

## *Electronic supplementary information*

# **Theoretical Exploration of the Nanoscale Host-Guest Interactions between [n]Cycloparaphenylenes (n=10, 8 and 9) and Fullerene C<sub>60</sub>: From Single- to Three-Potential Well**

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### **Contents:**

**Fig. S1** The configurations (Side view and Top view) of the [8]CPP $\supset$ C<sub>60</sub> host-guest complexes at B3LYP/DFT-D3/6-31G(D) level of theory

**Table S1** The Cartesian coordinates of [8]CPP $\supset$ C<sub>60</sub> optimized at B3LYP/DFT-D3/6-31G(D) level of theory

**Fig. S2** The configurations (Side view and Top view) of the F-[9]CPP $\supset$ C<sub>60</sub> host-guest complexes at B3LYP/DFT-D3/6-31G(D) level of theory

**Table S2** The Cartesian coordinates of F-[9]CPP $\supset$ C<sub>60</sub> optimized at B3LYP/DFT-D3/6-31G(D) level of theory

**Fig. S3** The configurations (Side view and Top view) of the I-[9]CPP $\supset$ C<sub>60</sub> host-guest complexes at B3LYP/DFT-D3/6-31G(D) level of theory

**Table S3** The Cartesian coordinates of I-[9]CPP $\supset$ C<sub>60</sub> optimized at B3LYP/DFT-

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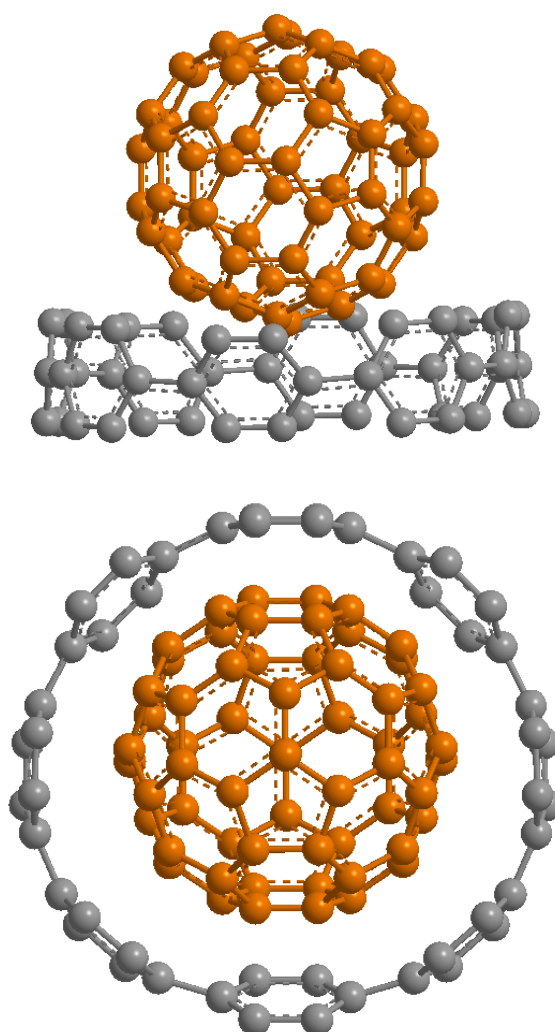
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D3/6-31G(D) level of theory

**Fig. S4** The configurations (Side view and Top view) of the [10]CPP $\supset$ C<sub>60</sub> host-guest complexes at B3LYP/DFT-D3/6-31G(D) level of theory

**Table S4** The Cartesian coordinates of [10]CPP $\supset$ C<sub>60</sub> optimized at B3LYP/DFT-D3/6-31G(D) level of theory

**Fig. S5** Energy profiles of the approach of C<sub>60</sub> through the cavities of [9]CPPs rings at B3LYP/DFT-D3/6-31G(D) level of theory



**Fig. S1** The configurations (Side view and Top view) of the [8]CPP $\supset$ C<sub>60</sub> host-guest complexes at B3LYP/DFT-D3/6-31G(D) level of theory.

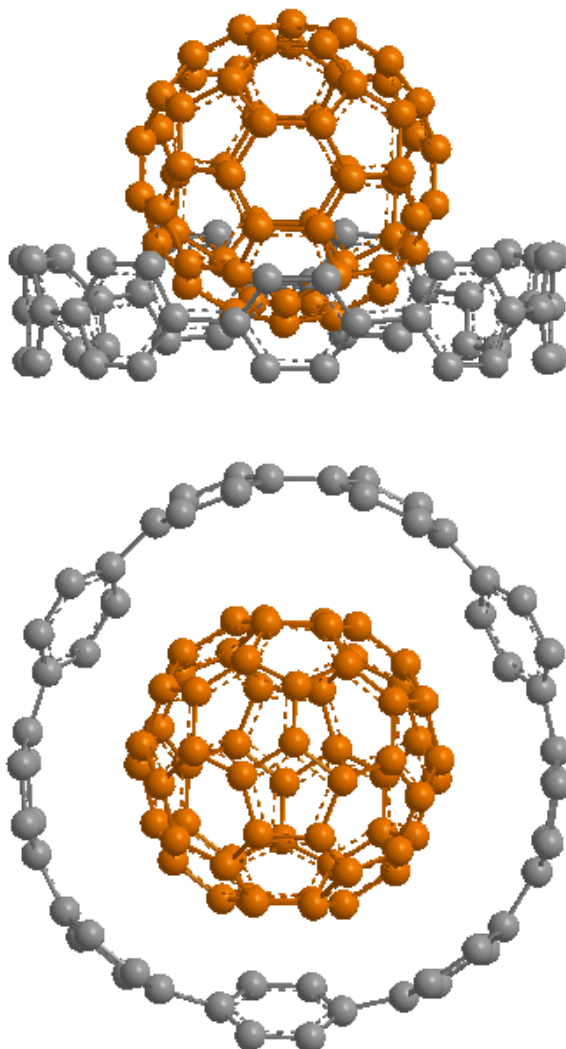
**Table S1** The Cartesian coordinates of [8]CPP $\supset$ C<sub>60</sub> optimized at B3LYP/DFT-D3/6-31G(D) level of theory

