

# Supplementary Information

## Designing of Organic Bridging Linkers of Metal-Organic Frameworks for Enhanced Carbon Dioxide Adsorption

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## 1. Binding Enthalpy of CO<sub>2</sub> Molecule in the Pure and Li-Decorated Linkers.

Table S1: After CO<sub>2</sub> adsorption, the value of  $\Delta H$  for the pure linkers at the center and side positions, calculated by both B3LYP and MP2 methods. The unit of  $\Delta H$  is expressed in kJ/mol.

Linkers	Positions	$\Delta H$ (B3LYP-D3)	$\Delta H$ (MP2)
<b>BDC</b>	Center	-9.61	-8.16
	Side	-8.07	-10.01
<b>FBDC</b>	Center	-13.34	-11.93
	Side	-13.33	-11.93
<b>DFBDC-1</b>	Center	-13.16	-11.77
	Side	-13.15	-11.77
<b>DFBDC-2</b>	Center	-13.29	-11.97
	Side	-13.29	-11.96
<b>TFBDC</b>	Center	-12.05	-11.00
	Side	-12.07	-11.04
<b>DCIBDC-1</b>	Center	-8.96	-8.34
	Side	-8.92	-8.26
<b>DCIBDC-2</b>	Center	-9.95	-11.99
	Side	-12.38	-10.91
<b>NDC</b>	Center	-14.09	-13.98
	Side	-9.39	-6.76

Table S2: After CO<sub>2</sub> adsorption, the value of  $\Delta H$  for the Li-decorated linkers at the center and side positions calculated by both B3LYP and MP2 methods. The unit of  $\Delta H$  is expressed in kJ/mol.

Linkers	Positions	$\Delta H$ (B3LYP)	$\Delta H$ (MP2)
<b>BDC</b>	Center	-34.64	-33.33
	Side	-34.64	-33.34
<b>FBDC</b>	Center	-35.21	-34.07
	Side	-35.22	-34.07
<b>DFBDC-1</b>	Center	-16.77	-15.22
	Side	-35.30	-34.06
<b>DFBDC-2</b>	Center	-11.25	-10.17
	Side	-35.32	-34.13

<b>TFBDC</b>	Center	-17.45	-15.72
	Side	-17.45	-15.73
<b>DCIBDC-1</b>	Center	-35.00	-33.69
	Side	-16.85	-15.81
<b>DCIBDC-2</b>	Center	-17.52	-16.45
	Side	-15.02	-14.86
<b>NDC</b>	Center	-16.53	-16.27
	Side	-16.55	-16.28

## 2. The Energies of HOMO and LUMO and Energy Gap ( $E_g$ )

**Table S3:** The HOMO and LUMO energies of the pure and Li-decorated linkers along with their energy gaps for CO<sub>2</sub> adsorbing at the side position of the linkers. The units are expressed in eV.

Linkers	$E_{\text{HOMO}}$ (eV)		$E_{\text{LUMO}}$ (eV)		$E_g$ (eV)	
	Pure	Li-decorated	Pure	Li-decorated	Pure	Li-decorated
<b>BDC</b>	-7.75	-6.69	-2.46	-1.37	5.29	5.33
<b>FBDC</b>	-7.64	-6.60	-2.65	-1.50	4.99	5.09
<b>DFBDC-1</b>	-7.53	-6.50	-2.83	-1.67	4.70	4.83
<b>DFBDC-2</b>	-7.62	-6.58	-2.76	-1.61	4.87	4.97
<b>TFBDC</b>	-7.56	-6.69	-2.62	-1.40	4.94	5.29
<b>DCIBDC-1</b>	-7.26	-6.51	-2.67	-1.67	4.60	4.83
<b>DCIBDC-2</b>	-7.41	-6.59	-2.46	-1.48	4.95	5.12
<b>NDC</b>	-6.58	-5.79	-2.61	-1.70	3.97	4.09

## 3. Coordinates of Optimized Geometries

### 3.1 Geometries of pure linkers

#### BDC

C	0.00365900	-0.02868600	-0.02024900
C	0.01286300	-0.01784300	1.37624400
C	1.21779300	0.00616900	2.05789100
C	2.42212100	0.01946800	1.35335000

C	2.41291300	0.00861900	-0.04314500
C	1.20798800	-0.01532000	-0.72479100
H	-0.92016500	-0.02820100	1.91864300
H	1.24678800	0.01494100	3.13775700
H	3.34595400	0.01897800	-0.58552400
H	1.17898400	-0.02401800	-1.80465700
C	3.68699100	0.04513200	2.13726200
O	3.74780600	0.05471300	3.34211300
O	4.79270100	0.05706500	1.35498400
H	5.55446700	0.07341000	1.95164400
C	-1.26122100	-0.05425500	-0.80413500
O	-1.32199800	-0.06458300	-2.00898900
O	-2.36689300	-0.06518300	-0.02188600
H	-3.12868700	-0.08145900	-0.61851200

**FBDC**

C	0.00264100	-0.02864000	-0.02000600
C	-0.00498300	-0.01840000	1.37125700
C	1.19678700	0.00537400	2.05617100
C	2.42729400	0.01957300	1.39096900
C	2.40538400	0.00891700	-0.01001600
C	1.21465400	-0.01485100	-0.71078100
H	-0.92686000	-0.02853400	1.93116200
H	3.34421600	0.01962000	-0.54093600
H	1.20243900	-0.02303300	-1.79031800

C	3.71126400	0.04469400	2.14389800
O	3.82947000	0.05277600	3.34128900
O	4.78490800	0.05806300	1.31109700
H	5.56821000	0.07363100	1.87900900
C	-1.25925600	-0.05408100	-0.81173600
O	-1.30825100	-0.06411800	-2.01620700
O	-2.36664200	-0.06510700	-0.03464000
H	-3.12838300	-0.08132200	-0.63149300
F	1.13919000	0.01453000	3.38959900

**DFBDC-1**

C	-0.00235900	-0.02874700	-0.05705900
C	0.00312300	-0.01906300	1.33885500
C	1.19090400	0.00460200	2.04215200
C	2.42815100	0.01973400	1.39017700
C	2.42267400	0.01006700	-0.00575200
C	1.23490700	-0.01361300	-0.70904000
H	-0.92462500	-0.02996600	1.88801900
H	3.35043500	0.02098500	-0.55489600
C	3.70919500	0.04513200	2.15152700
O	3.81462100	0.05424500	3.34925000
O	4.78486100	0.05732500	1.32437600
H	5.56823200	0.07336800	1.89236100
C	-1.28338700	-0.05422000	-0.81843400
O	-1.38882700	-0.06379000	-2.01614600

O	-2.35910900	-0.06592700	0.00872300
H	-3.14245100	-0.08211000	-0.55929700
F	1.11662000	0.01264900	3.37511600
F	1.30916200	-0.02162400	-2.04200900

