	0.035074
C	-8.799452	-6.776391	0.035074	C	8.799452	-6.776391	0.035074
C	-8.769967	7.751664	-1.017765	C	8.769967	7.751664	-1.017765
C	-8.769967	-7.751664	-1.017765	C	8.769967	-7.751664	-1.017765
C	-8.707366	9.706690	-3.059391	C	8.707366	9.706690	-3.059391
C	-8.707366	-9.706690	-3.059391	C	8.707366	-9.706690	-3.059391
C	-7.910340	6.915436	1.088020	C	7.910340	6.915436	1.088020
C	-7.910340	-6.915436	1.088020	C	7.910340	-6.915436	1.088020
C	-7.757473	9.734460	-2.063563	C	7.757473	9.734460	-2.063563
C	-7.757473	-9.734460	-2.063563	C	7.757473	-9.734460	-2.063563
C	-7.751664	8.769967	-1.017765	C	7.751664	8.769967	-1.017765
C	-7.751664	-8.769967	-1.017765	C	7.751664	-8.769967	-1.017765
C	-6.915436	7.910340	1.088020	C	6.915436	7.910340	1.088020
C	-6.915436	-7.910340	1.088020	C	6.915436	-7.910340	1.088020
C	-6.776391	8.799452	0.035074	C	6.776391	8.799452	0.035074
C	-6.776391	-8.799452	0.035074	C	6.776391	-8.799452	0.035074
C	-6.024812	10.892187	2.063563	C	6.024812	10.892187	2.063563
C	-6.024812	-10.892187	2.063563	C	6.024812	-10.892187	2.063563
C	-5.635648	11.759146	3.059391	C	5.635648	11.759146	3.059391
C	-5.635648	-11.759146	3.059391	C	5.635648	-11.759146	3.059391
C	-5.536421	9.627973	-0.035074	C	5.536421	9.627973	-0.035074
C	-5.536421	-9.627973	-0.035074	C	5.536421	-9.627973	-0.035074
C	-5.135960	10.517725	1.017765	C	5.135960	10.517725	1.017765
C	-5.135960	-10.517725	1.017765	C	5.135960	-10.517725	1.017765
C	-4.661779	9.416185	-1.088020	C	4.661779	9.416185	-1.088020
C	-4.661779	-9.416185	-1.088020	C	4.661779	-9.416185	-1.088020
C	-4.329968	12.299977	3.059391	C	4.329968	12.299977	3.059391
C	-4.329968	-12.299977	3.059391	C	4.329968	-12.299977	3.059391
C	-3.805482	11.068826	1.017765	C	3.805482	11.068826	1.017765
C	-3.805482	-11.068826	1.017765	C	3.805482	-11.068826	1.017765
C	-3.441754	11.962125	2.063563	C	3.441754	11.962125	2.063563
C	-3.441754	-11.962125	2.063563	C	3.441754	-11.962125	2.063563

C	-3.361873	9.954624	-1.088020	C	3.361873	9.954624	-1.088020
C	-3.361873	-9.954624	-1.088020	C	3.361873	-9.954624	-1.088020
C	-2.893164	10.722846	-0.035074	C	2.893164	10.722846	-0.035074
C	-2.893164	-10.722846	-0.035074	C	2.893164	-10.722846	-0.035074
C	-1.430520	11.013784	0.035074	C	1.430520	11.013784	0.035074
C	-1.430520	-11.013784	0.035074	C	1.430520	-11.013784	0.035074
C	-1.397941	12.368664	-2.063563	C	1.397941	12.368664	-2.063563
C	-1.397941	-12.368664	-2.063563	C	1.397941	-12.368664	-2.063563
C	-0.720049	11.682557	-1.017765	C	0.720049	11.682557	-1.017765
C	-0.720049	-11.682557	-1.017765	C	0.720049	-11.682557	-1.017765
C	-0.706629	13.020704	-3.059391	C	0.706629	13.020704	-3.059391
C	-0.706629	-13.020704	-3.059391	C	0.706629	-13.020704	-3.059391
C	-0.703504	10.483406	1.088020	C	0.703504	10.483406	1.088020
C	-0.703504	-10.483406	1.088020	C	0.703504	-10.483406	1.088020
H	-13.546774	1.248468	-3.840807	H	13.546774	1.248468	-3.840807