Atom	x	y	z
C	5.02496600	-2.55461900	-2.66909400
C	4.64209600	-3.04314600	-3.93492500
C	3.60301300	-3.95124400	-4.07432300
C	2.87990600	-4.41131500	-2.95655200
C	3.45486600	-4.15480900	-1.70069300
C	4.50855000	-3.25558900	-1.56238400
C	-2.82437200	-4.44478400	-2.95251400
C	-3.55446600	-3.99351400	-4.06941500
C	-4.60514600	-3.09912900	-3.92869000
C	-4.99404000	-2.61704600	-2.66223000
C	-4.46725600	-3.31171000	-1.55648800
C	-3.40110800	-4.19599900	-1.69597300
C	-5.59182500	-1.26265900	-2.51802700
C	5.60405500	-1.19207000	-2.52621900
C	5.62527800	-0.53370500	-1.28251800
C	5.55249100	0.85268700	-1.19491600
C	5.45861700	1.65426700	-2.34547400
C	5.75086000	1.01173300	-3.56483900
C	5.81842900	-0.37142100	-3.65284600
C	-2.79428300	4.92981000	-2.14530400
C	-3.60676000	4.61741300	-1.03845500
C	-4.59271600	3.63546000	-1.11301800
C	-4.82281200	2.91136000	-2.29930300
C	-4.12853300	3.35130400	-3.44110000
C	-3.14756000	4.32707500	-3.36647400
C	-5.82126800	-0.44521700	-3.64409700
C	-5.77308000	0.93879100	-3.55639100
C	-5.48672700	1.58548300	-2.33780600
C	-5.56591000	0.78276200	-1.18703300
C	-5.61851100	-0.60456000	-1.27434600
H	5.07871800	-2.62948800	-4.83713800
H	3.28475200	-4.22877100	-5.07447300
H	2.98626500	-4.54180900	-0.80256600
H	4.82604300	-3.00129500	-0.55835800
H	5.55704200	-1.10102700	-0.36193800
H	5.42034300	1.29624600	-0.21525300
H	5.83220900	1.59178900	-4.47853000
H	5.93198500	-0.81153000	-4.63743400
H	-5.93174400	-0.88706100	-4.62827500
H	-5.86505700	1.51762000	-4.46987200
H	-5.43649200	1.22820500	-0.20788300

H	-5.53812100	-1.17050000	-0.35388800
H	-2.92597600	-4.57620500	-0.79821400
H	-4.78761200	-3.06260100	-0.55210800
H	-3.23349600	-4.26626900	-5.06999800
H	-5.04746100	-2.69025600	-4.83031500
H	-5.14323100	3.38653300	-0.21109900
H	-3.42481800	5.09741800	-0.08163100
H	-4.25752200	2.83241600	-4.38395200
H	-2.55648600	4.52230700	-4.25390000
C	-1.46117700	5.57170500	-2.03485600
C	-0.73382600	5.52214300	-0.83365400
C	0.65864300	5.53196000	-0.83478400
C	1.38352800	5.59054800	-2.03704500
C	0.65128400	5.96426700	-3.18268800
C	-0.73561600	5.95530500	-3.18153000
H	-1.24272200	5.31363300	0.09970100
H	1.17188600	5.33121400	0.09775300
H	1.17015200	6.17668800	-4.11220600
H	-1.25868800	6.16134800	-4.11011700
C	3.08324900	4.36633600	-3.37066800
C	4.07592400	3.40259600	-3.44653100
C	4.77707800	2.97112700	-2.30569500
C	4.53920400	3.69194400	-1.11898200
C	3.54158700	4.66192600	-1.04316500
C	2.72420500	4.96480200	-2.14908000
H	2.48876100	4.55438400	-4.25736400
H	4.21016600	2.88557600	-4.38966100
H	5.09360800	3.44957900	-0.21768500
H	3.35494400	5.13939100	-0.08598600
C	-0.66595800	-4.28869200	-4.14776600
C	-1.40168400	-4.84190800	-3.08386700
C	-0.66313700	-5.50924000	-2.08874700
C	0.73251300	-5.50114500	-2.08971300
C	1.46185200	-4.82533700	-3.08589800
C	0.71824400	-4.28065600	-4.14874000
H	-1.18171700	-3.74046600	-4.92766000
H	-1.18243000	-5.99572900	-1.26808700
H	1.25859800	-5.98154300	-1.26975300
H	1.22654400	-3.72641200	-4.92927700
C	1.19767200	-1.53765000	5.30732300
C	0.76321100	-2.74284000	4.61724600
C	1.46632400	-3.20104700	3.50260700
C	2.63408700	-2.47214500	3.03033400
C	3.05050600	-1.31706300	3.69282600