**DFBDC-2**

C	-0.02842400	-0.02905600	0.00784600
C	0.00508600	-0.01738900	1.39972600
C	1.21941500	0.00668100	2.08666000
C	2.43180300	0.01975800	1.39975000
C	2.39239300	0.00803100	-0.00099300
C	1.19195100	-0.01587800	-0.67740100
H	3.32181400	0.01808300	-0.54726800
C	3.72421800	0.04475800	2.14162400
O	3.85086700	0.05180600	3.33764500
O	4.78663100	0.05892100	1.29735700
H	5.57796800	0.07410200	1.85436600
C	-1.27161700	-0.05441800	-0.82032600
O	-1.25792800	-0.06495900	-2.02659800
O	-2.41091100	-0.06410600	-0.10458600
H	-3.13879800	-0.08002600	-0.74369100
F	1.15873000	0.01662700	3.41371000
H	1.16258400	-0.02506900	-1.75643200
F	-1.10055200	-0.02847000	2.14163500

**TFBDC**

C	-0.02284600	-0.10917400	-0.01248900
C	0.03237800	-0.09100900	1.37839800
C	1.24764200	-0.08306400	2.04690500
C	2.45114300	-0.05977400	1.34700200
C	2.39566800	-0.06436000	-0.04404900
C	1.18095700	-0.10490500	-0.71232100
C	3.74854500	-0.08335300	2.09531500
O	3.97197600	-0.80787100	3.02533700
O	4.62466000	0.81088900	1.60226800
H	5.44381300	0.72282300	2.11294700
C	-1.31865700	-0.18497000	-0.76019900
O	-1.51888500	-0.93056100	-1.67877900
O	-2.22262800	0.68888100	-0.28110600
H	-3.03840000	0.56721800	-0.79031900
F	1.23970400	-0.06529700	3.37793700
F	1.18849700	-0.10691700	-2.04344800
F	3.51574000	-0.06419500	-0.76747700
F	-1.08735000	-0.11522500	2.10193000

**DCIBDC-1**

C	0.00999500	-0.06098800	-0.06838400
C	0.00648800	-0.03638200	1.32634700
C	1.18128000	-0.02855700	2.06184700
C	2.41692800	-0.01594900	1.40193600
C	2.41983300	-0.00267300	0.00695800

C	1.24557700	-0.03895500	-0.72835900
H	-0.93674500	-0.02951200	1.84813200
H	3.36246600	0.03044300	-0.51490000
C	3.72667000	-0.05815800	2.12179800
O	3.91399800	-0.52992600	3.21089900
O	4.72219000	0.48478000	1.37875000
H	5.53749200	0.38163000	1.89057100
C	-1.29760500	-0.15212400	-0.78780200
O	-1.46910700	-0.63939000	-1.87270200
O	-2.31052000	0.36457000	-0.04972400
H	-3.12193400	0.23035700	-0.56053700
Cl	1.39667500	0.00017900	-2.46201000
Cl	1.02854200	0.01987400	3.79510500

**DCIBDC-2**

C	-0.04361000	-0.13359800	0.06983000
C	-0.01992700	-0.10573700	1.46872900
C	1.20724100	-0.05219600	2.14988800
C	2.40685300	-0.01646300	1.42567200
C	2.36321400	-0.04354100	0.03208800
C	1.15792500	-0.12396900	-0.63392100
H	3.28896300	-0.01261000	-0.52105600
C	3.74967000	-0.02466900	2.08812800
O	4.03824400	-0.60993100	3.09637800
O	4.65194200	0.69115800	1.37221300



H	5.50218600	0.59798500	1.82649500
C	-1.28041600	-0.19254300	-0.77573300
O	-1.36652400	-0.88360500	-1.75862600
O	-2.24834200	0.65194600	-0.37934100
H	-2.98933700	0.54311700	-0.99421700
Cl	1.21406500	0.02017100	3.88277500
H	1.12397500	-0.17642200	-1.71194300
Cl	-1.49600100	-0.20897200	2.38054600

**NDC**

C	0.10172200	-0.04542000	0.09688800
C	0.06409300	-0.09400100	1.47334000
C	1.28278000	-0.04301600	2.22409900
C	2.53240700	0.04742400	1.51597200
C	2.51401300	0.10966700	0.08513600
C	1.31322800	0.07210500	-0.58950000
H	0.38224500	-0.16856600	4.17841400
H	-0.81863300	-0.08775300	-0.46376800
C	1.31189300	-0.10486100	3.64081900
C	3.73345300	0.09815500	2.26876600
H	1.30476000	0.12310500	-1.66676800
C	3.71459400	0.04589800	3.63704300
C	2.49596300	-0.06313300	4.32748100
H	4.67234200	0.16179300	1.74748400
H	4.64544400	0.08534900	4.18683800

H	2.48966000	-0.11092000	5.40821700
C	3.76616600	0.17335700	-0.72666300
O	4.86917100	-0.17759900	-0.38296600
O	3.54506400	0.66978000	-1.97128100
H	4.39607600	0.63333200	-2.43082000
C	-1.27551200	-0.15715300	2.13091400
O	-1.54473200	0.18476700	3.25719400
O	-2.23279200	-0.64133300	1.29805700
H	-3.06373800	-0.60521600	1.79300100

### 3.2 Geometries of Li-decorated linkers

#### BDC

C	-0.00211300	-0.00146700	0.00957700
C	0.01218300	-0.00189500	1.40500700
C	1.21784300	-0.00267500	2.08812200
C	2.42229400	-0.00304000	1.38325000
C	2.40798700	-0.00260200	-0.01217500
C	1.20233000	-0.00182200	-0.69529800
H	-0.92989500	-0.00159700	1.93359500
H	1.24863800	-0.00300800	3.16792200
H	3.35007100	-0.00287800	-0.54075700
H	1.17154400	-0.00146900	-1.77509500
C	3.72345100	-0.00390100	2.12064100
O	3.72197600	-0.00437100	3.39322500
O	4.81436700	-0.00429400	1.46517800

C	-1.30329300	-0.00062500	-0.72774800
O	-1.30178400	-0.00036300	-2.00049800
O	-2.39423500	-0.00041300	-0.07245900
Li	5.54756100	-0.00634600	3.15341400
Li	-3.12599800	-0.00039300	-1.76205300