H	-13.546774	-1.248468	-3.840807	H	13.546774	-1.248468	-3.840807
H	-12.993355	4.030692	3.840807	H	12.993355	4.030692	3.840807
H	-12.993355	-4.030692	3.840807	H	12.993355	-4.030692	3.840807
H	-12.392180	2.445722	2.055630	H	12.392180	2.445722	2.055630
H	-12.392180	-2.445722	2.055630	H	12.392180	-2.445722	2.055630
H	-12.384819	2.482729	-2.055630	H	12.384819	2.482729	-2.055630
H	-12.384819	-2.482729	-2.055630	H	12.384819	-2.482729	-2.055630
H	-12.037819	6.337560	3.840807	H	12.037819	6.337560	3.840807
H	-12.037819	-6.337560	3.840807	H	12.037819	-6.337560	3.840807
H	-10.512944	7.001835	-2.055630	H	10.512944	7.001835	-2.055630
H	-10.512944	-7.001835	-2.055630	H	10.512944	-7.001835	-2.055630
H	-10.491981	7.033208	2.055630	H	10.491981	7.033208	2.055630
H	-10.491981	-7.033208	2.055630	H	10.491981	-7.033208	2.055630
H	-10.461816	8.696215	-3.840807	H	10.461816	8.696215	-3.840807
H	-10.461816	-8.696215	-3.840807	H	10.461816	-8.696215	-3.840807
H	-9.978948	1.228520	1.894016	H	9.978948	1.228520	1.894016
H	-9.978948	-1.228520	1.894016	H	9.978948	-1.228520	1.894016
H	-9.689480	2.683774	-1.894016	H	9.689480	2.683774	-1.894016
H	-9.689480	-2.683774	-1.894016	H	9.689480	-2.683774	-1.894016
H	-8.749212	4.953783	-1.894016	H	8.749212	4.953783	-1.894016
H	-8.749212	-4.953783	-1.894016	H	8.749212	-4.953783	-1.894016
H	-8.696215	10.461816	-3.840807	H	8.696215	10.461816	-3.840807
H	-8.696215	-10.461816	-3.840807	H	8.696215	-10.461816	-3.840807
H	-7.924877	6.187487	1.894016	H	7.924877	6.187487	1.894016
H	-7.924877	-6.187487	1.894016	H	7.924877	-6.187487	1.894016
H	-7.033208	10.491981	2.055630	H	7.033208	10.491981	2.055630
H	-7.033208	-10.491981	2.055630	H	7.033208	-10.491981	2.055630
H	-7.001835	10.512944	-2.055630	H	7.001835	10.512944	-2.055630
H	-7.001835	-10.512944	-2.055630	H	7.001835	-10.512944	-2.055630

H	-6.337560	12.037819	3.840807	H	6.337560	12.037819	3.840807
H	-6.337560	-12.037819	3.840807	H	6.337560	-12.037819	3.840807
H	-6.187487	7.924877	1.894016	H	6.187487	7.924877	1.894016
H	-6.187487	-7.924877	1.894016	H	6.187487	-7.924877	1.894016
H	-4.953783	8.749212	-1.894016	H	4.953783	8.749212	-1.894016
H	-4.953783	-8.749212	-1.894016	H	4.953783	-8.749212	-1.894016
H	-4.030692	12.993355	3.840807	H	4.030692	12.993355	3.840807
H	-4.030692	-12.993355	3.840807	H	4.030692	-12.993355	3.840807
H	-2.683774	9.689480	-1.894016	H	2.683774	9.689480	-1.894016
H	-2.683774	-9.689480	-1.894016	H	2.683774	-9.689480	-1.894016
H	-2.482729	12.384819	-2.055630	H	2.482729	12.384819	-2.055630
H	-2.482729	-12.384819	-2.055630	H	2.482729	-12.384819	-2.055630
H	-2.445722	12.392180	2.055630	H	2.445722	12.392180	2.055630
H	-2.445722	-12.392180	2.055630	H	2.445722	-12.392180	2.055630
H	-1.248468	13.546774	-3.840807	H	1.248468	13.546774	-3.840807
H	-1.248468	-13.546774	-3.840807	H	1.248468	-13.546774	-3.840807
H	-1.228520	9.978948	1.894016	H	1.228520	9.978948	1.894016
H	-1.228520	-9.978948	1.894016	H	1.228520	-9.978948	1.894016