C	2.31740300	-0.83979100	4.85541200
C	0.01135700	-0.81111900	5.73370900
C	-1.15611700	-1.56762400	5.30763000
C	-0.69109000	-2.76138600	4.61747700
C	-1.38246900	-3.23754200	3.50305600
C	0.74527800	-3.69745900	2.34042500
C	2.63350200	-2.51765300	1.57609800
C	3.04393300	-1.40454300	0.84329000
C	3.47866400	-0.20145700	1.53452000
C	3.48388100	-0.15767800	2.92877500
C	3.02171300	1.03643800	3.61959700
C	2.29898900	0.61472600	4.80970800
C	1.16129100	1.31124200	5.21741600
C	-0.00646500	0.58305200	5.68929200
C	-2.29347300	-0.89869400	4.85598400
C	-2.31215000	0.55581000	4.81017700
C	-1.19257100	1.28123500	5.21773100
C	-0.75816300	2.44048800	4.45292800
C	0.69722000	2.45908700	4.45280000
C	1.38970700	2.86309000	3.31147600
C	2.57559100	2.13562900	2.88535300
C	2.57446000	2.08930200	1.43084700
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C	0.01332200	-1.03149800	-1.23769700
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C	-2.28838100	-1.06067800	-0.34997900
C	-2.30831200	0.39206100	-0.39670600
C	-0.75533100	2.29048200	-0.15662500
C	0.69721200	2.30867600	-0.15673200
C	1.16413000	1.11997800	-0.85348700
C	2.29851400	0.45093400	-0.39739300
C	2.31540300	-1.00188900	-0.35059900
C	1.19932500	-1.72814300	-0.76127600
C	-0.68930000	-2.90208400	0.00896700
C	-1.38109200	-3.31085800	1.14905600
C	-2.56706200	-2.58395600	1.57684500
C	-3.00609800	-1.48172800	0.84425900
C	-3.47116100	-0.29015500	1.53548000
C	-3.03561000	0.86752000	0.77073200
C	-2.62631600	2.02314800	1.43136600
C	-1.45801100	2.74761600	0.95799000
C	1.38806400	2.78348900	0.95779900

C	0.65673400	3.26454700	2.11907700
C	-0.73886800	3.24688400	2.11918600
C	-1.46105600	2.82675100	3.31173800
C	-2.62824600	2.06935500	2.88597200
C	-3.04568100	0.95899300	3.62042000
C	-3.47750600	-0.24655700	2.92972700
C	-3.01443200	-1.39461900	3.69355900
C	-2.56841000	-2.53858900	3.03098100
C	0.76361500	-2.88330000	0.00898700
C	-0.64938000	-3.71535100	2.34054900
C	-1.19174700	1.09008100	-0.85320700



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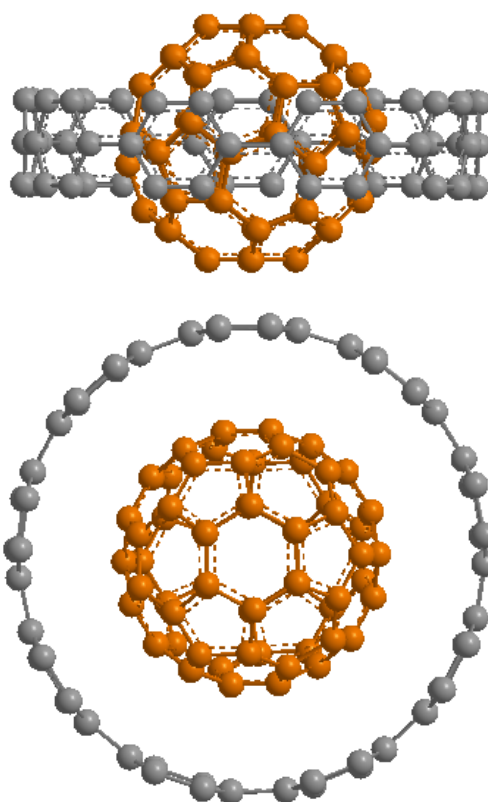
Atom	x	y	z
C	-3.27255200	5.48850100	-1.50942200
C	-2.63496500	5.73093400	-2.74283100
C	-1.28941800	6.05644800	-2.81258600
C	-0.49561300	6.13998800	-1.65323700
C	-1.18340600	6.14982400	-0.42916600
C	-2.54041400	5.84059300	-0.36024800
C	6.45893800	0.03968000	-1.44173000
C	6.47420900	-0.68819700	-2.65027200
C	6.07974200	-2.01596500	-2.70153300
C	5.64749400	-2.69631800	-1.54634500
C	5.90227400	-2.06094300	-0.32206000
C	6.29746200	-0.72471900	-0.27174200
C	4.70699300	-3.83819700	-1.64623000
C	-4.47476300	4.61556000	-1.44974000
C	-4.84834200	3.96930200	-0.25661800
C	-5.55442800	2.76977300	-0.27067700
C	-5.92101500	2.15952300	-1.48062800
C	-5.78940700	2.94318400	-2.64218400
C	-5.08937200	4.14081300	-2.62622000
C	-1.82597900	-6.11502400	-1.51929500
C	-1.04354000	-6.27004100	-0.35984100
C	0.34872400	-6.25397900	-0.41357200
C	1.02923900	-6.09665000	-1.63169500
C	0.25005100	-6.22048700	-2.79778400
C	-1.13509200	-6.22110400	-2.74364000
C	3.82807800	-3.86007000	-2.74404000
C	2.71109000	-4.67712300	-2.76505700
C	2.39899600	-5.53208400	-1.69227500
C	3.33350100	-5.59316900	-0.64204100
C	4.45629500	-4.76484600	-0.61744700
H	-3.16186600	5.55825600	-3.67404300
H	-0.82810300	6.15819000	-3.78981200
H	-0.63084900	6.25983200	0.49811700
H	-2.99293700	5.75559900	0.62155200
H	-4.46714000	4.31912800	0.69479800
H	-5.68321900	2.23304900	0.66257100
H	-6.16967100	2.56943800	-3.58821100
H	-4.94642300	4.66116900	-3.56691800
H	3.95292200	-3.13716900	-3.54227900
H	2.00606700	-4.55974200	-3.57981600
H	3.16171400	-6.26556000	0.19366000