**FBDC**

C	-0.00565500	-0.00203500	0.00213900
C	-0.00058200	-0.00202200	1.39269500
C	1.20472500	-0.00203900	2.07194100
C	2.43164600	-0.00206500	1.40208600
C	2.39722300	-0.00200700	0.00257900
C	1.20290100	-0.00203000	-0.69476300
H	-0.92927000	-0.00198200	1.94280700
H	3.34408400	-0.00196600	-0.51648100
H	1.18408500	-0.00203200	-1.77416600
C	3.76161300	-0.00221900	2.09331400
O	3.83388400	-0.00321400	3.35830500
O	4.81344500	-0.00073400	1.37373700
C	-1.30839500	-0.00201400	-0.73564100
O	-1.30361500	-0.00209800	-2.00688300
O	-2.39702100	-0.00203700	-0.07893700
F	1.14738100	-0.00194300	3.41149600
Li	5.64363300	-0.00174300	3.01987900
Li	-3.13312200	-0.00187300	-1.76938400

**DFBDC-1**

C	-0.01374900	0.00370800	0.00461000
C	-0.00052100	0.00211600	1.39946500
C	1.18784600	-0.00115700	2.10239500
C	2.42392300	-0.00299300	1.45044300
C	2.41070800	-0.00137800	0.05559500
C	1.22235000	0.00188900	-0.64734100
H	-0.93877900	0.00345900	1.93256300
H	3.34897700	-0.00270600	-0.47748800
C	3.74917900	-0.00653700	2.15446000
O	3.80592600	-0.00830400	3.41888500
O	4.80514600	-0.00798600	1.44352600
C	-1.33883800	0.00719700	-0.69942300
O	-1.39573800	0.00890200	-1.96387300
O	-2.39496700	0.00904200	0.01142500
F	1.10857800	-0.00249900	3.44102900
F	1.30157500	0.00325600	-1.98597600
Li	5.62393600	-0.01254500	3.09910400
Li	-3.21251500	0.01307800	-1.64359800

**DFBDC-2**

C	-0.00406000	0.01915900	0.01057300
C	0.01367400	0.01009900	1.40256000
C	1.21828500	-0.00576600	2.10771100
C	2.44082900	-0.01308900	1.44161500

C	2.41781400	-0.00394800	0.04213800
C	1.22755100	0.01177300	-0.65451800
H	3.36582500	-0.00960500	-0.47350900
C	3.76399100	-0.03005300	2.14999400
O	3.81891400	-0.03902600	3.41478600
O	4.82157800	-0.03563000	1.44164800
C	-1.26956800	0.03619600	-0.79639000
O	-1.16987200	0.04462000	-2.06518100
O	-2.39920100	0.04189300	-0.22467000
F	1.13127800	-0.01337000	3.43898400
H	1.21306600	0.01882300	-1.73359200
F	-1.10456400	0.01613000	2.13029400
Li	5.63522100	-0.05452500	3.09936800
Li	-3.01445900	0.06253100	-1.96344200

### **TFBDC**

C	-0.00594900	0.02324100	0.00434300
C	0.00288200	0.02066100	1.39362700
C	1.19411800	0.00934900	2.10327600
C	2.42000800	0.03776600	1.45017200
C	2.41097000	0.05877700	0.06104300
C	1.22014000	0.03320300	-0.64892000
C	3.71379400	0.04552300	2.22125800
O	3.90855000	-0.85653900	3.08385200
O	4.55716200	0.95378700	1.97742600

C	-1.29973300	0.01553800	-0.76674500
O	-1.47471200	-0.87582600	-1.64455800
O	-2.16289600	0.90070000	-0.50767500
F	1.14322400	0.00483000	3.44070800
F	1.27085400	0.05268800	-1.98622700
F	3.56299700	0.06974300	-0.62009700
F	-1.14898700	-0.00554100	2.07462400
Li	5.51474200	0.05631000	3.29478800
Li	-3.10070000	0.00495500	-1.84013900

#### DCIBDC-1

C	-0.01200100	0.01396000	0.00533500
C	0.00158700	0.02058800	1.39947300
C	1.18449900	0.01428200	2.12100300
C	2.41464200	0.03642800	1.45517900
C	2.40005100	0.08368000	0.06181200
C	1.21776700	0.05593700	-0.66020200
H	-0.94499700	0.03388200	1.91668900
H	3.34527400	0.14635900	-0.45425700
C	3.76467100	0.00137900	2.11840000
O	3.91158000	-0.56395500	3.23996200
O	4.74667900	0.52277700	1.50150100
C	-1.36020300	-0.05026600	-0.65937500
O	-1.48736000	-0.58862100	-1.79656100
O	-2.35988600	0.41810200	-0.02853700

Cl	1.35417200	0.14706700	-2.40131400
Cl	1.04565000	0.04896000	3.86395600
Li	-3.26082700	-0.13540800	-1.54539200
Li	5.66791500	-0.04059700	3.00238500

### DCIBDC-2

C	-0.01975400	-0.00639200	0.01390900
C	0.00341800	0.01133400	1.41251400
C	1.22862500	0.01232400	2.09866000
C	2.43325000	0.01404600	1.38718600
C	2.39250200	0.01441000	-0.00568000
C	1.18888600	-0.02276600	-0.67933800
H	3.32886500	0.03921300	-0.54275000
C	3.79812900	-0.02098800	2.02219300
O	4.01406000	-0.73317600	3.04414900
O	4.72554000	0.64654500	1.46503400
C	-1.27439400	0.02734300	-0.81785700
O	-1.29022900	-0.65555100	-1.88998800
O	-2.25221700	0.75310800	-0.47788000
Cl	1.23117000	0.07940400	3.83944400
H	1.15725700	-0.06005800	-1.75798600
Cl	-1.48281700	-0.03576500	2.32034500
Li	5.71831700	-0.04493000	2.86665000
Li	-2.99664300	0.04876900	-2.01401200

### NDC

C	-0.00117900	-0.00539500	-0.00414100
C	-0.01079700	-0.00826700	1.37308800
C	1.23089100	-0.00395100	2.08651000
C	2.46557200	-0.00617300	1.34379700
C	2.41712200	0.01396700	-0.08739500
C	1.19580800	0.02524400	-0.72398600
H	0.37599200	-0.02046000	4.05950000
H	-0.94573000	-0.02258300	-0.52636900
C	1.29766800	-0.02571400	3.50444000
C	3.68685600	-0.00073300	2.06761300
H	1.17712500	0.05380000	-1.80287400
C	3.70365700	-0.01139700	3.43683100
C	2.49928100	-0.03059900	4.16111300
H	4.60904900	-0.00582400	1.51346000
H	4.65032000	-0.00856400	3.96163000
H	2.51912300	-0.04576600	5.24322300
C	3.62493600	0.00352700	-0.98553400
O	4.75865400	-0.40461400	-0.57435900
O	3.48306900	0.38815900	-2.19149100
C	-1.36980200	0.00503600	2.01976100
O	-1.53524600	0.40825500	3.21600000
O	-2.37067900	-0.37158900	1.32781100
Li	5.26498400	-0.03493900	-2.30550100
Li	-3.30370900	0.04987000	2.85042400



