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Supporting Information

Synthesis, Crystal structure, Self-assembly of C_{60} Derivative Bearing Rigid Pyridine Substituent

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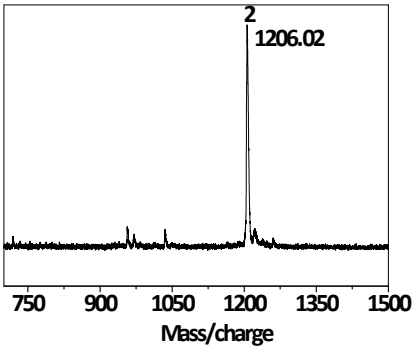

Figure S1. The MALDI-TOF spectra of **2**

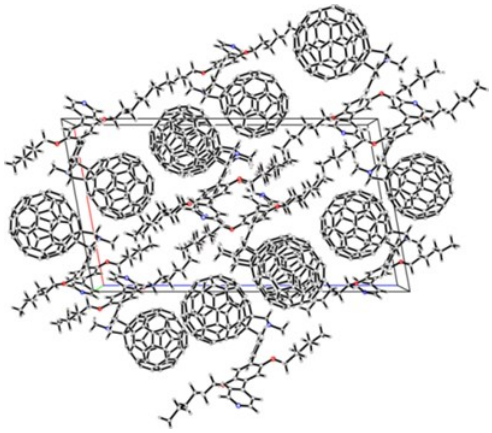

Figure S2. The crystal packing of **2**

Table S1 Redox potentials of compound **2** in comparison with C_{60}

Compound	$E^{0/-1}$	$E^{-1/-2}$	$E^{-2/-3}$	$E^{-3/-4}$

C_{60}	-1.07	-1.46	-1.91	-2.37
2	-1.20	-1.59	-2.11	-

Table S2. Cartesian coordinates of **2**.

2 xyz file

C	5.95273	1.71842	0.07351
C	5.53246	1.89094	1.45727
C	5.45608	0.78951	2.30394
C	6.1974	-0.70177	0.4802
C	6.28067	0.45324	-0.40323
C	4.48499	2.90886	1.48965
C	4.32977	0.65497	3.22605
C	5.70541	-1.83253	-0.29553
C	5.84046	0.03925	-1.73457
C	5.16814	2.62884	-0.75629
C	4.83493	-2.74924	0.28484
C	4.4122	-2.57667	1.67286
C	3.41702	2.78208	2.36934
C	3.96989	-0.75892	3.28597
C	3.33699	1.6253	3.25963
C	5.47766	-1.37336	-1.66397
C	5.09822	0.90761	-2.52441
C	4.75446	2.23658	-2.02323
C	4.2582	3.36169	0.11991
C	3.95828	0.41047	-3.29151
C	3.40374	2.55061	-2.47928
C	2.96978	3.65637	-0.30867
C	4.38575	-1.84426	-2.38318
C	1.93228	1.2366	3.36324
C	2.91648	1.42687	-3.26423
C	2.53014	3.23773	-1.63715
C	1.8456	3.51687	0.61256
C	0.71515	2.99337	-0.13496
C	0.44397	-0.6088	2.65899
C	1.1426	2.81855	-1.5396
C	0.67948	1.75324	-2.28387
C	-0.23758	0.74986	-1.68537
C	1.57888	1.04362	-3.17137
C	3.4634	-2.79188	-1.76524
C	-0.30016	0.25124	1.87819
C	3.60749	-0.93613	-3.21786
C	2.20706	-1.32658	-3.12897
C	0.06098	1.66138	1.81638

C	0.79425	-1.94814	2.13067
C	0.37365	-2.33475	0.87682
C	-0.14862	2.08971	0.44753
C	-0.64986	0.91838	-0.31168
C	1.21678	-0.36574	-3.1041
C	0.06703	-0.50104	-2.19365
C	-0.76511	-0.16315	0.54273
C	2.11809	-2.48818	-2.21223
C	1.27267	-3.03699	0.00539
C	1.05386	-2.61255	-1.34732
C	1.58883	-0.11306	3.41124
C	2.63316	-1.12941	3.36901
C	2.13979	-2.25189	2.57723
C	2.06303	3.09767	1.92453
C	1.14874	2.14746	2.54066
C	5.79348	-0.53691	1.80574
C	4.88031	-1.4961	2.41292
C	3.01122	-2.97053	1.76217
C	3.69078	-3.24765	-0.46896
C	2.56961	-3.36796	0.441
C	-0.23698	-1.78976	-1.47582
C	-0.72128	-1.59681	0.08414
C	-3.36602	-1.5967	0.13545
C	-4.3759	-1.91803	1.05556
C	-3.64794	-0.59501	-0.80927
C	-5.60862	-1.27367	1.0485
H	-4.18572	-2.67991	1.80513
C	-4.88341	0.04509	-0.83571
H	-2.90142	-0.29316	-1.53098
H	-6.4688	-1.7434	1.56263
H	-4.97299	1.02065	-1.35597
C	-2.07566	-2.40867	0.17364
C	-1.37512	-2.648	-2.10225
H	-0.97261	-3.34643	-2.84184
H	-2.06959	-2.96978	1.11454
C	-3.04038	-4.27421	-1.21356
H	-2.73471	-5.00855	-1.96587
H	-3.93528	-3.74299	-1.57393
H	-3.30102	-4.81086	-0.29581
N	-1.89965	-3.38276	-0.93973
H	-2.11723	-1.9993	-2.59423
C	-6.86042	0.22728	0.07547
C	-7.05166	1.39685	0.81082
C	-7.90662	-0.29828	-0.68379

C	-8.28844	2.04204	0.78644
H	-6.22729	1.81145	1.40896
C	-9.14321	0.34654	-0.70775
H	-9.86353	0.12358	-1.54372
C	-10.30875	2.02581	0.0078
C	-11.28773	1.69369	0.94402
C	-10.56627	3.00365	-0.95383
C	-12.52402	2.33983	0.91995
H	-11.08495	0.92342	1.70217
C	-11.80246	3.64925	-0.97813
H	-9.79425	3.2653	-1.69194
H	-13.29557	2.07815	1.65845
H	-12.00573	4.41994	-1.73589
C	-5.88542	-0.28098	0.09415
C	-9.33405	1.51701	0.0271
O	-8.61218	2.97096	1.82432
O	-7.71026	-1.49751	-1.43759
C	-8.69852	4.2887	1.27568
H	-9.68809	4.67008	1.41779
H	-7.9959	4.92723	1.76913
H	-8.47618	4.25477	0.22958
C	-8.97326	-1.98217	-1.90108
H	-9.64621	-2.07177	-1.07403
H	-9.3772	-1.29721	-2.61701
H	-8.8414	-2.9402	-2.35901
N	-12.78128	3.31761	-0.04094