H	5.12584600	-4.81357600	0.23674400
H	6.33968500	-0.24900500	0.70171500
H	5.63747200	-2.55610000	0.60627800
H	6.69909900	-0.19135900	-3.58704300
H	6.02310800	-2.50783600	-3.66776600
H	0.89953800	-6.21842300	0.52031800
H	-1.51258200	-6.27629500	0.61784600
H	0.73218400	-6.22686400	-3.77013100
H	-1.67746600	-6.19704700	-3.68174200
C	-3.19966000	-5.54675300	-1.47785200
C	-3.73872300	-5.02530000	-0.28719600
C	-4.70930700	-4.02772100	-0.30327700
C	-5.19560900	-3.50825400	-1.51312900
C	-4.85559000	-4.21848700	-2.68001600
C	-3.88577600	-5.21038300	-2.66252600
H	-3.30499200	-5.29024400	0.66906700
H	-4.97479200	-3.54943300	0.63315500
H	-5.29809200	-3.93527700	-3.63031900
H	-3.60192900	-5.66139100	-3.60694700
C	-5.41152400	-1.34613100	-2.69145600
C	-5.58813200	0.02771400	-2.68265100
C	-6.12306300	0.69420200	-1.56579200
C	-6.58289300	-0.10885500	-0.50652500
C	-6.40616300	-1.49242400	-0.51614000
C	-5.75988700	-2.14029200	-1.58460000
H	-4.88045100	-1.79404100	-3.52400200
H	-5.18957000	0.60656800	-3.50855700
H	-7.04246900	0.35729500	0.36049800
H	-6.73269700	-2.07013500	0.34390600
C	6.27246200	1.51657300	-1.44914700
C	6.09818800	2.20917200	-2.66574600
C	5.38909300	3.39841800	-2.72726400
C	4.81153300	3.96622100	-1.57523000
C	5.21985500	3.42781100	-0.34619100
C	5.93362000	2.23132700	-0.28546500
H	6.42852500	1.76882300	-3.59936900
H	5.20358000	3.84835000	-3.69788200
H	4.84206600	3.85239000	0.57825700
H	6.09808400	1.79263300	0.69251300
C	2.73931800	4.59758200	-2.75329900
C	3.61724400	4.83818400	-1.68116400
C	3.16881400	5.71708200	-0.67860200
C	1.87764800	6.24682900	-0.70170900
C	0.96844600	5.91765500	-1.72345600



C	1. 45707800	5. 11764800	-2. 77239600
H	3. 02364600	3. 89283100	-3. 52646400
H	3. 82363300	5. 96167000	0. 15316400
H	1. 56090000	6. 89250900	0. 11255100
H	0. 78479500	4. 79874500	-3. 56043100
C	0. 63859700	-2. 33382800	4. 17015900
C	1. 96602500	-2. 17207700	3. 59625300
C	2. 64986600	-0. 96512600	3. 75412500
C	2. 03575000	0. 12943400	4. 49154500
C	0. 76346800	-0. 02732100	5. 04166600
C	0. 04991800	-1. 28485700	4. 87823900
C	-0. 15870200	-3. 12159200	3. 24294400
C	0. 67483600	-3. 44592700	2. 09507100
C	1. 98857100	-2. 85910900	2. 31395700
C	2. 68858200	-2. 30976100	1. 23944800
C	3. 38406200	-0. 39633300	2. 63597500
C	2. 39356800	1. 37568800	3. 82998300
C	1. 46470400	2. 41442200	3. 74603700
C	0. 13766600	2. 24981400	4. 32045300
C	-0. 20560600	1. 05514400	4. 95511100
C	-1. 51792800	0. 46636700	4. 73774500
C	-1. 36008600	-0. 97961000	4. 69057000
C	-2. 12447800	-1. 73513600	3. 80058600
C	-1. 51057400	-2. 82736500	3. 06231100
C	0. 12375700	-3. 44702100	0. 81510600
C	-1. 28293800	-3. 14435700	0. 62582500
C	-2. 08248200	-2. 84060600	1. 72524700
C	-3. 05517000	-1. 76327200	1. 63675400
C	-3. 07997400	-1. 07838600	2. 92025600
C	-3. 23118400	0. 30717600	2. 96539700
C	-2. 43387000	1. 09597000	3. 89365000
C	-2. 07525400	2. 34000000	3. 23125500
C	-0. 81724500	2. 90541800	3. 44052900
C	3. 22562800	1. 05207100	2. 68291300
C	0. 20206600	3. 12791500	-0. 11106300
C	1. 55048700	2. 83630600	0. 07054900
C	2. 16255600	1. 74549200	-0. 66948100
C	1. 40154600	0. 99183500	-1. 56485700
C	-0. 00952500	1. 29736200	-1. 75330200
C	-1. 92241300	2. 17866800	-0. 46504700
C	-1. 93973600	2. 85811600	0. 82177500
C	-0. 62853200	3. 44397000	1. 04085600
C	-0. 08050900	3. 47461500	2. 32167000
C	1. 33020500	3. 17143200	2. 51139800

C	2.12494400	2.85691200	1.40883000
C	3.10738500	1.08504200	0.21424400
C	3.25800000	-0.29465900	0.16884300
C	2.47238900	-1.08462800	-0.76379900
C	1.55953100	-0.45527400	-1.61248300
C	0.24624700	-1.04479100	-1.83090600
C	-0.72457800	0.03864200	-1.91647100
C	-1.99728200	-0.11848100	-1.36490500
C	-2.60847400	0.97558700	-0.62367900
C	-2.64815700	2.31820700	1.89353900
C	-3.36351500	1.06236400	1.72858800
C	-3.33883700	0.40447800	0.49847900
C	-3.18205300	-1.03859100	0.45134600
C	-2.35360700	-1.36471100	-0.70033400
C	-1.42288900	-2.39868900	-0.61509100
C	-0.09605400	-2.23899600	-1.19373000
C	0.85932400	-2.88955500	-0.30932700
C	2.11417700	-2.32653100	-0.09901900
C	3.08616000	1.77195300	1.49854700
C	3.39211700	-1.05099600	1.40642300
C	-0.59683600	2.34566800	-1.04221300



**Fig. S3** The configurations (Side view and Top view) of the I-[9]CPP@C<sub>60</sub> host-guest complexes at B3LYP/DFT-D3/6-31G(D) level of theory.