### 3.3 Geometries of adsorbed CO<sub>2</sub> molecule placed at the Center and Side positions of pure linkers.

#### BDC – Center

C	-0.17688600	-0.22326000	-0.17003400
C	-0.18134000	0.38986800	1.08452300
C	1.01693200	0.67772300	1.71609800
C	2.22807500	0.35657600	1.10104800
C	2.23241200	-0.25996300	-0.15200800
C	1.03409900	-0.54621800	-0.78348100
H	-1.11901000	0.63744300	1.55805000
H	1.03066200	1.15207500	2.68639300
H	3.17069200	-0.50663700	-0.62486500
H	1.01535900	-1.01977500	-1.75423600
C	3.48579200	0.70138900	1.81579400
O	3.53635300	1.32342500	2.85049100
O	4.59394400	0.25009400	1.18858600
H	5.35176600	0.53917100	1.71683200
C	-1.43451500	-0.55385100	-0.89500800
O	-1.48274900	-1.08343500	-1.97774000
O	-2.54695900	-0.19662400	-0.21071500
H	-3.30375200	-0.44987700	-0.75820800
C	2.19457600	3.87879700	2.29741700
O	1.43836300	3.79445700	3.17327900
O	2.93566100	3.98100000	1.41036900

#### BDC – Side

C	0.16540500	0.25267600	0.14138200
C	0.16421300	0.10368300	1.52893600
C	1.35080000	-0.14927700	2.19678600
C	2.54662600	-0.25657600	1.48637500
C	2.54677900	-0.11274100	0.09668500
C	1.36049400	0.14191300	-0.57014100
H	-0.76112500	0.19325400	2.07684600
H	1.37273600	-0.26147300	3.27103100
H	3.47409400	-0.19397900	-0.44939700
H	1.33961700	0.26272800	-1.64343300
C	3.79646100	-0.50283100	2.25762700
O	3.85055600	-0.59937700	3.45872700
O	4.88949900	-0.60717900	1.46799500
H	5.64622000	-0.74389800	2.05549700
C	-1.07690900	0.54068800	-0.62604900
O	-1.12528600	0.68467700	-1.82276600
O	-2.17479400	0.62817600	0.16130100
H	-2.92184300	0.81915900	-0.42349400
C	2.75742800	3.02874500	1.43117300
O	1.64708000	3.27668400	1.20525500
O	3.86965200	2.78570100	1.65796800
<b>FBDC – Center</b>			
C	-0.13882800	-0.42391000	-0.21346100
C	-0.15235500	0.16784300	1.04608300

C	1.04698200	0.47290600	1.66042700
C	2.27887200	0.20441000	1.05907900
C	2.26448300	-0.40065000	-0.20378100
C	1.07572000	-0.70819300	-0.83796500
H	-1.07619400	0.39385800	1.55468300
H	3.20602000	-0.61855100	-0.68318300
H	1.06699800	-1.16766900	-1.81490000
C	3.55830300	0.57262200	1.72083100
O	3.67912800	1.31591400	2.66181100
O	4.62329200	-0.02348700	1.13170200
H	5.40883000	0.28852400	1.60342400
C	-1.39789000	-0.77152600	-0.93057500
O	-1.44191400	-1.28414800	-2.02062200
O	-2.50792600	-0.45060500	-0.22726700
H	-3.26801300	-0.70946100	-0.76768700
F	0.98894200	1.02833500	2.87720800
C	2.07851100	3.71852700	2.70052500
O	1.91241200	3.55754100	1.56155900
O	2.22937600	3.91267400	3.83256300

**FBDC – Side**

C	0.07486400	-0.01977100	-0.06532200
C	0.17320800	0.45478100	1.23927700
C	1.40368600	0.44929500	1.86756000
C	2.55782800	-0.02046900	1.23625100

C	2.42945800	-0.50168200	-0.07257800
C	1.20893800	-0.49935900	-0.72088100
H	-0.68770900	0.82647500	1.77210200
H	3.30910800	-0.87142900	-0.57586400
H	1.11373500	-0.86404000	-1.73258500
C	3.87939800	0.01473700	1.91645200
O	4.14400000	0.63501200	2.91533800
O	4.80154400	-0.74020200	1.27123400
H	5.63031400	-0.64035400	1.76124400
C	-1.22205300	-0.03501500	-0.79885300
O	-1.36216300	-0.43580400	-1.92697300
O	-2.24667800	0.45326700	-0.06295100
H	-3.03889500	0.40500900	-0.61688800
F	1.45141600	0.90124800	3.12686800
C	3.08407600	3.30919800	3.16464100
O	2.89900100	3.28067200	2.01761000
O	3.26131600	3.37381500	4.30760800

**DFBDC-1 – Center**

C	-0.13988100	-0.41372200	-0.19588000
C	-0.13137200	0.16137500	1.07641500
C	1.05838400	0.46081200	1.70559800
C	2.29309600	0.20275300	1.10556700
C	2.28598500	-0.38086600	-0.16157900
C	1.09562100	-0.67668000	-0.79603000

H	-1.05758800	0.37926800	1.58325200
H	3.21286200	-0.60256700	-0.66598300
C	3.57445800	0.55781700	1.77485900
O	3.68943800	1.27258500	2.73725700
O	4.63794000	-0.01508800	1.16395500
H	5.42629100	0.28249100	1.64047000
C	-1.42307300	-0.73413600	-0.88314800
O	-1.53140000	-1.23206800	-1.97208200
O	-2.49636200	-0.39399800	-0.12580300
H	-3.28170200	-0.63143300	-0.63905600
F	0.99159000	0.99964300	2.92957400
F	1.16628900	-1.22600800	-2.01026600
C	2.09341200	3.69089600	2.77806700
O	1.94082700	3.52985600	1.63710500
O	2.23215900	3.88300200	3.91185800

**DFBDC-1 – Side**

C	0.06204600	-0.01105000	-0.05016700
C	0.17448900	0.45128400	1.26254200
C	1.39323300	0.45015700	1.90725900
C	2.55493500	-0.01068000	1.28342200
C	2.44209700	-0.48206100	-0.02476700
C	1.22357700	-0.47663800	-0.67455600
H	-0.69268400	0.81624900	1.78889200
H	3.30901200	-0.85128300	-0.54898700

C	3.87437900	0.02061200	1.97188700
O	4.12362400	0.62204400	2.98505500
O	4.80342400	-0.71236900	1.31464000
H	5.63078700	-0.62084900	1.80881300
C	-1.25180500	-0.00644500	-0.75398800
O	-1.44780200	-0.38514100	-1.87810400
O	-2.24084300	0.48709000	0.03306500
H	-3.05234300	0.45700900	-0.49336400
F	1.42523900	0.89676100	3.16918100
F	1.19325500	-0.93461300	-1.92773500
C	3.06094500	3.30844000	3.21406300
O	2.89045700	3.26682500	2.06504000
O	3.22439100	3.38388400	4.35829200

