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A theoretical study on ionic liquid endohedral C540 fullerene

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Electronic supplementary information

Table S1 NBO charge transfer energies, ❒*E* (NBO), AIM parameters (electron density, ρ, laplacian of electron density, $\nabla^2\rho$, and ellipticity, ε) and distance, *d*, between donor and acceptor for interionic interactions. All values calculated for the cluster formed by 6_CH_BE confined inside C540. The most relevant interactions are reported in bold. Atom labelling as in Figure 13

NBO			AIM			
Donor	Acceptor	❒*E* (NBO) / kcal mol^{-1}	ρ /a. u.	$\nabla^2\rho$/a. u.	ε/a. u.	*d*/ Å
LP O162	BD* C 57 - H 61	5.22	0.0242	0.0418	0.0175	2.091
BD C161 - O162	BD* C 57 - H 61	0.67				
LP O162	BD* C 45 - H 49	6.60	0.0217	0.0392	0.0042	2.124
LP O162	BD* C 46 - H 47	4.05	0.0171	0.0377	0.0759	2.193
LP O190	**BD* O 62 - H 63**	**10.91**	**0.0230**	**0.0410**	**0.0773**	**2.019**
LP O190	BD* C 23 - H 32	3.34	0.0135	0.0257	0.1697	2.348
LP O190	BD* C 36 - H 40	1.59	0.0099	0.0243	0.2097	2.512
LP O204	BD* C 65 - H 73	5.11	0.0196	0.0330	0.0222	2.158
LP O204	BD* C 78 - H 81	1.87	0.0096	0.0172	0.0872	2.500
LP O 204	**BD* O 125 - H 126**	**19.05**	**0.0350**	**0.0586**	**0.0270**	**1.848**
LP O 205	BD* C 120 - H 123	4.81	0.0268	0.0459	0.0526	2.039
BD C189 - O191	BD* C 24 - H 27	1.18	0.0216	0.0363	0.0259	2.095
LP O191		7.71				
BD C189 - O191	BD* C 44 - H 52	0.98	0.0098	0.0316	0.0664	2.491
LP O191		0.81				
BD C169 - C170	BD* C 44 - H 51	0.87	0.0111	0.0211	0.8147	2.532
BD C170 - H179		1.15				
BD C175 - O176	**BD* C 99 - H103**	**3.10**	**0.0351**	**0.0628**	**0.0507**	**1.875**
LP O176		**8.75**				
C175 - O176	BD* C109 - H110	0.73	0.0141	0.0257	0.0604	2.288
LP O176		1.83				
LP O176	BD* C 87 - H 91	1.92	0.0117	0.0208	0.1822	2.402
LP O176	BD* C107 - H115	2.03	0.0112	0.0252	0.0717	2.432
LP O177	BD* C 65 - H 72	1.38	0.0172	0.0363	0.0834	2.228
LP O177	BD* O104 - H105	3.77	0.0147	0.0267	0.0895	2.247
LP O177	BD* C119 - H121	1.24	0.0099	0.0262	0.0358	2.487
BD C156 - C157	BD* C 57 - H 61	0.36	0.0157	0.0302	0.9701	2.305
BD C157 - C160		0.21				
BD C157 - H166		0.67				
BD C161 - O163	BD* C 88 - H 97	0.24	0.0120	0.0213	0.0542	2.390
LP O163		2.45				
LP O163	BD* C 86 - H 94	1.27	0.0082	0.0253	0.0759	2.520
BD C144 - C146	BD* C 2 - H 10	1.44	0.0158	0.0294	0.4044	2.299
BD C147 - O148	BD* C 4 - H 12	1.13	0.0120	0.0254	0.3916	2.532
LP O148	BD* C 3 - H 7	3.03	0.0160	0.0263	0.0404	2.378
LP O149	BD* C 23 - H 31	6.33	0.0259	0.0451	0.0243	2.036
LP O149	BD* C 25 - H 26	2.88	0.0162	0.0288	0.1139	2.281
LP O149	BD* C 36 - H 39	5.50	0.0214	0.0392	0.0918	2.085
LP O134	BD* O 20 - H 21	7.64	0.0198	0.0289	0.0628	2.176
LP O134	BD* C 87 - H 92	4.51	0.0179	0.0244	0.2214	2.336
LP O134	BD* C 99 - H102	3.84	0.0157	0.0341	0.1036	2.171
BD C133 - O135	BD* C107 - H114	0.53	0.0237	0.0407	0.0842	2.082
LP O135		6.71				
LP O135	BD* C 87 - H 92	1.91	0.0134	0.0235	0.3388	2.349
LP O135	BD* C109 - H117	2.62	0.0128	0.0240	0.1562	2.297