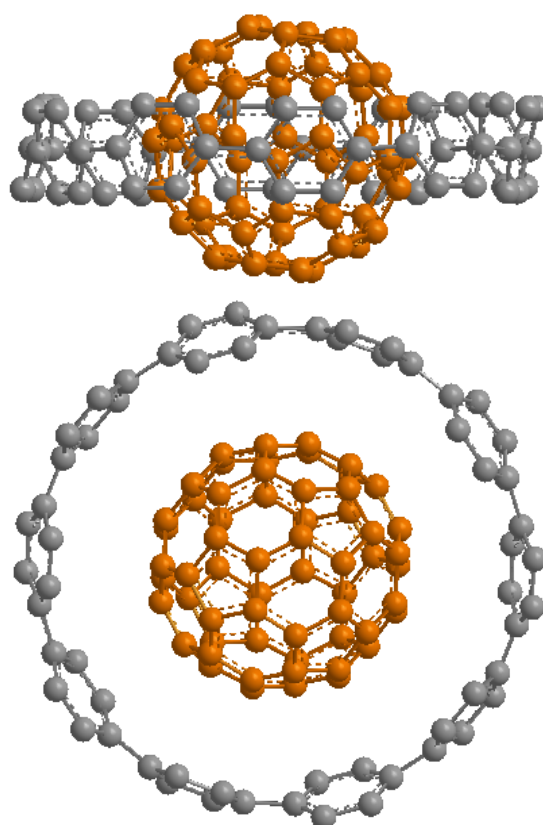
**Table S3** The Cartesian coordinates of I-[9]CPP $\supset$ C<sub>60</sub> optimized at B3LYP/DFT-D3/6-31G(D) level of theory

Atom	x	y	z
C	-2.93266600	5.64565800	-0.02478600
C	-3.60996500	5.27727800	1.15977500
C	-4.68370600	4.38508600	1.16510400
C	-5.16609800	3.77798400	-0.01487600
C	-4.64242500	4.32849700	-1.20442400
C	-3.57232800	5.22607600	-1.20982800
C	-3.42362500	-5.36245600	-0.02406300
C	-2.76956700	-5.77928700	1.15761300
C	-1.45984300	-6.26238200	1.16070100
C	-0.68961300	-6.36179700	-0.01868500
C	-1.42478100	-6.16942200	-1.20796600
C	-2.73713100	-5.69144700	-1.21122100
C	0.81543900	-6.34795800	-0.00663600
C	-1.51666300	6.15937200	-0.01935700
C	-0.75212600	6.27415200	-1.20326500
C	0.64327000	6.29024300	-1.19850400
C	1.39469300	6.18792900	-0.00827400
C	0.62804100	6.30810800	1.17386400
C	-0.76762500	6.29740400	1.16907800
C	6.09414900	-1.76707600	-0.01654900
C	5.80557000	-2.48234100	-1.20161900
C	5.12136500	-3.69858200	-1.19822000
C	4.66161100	-4.30179500	-0.00810100
C	5.15234600	-3.70126600	1.17435400
C	5.84153000	-2.48754000	1.17077700
C	1.54780500	-6.14726100	1.18312300
C	2.85069700	-5.64365200	1.18781500
C	3.52933200	-5.29495700	0.00171800
C	2.88288800	-5.71987400	-1.18126700
C	1.58292500	-6.22818000	-1.18583500
H	-3.23169900	5.60299800	2.12285800
H	-5.07040800	4.07930100	2.13158600
H	-4.98516300	3.96386900	-2.16671800
H	-3.16529200	5.50416300	-2.17587100
H	-1.24331100	6.24317500	-2.16969500
H	1.14294700	6.26596200	-2.16096900
H	1.12032600	6.30723200	2.14039900
H	-1.26749400	6.28340700	2.13172200
H	1.05967900	-6.26143200	2.14495100
H	3.28681500	-5.40969900	2.15286000

H	3. 35554900	-5. 55806200	-2. 14416900
H	1. 13186800	-6. 43074400	-2. 15159200
H	-3. 17716100	-5. 46137400	-2. 17539400
H	-0. 93379600	-6. 26867600	-2. 16994200
H	-3. 24587200	-5. 63056600	2. 12089300
H	-1. 00506600	-6. 45956400	2. 12580800
H	4. 84430900	-4. 11472500	-2. 16082400
H	6. 01938100	-2. 03771800	-2. 16744800
H	4. 90814500	-4. 12999800	2. 14030600
H	6. 08334300	-2. 05059200	2. 13380700
C	6. 35785700	-0. 28409000	-0. 01983800
C	6. 31772800	0. 48061100	-1. 20439400
C	6. 07543700	1. 85610800	-1. 19887500
C	5. 85681900	2. 58398600	-0. 00948300
C	6. 13957800	1. 86212400	1. 17062100
C	6. 37488700	0. 48601500	1. 16521500
H	6. 35888700	-0. 01031300	-2. 17057300
H	5. 93387100	2. 33571900	-2. 16133400
H	6. 06711200	2. 34958900	2. 13721100
H	6. 46495700	-0. 00506300	2. 12826400
C	4. 55200200	4. 41906000	1. 18698500
C	3. 46369500	5. 29475300	1. 18901800
C	2. 82058200	5. 70259000	0. 00196200
C	3. 50959500	5. 34903200	-1. 18030300
C	4. 60020900	4. 47782000	-1. 18229700
C	5. 09092400	3. 87993600	-0. 00097500
H	4. 89716700	4. 05937800	2. 15024300
H	3. 04483500	5. 56044800	2. 15347600
H	3. 13001200	5. 67001900	-2. 14442300
H	4. 99740400	4. 18187900	-2. 14754600
C	-4. 57663900	-4. 39332700	-0. 01244100
C	-5. 05259000	-3. 80416600	1. 17847500
C	-5. 75984600	-2. 60093400	1. 18419600
C	-6. 05727300	-1. 88683300	0. 00067700
C	-5. 78704000	-2. 59768500	-1. 18844400
C	-5. 07486300	-3. 79786500	-1. 19429400
H	-4. 77114300	-4. 21944300	2. 14023200
H	-5. 98560500	-2. 16386700	2. 15079000
H	-6. 03408900	-2. 16155600	-2. 15048200
H	-4. 81919300	-4. 21807600	-2. 16103700
C	-6. 32676000	0. 35554700	1. 19031200
C	-6. 35098600	-0. 40963500	0. 00563900
C	-6. 38352300	0. 35969700	-1. 17953600
C	-6. 17480300	1. 73989300	-1. 18526000