**DFBDC-2 – Center**

C	-0.11828100	-0.40842200	-0.26458900
C	-0.16294400	0.27618800	0.94732400
C	1.00740100	0.55576900	1.64972200
C	2.25017000	0.16310600	1.16313700
C	2.29057700	-0.53431800	-0.05043000
C	1.13316500	-0.80757600	-0.74749800
H	3.24616800	-0.84833000	-0.43896200
C	3.49695700	0.51108000	1.89841500
O	3.59434700	1.34447000	2.76274000
O	4.55320800	-0.21923600	1.47101100

H	5.32264000	0.08508100	1.97370500
C	-1.30901900	-0.75540600	-1.09790200
O	-1.22937800	-1.35980000	-2.13877700
O	-2.47993900	-0.33415300	-0.58655300
H	-3.16924300	-0.61264500	-1.20764100
F	0.87830900	1.20078800	2.80826900
H	1.16276900	-1.33816700	-1.68710300
F	-1.30335300	0.69184400	1.49404200
C	2.11443500	3.82308300	2.42847000
O	1.99386300	3.52925500	1.31027700
O	2.22367300	4.14657700	3.53520200

**DFBDC-2 – Side**

C	0.06318400	-0.01328900	-0.03510800
C	0.17039600	0.41133900	1.28682200
C	1.40139100	0.40136600	1.93948800
C	2.55546600	-0.02935400	1.29289300
C	2.44230400	-0.46523100	-0.03302300
C	1.22527400	-0.45169200	-0.68016500
H	3.32737700	-0.80505000	-0.54669200
C	3.87266600	0.00987000	1.98548900
O	4.12173700	0.62808900	2.98888100
O	4.80166200	-0.73454400	1.34150700
H	5.62861100	-0.63370800	1.83476900
C	-1.20346900	-0.03972600	-0.82727500

O	-1.25646900	-0.42338100	-1.96966500
O	-2.28185600	0.40256700	-0.15537100
H	-3.03232000	0.34015300	-0.76476100
F	1.41684400	0.80875600	3.20782100
H	1.13730900	-0.77986700	-1.70477100
F	-0.87620200	0.84006100	1.98900300
C	2.97176000	3.28299400	3.26174400
O	2.75943300	3.24149800	2.11963400
O	3.17624200	3.35710500	4.39934100

**TFBDC – Center**

C	-0.20465100	-0.24899800	-0.02024700
C	-0.16099000	-0.70529600	1.29422800
C	0.98456300	-0.56576800	2.06387600
C	2.11697900	0.06402500	1.55456800
C	2.06859800	0.52667100	0.24351000
C	0.93454800	0.36378700	-0.53533800
C	3.34406600	0.19026300	2.40178200
O	3.79389500	-0.69398300	3.07487700
O	3.87872800	1.42628600	2.32249900
H	4.68594900	1.43236200	2.85885600
C	-1.40590500	-0.44099200	-0.89447100
O	-1.35257600	-0.83335300	-2.02723600
O	-2.54418900	-0.11262200	-0.25748300
H	-3.27623400	-0.28368700	-0.86936800



F	0.96803100	-1.01721400	3.31588300
F	0.94452500	0.83928800	-1.77804900
F	3.12958100	1.12775300	-0.30223200
F	-1.21380800	-1.31937400	1.83440800
C	2.93999100	3.86253200	0.99347700
O	4.03624900	4.23960400	0.99800800
O	1.83638500	3.50163700	0.98853800

**TFBDC – Side**

C	0.01685300	-0.00450000	0.03039400
C	-0.02169400	-0.07309500	1.42028300
C	1.14535700	-0.12587100	2.16815400
C	2.39313300	-0.08007200	1.55221100
C	2.42957500	-0.00320400	0.16368300
C	1.26497700	0.02211100	-0.58615700
C	3.63667300	-0.15135800	2.38165800
O	3.79973400	-0.91695300	3.28972500
O	4.55079900	0.75920200	1.98775500
H	5.34168200	0.63719200	2.53450800
C	-1.22601100	-0.00851400	-0.80588500
O	-1.37102400	-0.68732500	-1.78473800
O	-2.15042500	0.84489800	-0.33003300
H	-2.93036900	0.77222700	-0.90096500
F	1.04822600	-0.18674600	3.49421100
F	1.36456700	0.10952600	-1.91014300

F	3.59844300	0.03119400	-0.48238200
F	-1.18755800	-0.12315400	2.06493400
C	4.40886100	2.91161200	0.00261900
O	3.24970900	2.95709000	0.05312700
O	5.56648100	2.88308000	-0.05302400

**DCIBDC-1 – Center**

C	-0.18035200	-0.34214800	-0.16460800
C	-0.31402700	-0.47571300	1.21780900
C	0.75691900	-0.28892400	2.07662100
C	2.00670100	0.07269500	1.56212700
C	2.13306400	0.24234000	0.18470500
C	1.06992600	0.02741100	-0.67770000
H	-1.27603700	-0.73499600	1.62916100
H	3.08364600	0.54745900	-0.22230600
C	3.21386800	0.25986100	2.42023900
O	3.45685200	-0.33170700	3.43596500
O	4.05350000	1.19301700	1.89717200
H	4.82847000	1.23482700	2.47655400
C	-1.36214500	-0.63722000	-1.03155300
O	-1.31961000	-1.01489200	-2.17155100
O	-2.52849400	-0.45554500	-0.36492100
H	-3.23767200	-0.70494700	-0.97495300
Cl	1.36181900	0.29619500	-2.37248700
Cl	0.45313100	-0.45913500	3.78209800

C	2.76603700	3.80249900	1.89066500
O	1.73300600	3.32030900	1.67361800
O	3.79324900	4.29475100	2.11124700

**DCIBDC-1 – Side**

C	-0.06130500	-0.14010900	-0.01332700
C	0.01380900	0.13156200	1.35314900
C	1.21985000	0.12041800	2.03492600
C	2.40794100	-0.13959700	1.34325100
C	2.33861500	-0.37538800	-0.02852300
C	1.12999900	-0.39311800	-0.70600800
H	-0.89169000	0.35256300	1.89457000
H	3.24923100	-0.55040500	-0.57851800
C	3.74046000	-0.19970800	2.01369100
O	3.94961600	-0.56431400	3.13797500
O	4.73500900	0.19739500	1.17548300
H	5.56951300	0.09640500	1.65651500
C	-1.40726500	-0.18737900	-0.66249700
O	-1.69291400	-0.82456700	-1.64046600
O	-2.31183700	0.56784100	0.00770900
H	-3.15920000	0.45236300	-0.44606700
Cl	1.19129900	-0.67864500	-2.42192300
Cl	1.18141100	0.50091900	3.73311400
C	4.41689000	2.98655500	0.41936000
O	5.57135300	3.10228300	0.41987300

