

Supporting Information

The Encapsulated Lithium Effect of $\text{Li}@C_{60}\text{Cl}_8$ Remarkably Enhances the Static First Hyperpolarizability

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Table S1. The NBO charge of all the atoms in C_{60} (C_{2v}), $C_{60}Cl_8$ and $Li@C_{60}Cl_8$ at B3LYP/6-31G(d) level

	$Li@C_{60}Cl_8$	$C_{60}Cl_8$	C_{60} (C_{2v})		$Li@C_{60}Cl_8$	$C_{60}Cl_8$	C_{60} (C_{2v})
$C_{(1)}$	0.00486	0.00551	0.01451	$C_{(35)}$	-0.04086	0.00582	0.003
$C_{(2)}$	-0.00776	-0.00004	0.01451	$C_{(36)}$	-0.02291	0.02748	0.00115
$C_{(3)}$	-0.00776	-0.00003	-0.00922	$C_{(37)}$	-0.05076	0.00038	0.00115
$C_{(4)}$	0.00486	0.00552	0.01662	$C_{(38)}$	-0.04712	-0.05194	-0.00173
$C_{(5)}$	-0.00073	0.00294	-0.00922	$C_{(39)}$	0.01544	0.01615	0.00208
$C_{(6)}$	-0.00073	0.00293	-0.01253	$C_{(40)}$	0.01544	0.01612	0.00134
$C_{(7)}$	-0.00054	-0.00133	0.01356	$C_{(41)}$	0.00891	0.01491	-0.00346
$C_{(8)}$	-0.00054	-0.00137	-0.01253	$C_{(42)}$	-0.00992	-0.00292	-0.00346
$C_{(9)}$	0.00486	0.00553	-0.00302	$C_{(43)}$	0.00463	0.00284	0.00134
$C_{(10)}$	-0.00073	0.00293	0.003	$C_{(44)}$	0.00611	0.0032	0.00208
$C_{(11)}$	0.00486	0.0055	-0.00909	$C_{(45)}$	-0.00294	0.01192	0.00208
$C_{(12)}$	-0.00054	-0.00138	-0.00909	$C_{(46)}$	-0.04484	-0.05204	-0.00173
$C_{(13)}$	0.00923	0.00873	-0.00922	$C_{(47)}$	-0.02291	0.0275	0.0035
$C_{(14)}$	0.00891	0.01489	0.01662	$C_{(48)}$	-0.04086	0.00573	-0.00056
$C_{(15)}$	-0.00992	-0.00288	-0.00922	$C_{(49)}$	-0.04484	-0.05202	-0.00192
$C_{(16)}$	0.00463	0.00285	-0.00909	$C_{(50)}$	-0.04484	-0.05206	0.01356
$C_{(17)}$	-0.00992	-0.00291	-0.00909	$C_{(51)}$	-0.02291	0.02749	-0.00056
$C_{(18)}$	0.00891	0.0149	0.003	$C_{(52)}$	-0.05076	0.00034	0.0035
$C_{(19)}$	0.00923	0.00872	-0.00302	$C_{(53)}$	-0.05076	0.0004	-0.00173
$C_{(20)}$	0.00923	0.00871	0.0035	$C_{(54)}$	-0.04712	-0.05209	0.00208
$C_{(21)}$	0.01544	0.01619	-0.00056	$C_{(55)}$	0.005	0.01455	0.00134
$C_{(22)}$	0.01544	0.01607	-0.00192	$C_{(56)}$	0.00891	0.01487	-0.00021
$C_{(23)}$	-0.04712	-0.05193	-0.00056	$C_{(57)}$	-0.00992	-0.00287	-0.00021
$C_{(24)}$	0.005	0.01456	0.0035	$C_{(58)}$	0.00923	0.0087	0.00134
$C_{(25)}$	-0.00294	0.01197	-0.00173	$C_{(59)}$	-0.00073	0.00295	-0.00346
$C_{(26)}$	0.00611	0.0032	0.00115	$C_{(60)}$	-0.02291	0.02759	-0.00346
$C_{(27)}$	-0.00294	0.01198	0.00115	$Cl_{(1)}$	-0.0158	-0.01793	
$C_{(28)}$	0.005	0.01451	0.003	$Cl_{(2)}$	-0.0158	-0.01818	
$C_{(29)}$	-0.00054	-0.00132	-0.00302	$Cl_{(3)}$	0.01742	0.01792	
$C_{(30)}$	-0.05076	0.00031	-0.01253	$Cl_{(4)}$	0.01742	0.01785	
$C_{(31)}$	-0.04712	-0.05199	0.01451	$Cl_{(5)}$	0.01742	0.01783	
$C_{(32)}$	0.005	0.01453	0.01451	$Cl_{(6)}$	0.01742	0.01831	
$C_{(33)}$	-0.00294	0.01198	-0.01253	$Cl_{(7)}$	-0.0158	-0.01808	
$C_{(34)}$	-0.04484	-0.05233	-0.00302	$Cl_{(8)}$	-0.0158	-0.01819	