C	-5.90613700	2.46710200	-0.00508600
C	-6.11172500	1.73568100	1.18452400
H	-6.35874300	-0.13632200	2.15648300
H	-6.46534900	-0.13329100	-2.14237300
H	-6.11181700	2.22862900	-2.15183500
H	-5.98153500	2.21896700	2.14681000
C	1.26487500	-0.68559400	-3.26567200
C	0.01180000	-1.42500200	-3.27087600
C	-1.20575100	-0.73788500	-3.27656100
C	-1.21968500	0.71712900	-3.27607400
C	-0.01581300	1.42813900	-3.27088900
C	1.25098500	0.71240200	-3.26465000
C	2.20395200	-1.40298000	-2.41458700
C	1.53294900	-2.58176000	-1.89222100
C	0.18025900	-2.59805100	-2.42451200
C	-0.86831000	-3.01973700	-1.60977800
C	-2.30214300	-1.19613200	-2.43482300
C	-2.32517600	1.15411400	-2.43482900
C	-2.17167600	2.26976900	-1.61420300
C	-0.92589400	3.00938200	-1.60946700
C	0.13007100	2.60293800	-2.42264300
C	1.48255500	2.61228100	-1.89050300
C	2.17676600	1.44772900	-2.41440200
C	3.06082100	0.75337500	-1.59098100
C	3.07824900	-0.69524700	-1.59256900
C	1.76004600	-2.98025300	-0.57656000
C	2.67720900	-2.25519200	0.27181600
C	3.31277900	-1.13359300	-0.22580800
C	3.45780100	0.02872400	0.61910700
C	3.28920800	1.19092200	-0.22479700
C	2.63456700	2.29912700	0.27266200
C	1.70542400	3.01279200	-0.57467800
C	0.61304200	3.44692400	0.26464400
C	-0.67264600	3.43528400	-0.24202300
C	-2.99063900	-0.02792700	-1.91176100
C	-2.20171100	1.40780700	2.43526000
C	-3.07379700	0.69866800	1.61173400
C	-3.06636800	-0.75014100	1.61245400
C	-2.17927400	-1.44295400	2.43381900
C	-1.25265100	-0.70960200	3.28488800
C	-0.00902000	1.42600700	3.29147500
C	-0.17537400	2.59894400	2.44445800
C	-1.52796000	2.58516000	1.91264200
C	-1.75724100	2.98183000	0.59674600

C	-2.67380300	2.25249600	-0.25113000
C	-3.30950800	1.13307000	0.24567200
C	-3.29321000	-1.19153100	0.24510100
C	-2.63757300	-2.30127800	-0.25320000
C	-1.70822300	-3.01127100	0.59492800
C	-1.48782800	-2.60955700	1.91079200
C	-0.13490900	-2.60259500	2.44299400
C	0.01309400	-1.42722600	3.28988700
C	1.21869800	-0.71922400	3.29628600
C	1.20681800	0.73584100	3.29580300
C	0.87355300	3.02471200	1.63183000
C	2.13180800	2.30627500	1.63583200
C	2.30453400	1.19264300	2.45527700
C	2.99099400	0.02269900	1.93193100
C	2.32316300	-1.15790900	2.45435000
C	2.17271800	-2.27574700	1.63578900
C	0.92117200	-3.00605400	1.62844600
C	0.67190100	-3.43137500	0.26183400
C	-0.61206300	-3.44223000	-0.24373400
C	-3.45795900	-0.03118600	-0.59908300
C	-2.13199700	-2.31124000	-1.61671900
C	-1.26321500	0.68840900	3.28502300



**Fig. S4** The configurations (Side view and Top view) of the [10]CPP $\supset$ C<sub>60</sub> host-guest complexes at B3LYP/DFT-D3/6-31G(D) level of theory.

**Table S4** The Cartesian coordinates of [10]CPP $\supset$ C<sub>60</sub> optimized at B3LYP/DFT-D3/6-31G(D) level of theory

Atom	x	y	z
C	-4.37002700	5.31798600	-0.04803300
C	-5.17078700	5.03888900	1.07331500
C	-6.05729400	3.96747500	1.07363200
C	-6.18093100	3.12784800	-0.04676500
C	-5.50501600	3.51239200	-1.21705300
C	-4.62042200	4.58128800	-1.21749200
C	-3.73763100	-5.78941000	0.03627800
C	-2.98457600	-5.84990400	1.21957100
C	-1.68662400	-6.34555900	1.21967800
C	-1.08253000	-6.80751300	0.03817600
C	-1.90191800	-6.91603900	-1.09986500
C	-3.19866300	-6.41766700	-1.10107300
C	0.39283800	-6.87887200	-0.04180900
C	-3.13480800	6.12722000	0.03670200
C	-2.53676000	6.70192200	-1.09938500
C	-1.19730400	7.07029500	-1.09733700
C	-0.39254700	6.87946000	0.04029600