O 3.26103100 2.88310100 0.41907200

**DCIBDC-2 -Center**

C 0.25944500 0.11118500 0.08770500

C 0.36403000 0.28018600 1.47139000

C 1.59114600 0.06708400 2.11679400

C 2.71431000 -0.31214600 1.36852900

C 2.59062200 -0.47944800 -0.01026800

C 1.37648900 -0.29196000 -0.63797900

H 3.45886200 -0.76797500 -0.58189500

C 4.03728800 -0.61765700 1.99967400

O 4.20816800 -1.13479400 3.07014700

O 5.06106500 -0.27532300 1.17923000

H 5.87631500 -0.54704200 1.62581500

C -0.98600400 0.32808500 -0.71550900

O -1.34514200 -0.41567600 -1.59035500

O -1.62265700 1.47857800 -0.41787900

H -2.40771700 1.53153400 -0.98322400

Cl 1.70815000 0.33330100 3.82601000

H 1.27399500 -0.44588200 -1.70187500

Cl -1.03554100 0.70209000 2.41504300

C -0.53496800 3.79996300 0.98927600

O 0.54889000 3.39730700 0.88671200

O -1.61079400 4.22069500 1.09213500

**DCIBDC-2 – Side**

C	0.14595300	0.03159000	-0.07426500
C	0.09151300	0.17173900	1.31730500
C	1.25725200	0.01828200	2.08453100
C	2.47457700	-0.26511200	1.45206000
C	2.51071600	-0.40434100	0.06530300
C	1.35858200	-0.27928300	-0.68380400
H	3.45254700	-0.61403500	-0.41744500
C	3.74473700	-0.47785500	2.21375300
O	3.85970000	-1.05910700	3.25682100
O	4.80468100	0.04478300	1.54274300
H	5.59549500	-0.16575800	2.06071200
C	-1.02161300	0.17176200	-1.00478700
O	-1.20721500	-0.56964700	-1.93550200
O	-1.79117700	1.24365000	-0.74770400
H	-2.50241100	1.24768100	-1.40586200
Cl	1.18451200	0.23789900	3.80191900
H	1.37887000	-0.41269200	-1.75508600
Cl	-1.42150000	0.46917300	2.11796600
C	3.80633500	2.66330500	0.37899500
O	3.36829400	2.90102000	1.42680300
O	4.23793300	2.43329200	-0.67312200

**NDC – Center**

C	0.00104400	0.02215300	-0.00222800
C	0.00274200	0.01511400	1.37414100

C	1.24046600	0.00918400	2.09085800
C	2.47193700	0.06261800	1.35137900
C	2.41631900	0.10498800	-0.07953200
C	1.19846200	0.06565300	-0.72263600
H	0.38555100	-0.11830400	4.06885400
H	-0.93697100	0.01754800	-0.53515100
C	1.30130700	-0.07605500	3.50468900
C	3.69272500	0.04016900	2.07259500
H	1.16374200	0.08876600	-1.80030200
C	3.70639800	-0.03057400	3.44057000
C	2.50258900	-0.09107100	4.16234800
H	4.61983400	0.08983600	1.52895400
H	4.65182800	-0.04476200	3.96601500
H	2.52047800	-0.15130600	5.24206900
C	3.64523400	0.22964200	-0.91842800
O	4.71876600	0.65504700	-0.56570000
O	3.43830900	-0.18003700	-2.19646000
H	4.26899800	-0.02312400	-2.66763600
C	-1.31239100	0.08061400	2.07227300
O	-1.52328400	0.57532600	3.15519500
O	-2.31358100	-0.46222400	1.33902800
H	-3.12839100	-0.32486400	1.84363500
C	0.05873100	2.94693900	3.77343500
O	0.04540800	2.75852300	4.91772300

**NDC – Side**

O	0.08563900	3.16169000	2.63295000
C	0.18245300	0.53478500	0.10875400
C	0.17475200	0.38980800	1.47903000
C	1.38993400	0.08454000	2.17384200
C	2.60968100	-0.03407900	1.42026800
C	2.56770400	0.15670800	0.00156300
C	1.36807600	0.41903100	-0.62258100
H	0.53076700	-0.04533300	4.14708700
H	-0.73255400	0.75754000	-0.41575500
C	1.43602600	-0.13952200	3.57339300
C	3.80186100	-0.36942400	2.11130600
H	1.34022200	0.55339200	-1.69235900
C	3.80119700	-0.57683600	3.46494100
C	2.61011700	-0.46111600	4.20088300
H	4.72018600	-0.45189200	1.55677400
H	4.72405700	-0.83361500	3.96759700
H	2.61701600	-0.62896400	5.26955300
C	3.79966800	0.12080000	-0.84186600
O	4.93232600	0.31470500	-0.47147800
O	3.52141400	-0.14077700	-2.14476200
H	4.36646600	-0.09996300	-2.61484200
C	-1.11631900	0.59805400	2.19690800
O	-1.25958600	0.90509600	3.35479800

O	-2.19447600	0.42321700	1.38363400
H	-2.97815700	0.61585300	1.91895600
C	-3.70836400	1.30204500	-0.90118800
O	-2.85157700	1.30496100	-1.68303400
O	-4.57453100	1.30551900	-0.12833400

### 3.4 Geometries of adsorbed CO<sub>2</sub> molecule placed at the Center and Side positions of Li-decorated linkers.

#### BDC – Center

C	-0.46793600	-0.58113500	-0.33667000
C	-0.51185100	0.07256200	0.89546500
C	0.65824300	0.52271900	1.48590000
C	1.88501700	0.32494000	0.85082700
C	1.92860100	-0.32868300	-0.38140700
C	0.75877000	-0.77951900	-0.97179100
H	-1.47034900	0.21688300	1.37232700
H	0.64378200	1.02970900	2.43969100
H	2.88719200	-0.47281600	-0.85817600
H	0.77335200	-1.28774900	-1.92490500
C	3.14844700	0.81290700	1.48746400
O	3.09040500	1.40125600	2.61545300
O	4.25610500	0.63478500	0.89440600
C	-1.73050400	-1.06765600	-0.97371900
O	-1.67590000	-1.66285700	-2.09731800
O	-2.84236700	-0.87999400	-0.38346100
Li	4.95403700	1.53438400	2.36132100



Li	-3.49941100	-1.75129400	-1.86550700
C	4.13507200	3.86797900	3.50439800
O	3.17054300	4.40673900	3.82234100
O	5.14961100	3.36743600	3.19869000