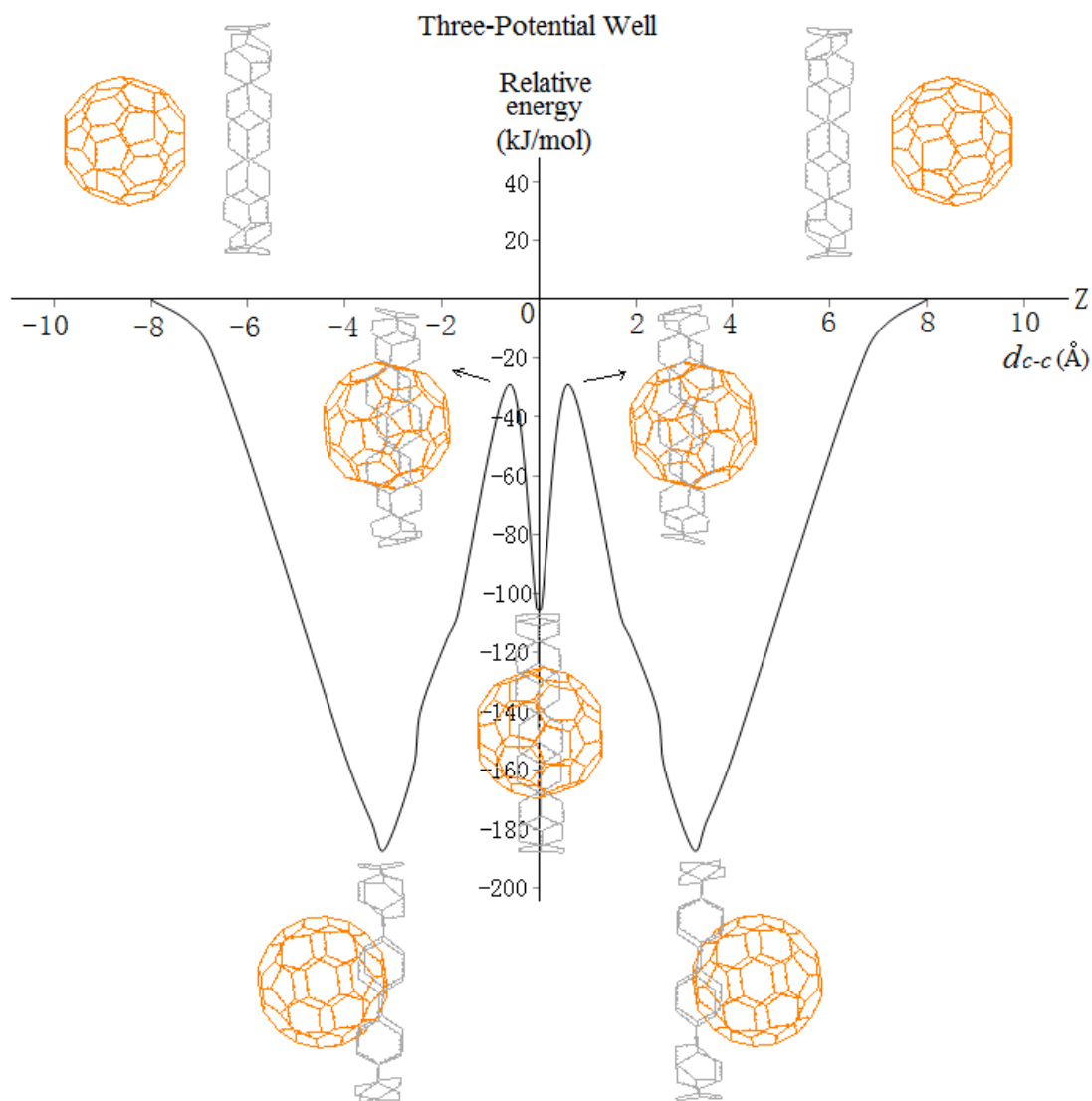
C	-1.03874200	6.47487900	1.22059300
C	-2.37905800	6.10931400	1.21953500
C	1.08282900	6.80803300	-0.03975800
C	1.68659500	6.34492200	-1.22096600
C	2.98448000	5.84910800	-1.22070200
C	3.73773400	5.78950900	-0.03749700
C	3.19904300	6.41864800	1.09948800
C	1.90238000	6.91727500	1.09809000
C	6.18127400	-3.12784400	0.04631800
C	6.05822900	-3.96769100	-1.07396600
C	5.17175200	-5.03914800	-1.07384600
C	4.37050400	-5.31800400	0.04720200
C	4.62023800	-4.58100800	1.21661100
C	5.50477800	-3.51207700	1.21637100
C	1.19750900	-7.07019300	1.09580500
C	2.53702200	-6.70202500	1.09805200
C	3.13523700	-6.12713900	-0.03784300
C	2.37956800	-6.10872800	-1.22071500
C	1.03917700	-6.47400000	-1.22194300
H	-5.05785200	5.63372000	1.97509900
H	-6.61948500	3.74509900	1.97604800
H	-5.56095500	2.88252500	-2.09813500
H	-4.01356500	4.75526400	-2.09940200
H	1.08928600	6.23303600	-2.11954800
H	3.35752500	5.36529900	-2.11754800
H	3.78309400	6.46559500	2.01385700
H	1.49967400	7.34452800	2.01172300
H	0.75443900	-7.45800200	2.00834200
H	3.11362600	-6.80793800	2.01223500
H	2.79876600	-5.66171800	-2.11621900
H	0.45561500	-6.30160000	-2.11984900
H	-3.78256200	-6.46411700	-2.01555900
H	-1.49904200	-7.34257400	-2.01375500
H	-3.35787400	-5.36698400	2.11679200
H	-1.08954600	-6.23442500	2.11850700
H	5.05919900	-5.63416500	-1.97555900
H	6.62082200	-3.74542100	-1.97615900
H	4.01259600	-4.75457300	2.09804400
H	5.56001700	-2.88174200	2.09716500
H	-0.75432300	7.45789000	-2.01000900
H	-3.11344000	6.80755500	-2.01354900
H	-0.45513800	6.30318800	2.11861100
H	-2.79809600	5.66250300	2.11521000
C	6.73116300	-1.75750500	-0.04095700