**BDC – Side**

C	-0.26155000	-0.12613000	-0.26753200
C	-0.22600000	0.30293300	1.05987200
C	0.98915200	0.46382300	1.70633500
C	2.18212700	0.19813900	1.03279500
C	2.14626200	-0.23086600	-0.29468800
C	0.93126900	-0.39239200	-0.94122400
H	-1.15929500	0.50388700	1.56536100
H	1.03609100	0.79413400	2.73378400
H	3.07964800	-0.43179200	-0.80005500
H	0.88419300	-0.72392400	-1.96826400
C	3.49449900	0.37400100	1.73029200
O	3.50779700	0.76020800	2.94377400
O	4.57203100	0.13766200	1.10309700
C	-1.57284200	-0.30042600	-0.96522100
O	-1.59071300	-0.69297900	-2.17571400
O	-2.65303600	-0.05404200	-0.33885300
Li	5.37407600	0.65602600	2.69581200
Li	-3.41030500	-0.54710200	-1.94221500
C	4.89256800	2.85847000	4.22559200

O	5.82638700	2.27151300	3.82964500
O	4.01371100	3.47327600	4.63949500

**FBDC – Center**

C	-0.41336300	-0.59593500	-0.35724400
C	-0.49978400	0.03470600	0.87946400
C	0.64244800	0.55310800	1.46217900
C	1.89295100	0.46824900	0.84470300
C	1.94984800	-0.16219500	-0.40346300
C	0.82060400	-0.69290400	-1.00066400
H	-1.45040800	0.12194200	1.38322900
H	2.91391200	-0.21982200	-0.88668200
H	0.87225200	-1.18291500	-1.96125100
C	3.15863900	1.00357200	1.44522200
O	3.18341500	1.38604300	2.65348900
O	4.19697200	1.05100700	0.71488400
C	-1.64673200	-1.16195900	-0.98939400
O	-1.55872600	-1.73802700	-2.11922200
O	-2.76107800	-1.05745700	-0.38610100
F	0.49833800	1.16308100	2.64903700
Li	4.97361000	1.79768200	2.23385800
Li	-3.37354500	-1.95680500	-1.87434400
C	4.06645300	3.79153200	3.86876700
O	3.10701600	4.15075600	4.38960600
O	5.07330800	3.47323300	3.35983500

**FBDC – Side**

C	-0.27672800	-0.13933700	-0.16453800
C	-0.18173800	0.41218200	1.10874600
C	1.06507000	0.63212700	1.66581000
C	2.24552500	0.31975500	0.98658500
C	2.12122600	-0.22473200	-0.29674700
C	0.88400900	-0.45819500	-0.86958400
H	-1.07283800	0.66936500	1.66091000
H	3.03261900	-0.45787000	-0.82705800
H	0.79514600	-0.88337200	-1.85793000
C	3.61704200	0.52919600	1.55604900
O	3.76487800	0.82787400	2.77915700
O	4.61613200	0.38967700	0.78402400
C	-1.62436500	-0.38267900	-0.76938000
O	-1.70209100	-0.88813700	-1.93325700
O	-2.66817100	-0.08029500	-0.10934900
F	1.09719300	1.17896700	2.89107700
Li	5.58694200	0.86192800	2.30193600
Li	-3.51168700	-0.72618500	-1.61607100
C	5.18229100	2.93564200	4.03621600
O	6.08144200	2.42770400	3.48157600
O	4.33871100	3.47306400	4.60223000

**DFBDC-1 – Center**

C	-0.15339800	-0.17320200	-0.29328500
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C	-0.18931900	0.47966500	0.93912900
C	0.96632500	0.70516000	1.65679400
C	2.21494200	0.29180700	1.18939500
C	2.25008500	-0.37257700	-0.03601000
C	1.09481100	-0.59355500	-0.75967000
H	-1.13910500	0.80997300	1.33047100
H	3.19781000	-0.71611200	-0.42116200
C	3.50507600	0.52382000	1.91522000
O	3.55205000	1.31829100	2.90341900
O	4.54381800	-0.08459800	1.51066000
C	-1.44371500	-0.38103500	-1.03141100
O	-1.45197500	-0.93986800	-2.16670800
O	-2.51868600	0.02302000	-0.48263700
F	0.84262700	1.32847600	2.84272700
F	1.21864300	-1.23379100	-1.93081500
Li	5.32945900	0.81994300	2.92290900
Li	-3.26876500	-0.64230100	-2.03446600
C	2.29838700	3.81526400	2.80653100
O	2.16888800	3.72937600	1.65580500
O	2.42231900	3.95773800	3.95088400

**DFBDC-1 – Side**

C	-0.30381800	-0.15250000	-0.13913100
C	-0.20374600	0.37571500	1.14825500
C	1.02627100	0.61555600	1.72724200

C	2.21917600	0.34490700	1.05231100
C	2.11919400	-0.17531600	-0.23789200
C	0.88916200	-0.42037900	-0.81559400
H	-1.10706000	0.59886500	1.69483800
H	3.02254000	-0.38714200	-0.78904100
C	3.58610200	0.57575600	1.62968500
O	3.71809500	0.89849200	2.84688600
O	4.59008300	0.43056700	0.86687700
C	-1.67013900	-0.39504600	-0.70993800
O	-1.80525700	-0.88700000	-1.86834500
O	-2.68022900	-0.09344300	0.00394600
F	1.03166700	1.13404400	2.96517900
F	0.88457700	-0.92519000	-2.05803100
Li	5.54921700	0.93097200	2.38642700
Li	-3.59874400	-0.72150000	-1.46969500
C	5.15702600	2.98330700	4.15660800
O	6.04731500	2.47363300	3.58957200
O	4.32049200	3.51942000	4.73406600

**DFBDC-2 – Center**

C	0.12725700	0.08497000	-0.19761200
C	0.26458000	0.83130700	0.96810200
C	1.45062500	0.81554400	1.69957100
C	2.53945800	0.05301900	1.28993700
C	2.39536700	-0.70400900	0.12175200

C	1.22109200	-0.68844700	-0.60240300
H	3.23810800	-1.29901000	-0.19522300
C	3.84283700	0.01394400	2.03318600
O	4.01827800	0.72986500	3.06258000
O	4.75882300	-0.75231700	1.59450800
C	-1.12259500	0.07938700	-1.02863300
O	-1.15569700	-0.67292100	-2.05409500
O	-2.10814900	0.80899600	-0.71346700
F	1.48050500	1.57142300	2.80237800
H	1.11468900	-1.27082400	-1.50474300
F	-0.71950300	1.60089800	1.44528800
Li	5.68524300	-0.05987300	3.03623500
Li	-2.84702000	0.05254300	-2.22507500
C	0.51209300	4.19061500	1.97311700
O	1.10977300	3.98358200	0.99947500
O	-0.08218600	4.42098000	2.94170300