C	6.55832600	-1.02296700	-1.22518100
C	6.62872000	0.36444500	-1.22611200
C	6.87456700	1.07928000	-0.04270100
C	7.23754100	0.33515600	1.09422300
C	7.16745000	-1.05248000	1.09510500
H	6.21560500	-1.52775100	-2.12242300
H	6.33904000	0.90025700	-2.12409600
H	7.51573300	0.85219600	2.00784900
H	7.39241700	-1.59386600	2.00930300
C	5.82862700	2.94694700	1.21396700
C	5.05971800	4.10161700	1.21577600
C	4.88622400	4.86108800	0.04678600
C	5.65393100	4.50208700	-1.07477600
C	6.42755600	3.34636900	-1.07559400
C	6.46389500	2.49762200	0.04397900
H	5.81853300	2.31289000	2.09378500
H	4.47325200	4.33598200	2.09740100
H	5.60166700	5.10567400	-1.97630000
H	6.96494500	3.06875500	-1.97778300
C	-4.88617400	-4.86102800	-0.04766300
C	-5.65366400	-4.50205500	1.07406600
C	-6.42730900	-3.34635200	1.07507300
C	-6.46398800	-2.49759000	-0.04449300
C	-5.82902900	-2.94693800	-1.21463100
C	-5.06002500	-4.10153800	-1.21659300
H	-5.60121900	-5.10562800	1.97558900
H	-6.96446800	-3.06876700	1.97740700
H	-5.81930900	-2.31305300	-2.09458100
H	-4.47380400	-4.33582200	-2.09839600
C	-6.62878600	-0.36443100	1.22569100
C	-6.87464000	-1.07925800	0.04227600
C	-7.23754300	-0.33506700	-1.09463200
C	-7.16732000	1.05255800	-1.09550600
C	-6.73094500	1.75756400	0.04054400
C	-6.55825600	1.02297600	1.22476400
H	-6.33919400	-0.90023900	2.12370600
H	-7.51576200	-0.85204500	-2.00828500
H	-7.39226700	1.59392400	-2.00971800
H	-6.21551900	1.52766900	2.12204700
C	2.00459700	1.07137000	-2.73149100
C	0.76687000	0.69470600	-3.39717700
C	-0.38586000	1.46031700	-3.21374100
C	-0.35055600	2.63570500	-2.35729100
C	0.83594200	2.99285900	-1.71592100

C	2.03955700	2.19804600	-1.90845600
C	2.68498700	-0.14989700	-2.32363000
C	1.86651500	-1.28042600	-2.73835700
C	0.68161000	-0.75799200	-3.40148200
C	-0.55268100	-1.38511400	-3.22306800
C	-1.67277700	0.80653700	-3.02750300
C	-1.61655000	2.70935100	-1.64050700
C	-1.64020500	3.13444700	-0.31299800
C	-0.40202700	3.50532400	0.35387300
C	0.80771400	3.43577200	-0.33020700
C	1.99369300	2.91852100	0.33326000
C	2.75532400	2.15122100	-0.64032500
C	3.40505700	0.98150500	-0.24984800
C	3.36526400	-0.19363200	-1.10756600
C	1.76943700	-2.40882600	-1.92273700
C	2.48555400	-2.45442100	-0.65502100
C	3.26664200	-1.37071200	-0.25732600
C	3.24283500	-0.92266800	1.12722300
C	3.32849500	0.53057200	1.13205600
C	2.60053300	1.26992400	2.06586000
C	1.92096500	2.49131100	1.65850500
C	0.65485900	2.56168400	2.37486000
C	-0.48187700	3.06011000	1.73686400
C	-2.43381300	1.57812500	-2.05561200
C	-2.68519600	0.14974500	2.32463300
C	-3.36546300	0.19348100	1.10856800
C	-3.40525100	-0.98166000	0.25084300
C	-2.75553000	-2.15137700	0.64131600
C	-2.03976500	-2.19820000	1.90945400
C	-0.76707600	-0.69486000	3.39817400
C	-0.68181400	0.75783800	3.40248400
C	-1.86672000	1.28027000	2.73936500
C	-1.76963900	2.40866600	1.92374100
C	-2.48575300	2.45425700	0.65602200
C	-3.26685300	1.37056400	0.25832200
C	-3.32864800	-0.53071400	-1.13104500
C	-2.60074400	-1.27009200	-2.06487900
C	-1.92116200	-2.49146900	-1.65751300
C	-1.99389500	-2.91867400	-0.33227000
C	-0.80790900	-3.43589100	0.33119400
C	-0.83614900	-2.99300000	1.71691300
C	0.35034600	-2.63584200	2.35828400
C	0.38565500	-1.46046700	3.21474000
C	0.55248000	1.38495800	3.22406900

C	1.75439300	0.58630400	3.03316800
C	1.67257500	-0.80668900	3.02850100
C	2.43360200	-1.57827300	2.05660100
C	1.61634000	-2.70950000	1.64151600
C	1.64002400	-3.13463600	0.31400600
C	0.40182400	-3.50549000	-0.35286800
C	0.48167900	-3.06028900	-1.73586500
C	-0.65505600	-2.56184800	-2.37385900
C	-3.24300200	0.92249500	-1.12622100
C	-1.75459300	-0.58646100	-3.03217300
C	-2.00480100	-1.07152500	2.73248900



**Fig. S5** Energy profiles of the approach of  $C_{60}$  through the cavities of [9]CPPs rings at B3LYP/DFT-D3-D3/6-31G(D) level of theory.