**DFBDC-2 – Side**

C	-0.26964400	-0.06834400	-0.22079300
C	-0.21876200	0.51011900	1.04470300
C	1.00215300	0.76359900	1.67137700
C	2.20783400	0.45106500	1.05054200
C	2.15214300	-0.12155000	-0.22512000
C	0.94554400	-0.37837400	-0.84239700
H	3.08774700	-0.35566200	-0.70960700

C	3.54669300	0.69317700	1.68628200
O	3.62460800	1.02115100	2.90721500
O	4.58350100	0.54953100	0.96879300
C	-1.55368600	-0.36716200	-0.93795000
O	-1.48429800	-0.88659600	-2.09798500
O	-2.66959300	-0.10862200	-0.39823700
F	0.94923500	1.33137900	2.87882300
H	0.90517700	-0.82474400	-1.82413600
F	-1.31893400	0.85220200	1.71774800
Li	5.47242600	1.06414000	2.52705900
Li	-3.32510000	-0.80361800	-1.97505600
C	4.99232100	3.12408400	4.26622600
O	5.90913400	2.61632000	3.74113500
O	4.12873100	3.65867800	4.80381100

**TFBDC – Center**

C	-0.25675600	-0.26484600	0.00148100
C	-0.16324200	-0.73637600	1.30516800
C	0.98041200	-0.53192400	2.06257700
C	2.05805500	0.18233300	1.55516300
C	1.95773900	0.66435500	0.25705900
C	0.82894200	0.43417900	-0.51191700
C	3.28702200	0.43650600	2.38460600
O	3.88222000	-0.54071800	2.91352100
O	3.68819200	1.63000200	2.51724700

C	-1.49231000	-0.50229800	-0.82680500
O	-1.36117800	-1.01947000	-1.97183200
O	-2.61367500	-0.17510500	-0.34686900
F	1.01628900	-1.00692100	3.31297800
F	0.78806600	0.92932200	-1.75362300
F	2.97604400	1.34842000	-0.28606000
F	-1.17133900	-1.43070900	1.84477600
Li	5.04402600	0.80489100	3.48360600
Li	-3.21104600	-0.82389200	-1.98409300
C	2.95052800	3.94442000	1.12790900
O	1.81815100	3.69313400	1.15932200
O	4.07086600	4.24349500	1.07993900

**TFBDC – Side**

C	-0.00938900	-0.00733000	0.05303500
C	-0.03234000	-0.16430700	1.43343800
C	1.14019500	-0.18204800	2.17385500
C	2.37580800	-0.00792300	1.56395400
C	2.39607900	0.16219800	0.18623700
C	1.22844400	0.14879400	-0.55874500
C	3.64787700	0.00840900	2.36671100
O	3.90023400	-0.95845100	3.13507400
O	4.42994300	0.99552500	2.23615500
C	-1.28210100	-0.00573700	-0.75273200
O	-1.37322200	-0.79024800	-1.73863200



O	-2.21089100	0.77998400	-0.41389700
F	1.05990800	-0.33532000	3.50066900
F	1.31101400	0.32419600	-1.88204600
F	3.56438500	0.32004900	-0.45403200
F	-1.19468200	-0.33595300	2.07306600
Li	5.46500200	0.01688700	3.42918900
Li	-3.04990800	0.00300000	-1.88049300
C	4.46012800	3.03156000	0.31792000
O	3.31076100	3.18642000	0.35515900
O	5.61354000	2.92052100	0.25292300

**DCIBDC-1 – Center**

C	-0.48493200	-0.52113000	-0.29554700
C	-0.58722400	-0.49857500	1.09492100
C	0.46757700	-0.10107600	1.90043300
C	1.66898300	0.32742800	1.32682400
C	1.75211000	0.35632300	-0.06434000
C	0.70966400	-0.07359300	-0.86986900
H	-1.52239500	-0.79969300	1.54045600
H	2.66002800	0.72959700	-0.51171200
C	2.89412000	0.75366800	2.09074100
O	3.14575600	0.25160500	3.22004900
O	3.66995000	1.60045100	1.54443300
C	-1.67541000	-1.04038400	-1.05466400
O	-1.52372600	-1.59451200	-2.18126500

O	-2.82119600	-0.93547900	-0.51316700
Cl	0.94858000	0.04440700	-2.59840600
Cl	0.18740500	-0.09690200	3.62701000
Li	-3.35971900	-1.76934000	-2.07286000
Li	4.62108900	1.39042500	3.17008600
C	4.73441500	4.06138900	2.56442800
O	4.33237200	4.82701100	1.80722900
O	5.16962300	3.32128700	3.36185200

**DCIBDC-1 – Side**

C	0.00873000	0.02680600	-0.01493400
C	-0.00829100	0.19929100	1.36892800
C	1.15892000	0.28776700	2.10728100
C	2.40186600	0.23781300	1.47032200
C	2.41927300	0.12354100	0.08201100
C	1.25210900	0.00123200	-0.65567100
H	-0.96585800	0.26481100	1.86111900
H	3.37456600	0.13161200	-0.41930800
C	3.73264300	0.28141400	2.16466500
O	3.86819400	-0.23640100	3.31394100
O	4.71256400	0.81315400	1.56023000
C	-1.32499700	-0.12934100	-0.69404600
O	-1.42137200	-0.78277100	-1.77212100
O	-2.34416200	0.38280100	-0.13205200
Cl	1.42684400	-0.11226800	-2.39125900

Cl	0.99181900	0.53277600	3.83291600
Li	-3.20858000	-0.34773900	-1.59486800
Li	5.60512600	0.36531300	3.12558400
C	2.53162900	-2.47245100	4.27237600
O	2.98643300	-2.30046300	5.32614500
O	2.06382300	-2.69739200	3.23435200

**DCIBDC-2 – Center**

C	0.31261800	0.11610700	0.13343300
C	0.44349200	0.28048600	1.51473500
C	1.67355900	0.03956600	2.14415900
C	2.78180500	-0.35676300	1.38682500
C	2.63755700	-0.50514600	0.00878000
C	1.41844600	-0.29858000	-0.60417700
H	3.50636800	-0.78959000	-0.56559300
C	4.13691700	-0.67599800	1.96106400
O	4.24187800	-1.27095800	3.07165200
O	5.15793200	-0.37039100	1.26818700
C	-0.94685600	0.40091800	-0.63575500
O	-1.27821200	-0.40023800	-1.56085100
O	-1.62409000	1.44344500	-0.38887200
Cl	1.81840800	0.30608800	3.85855800
H	1.29998900	-0.44482000	-1.66755500
Cl	-0.94014600	0.72869100	2.47823100
Li	6.04663600	-1.10001200	2.71777600

Li	-2.72108200	0.76136400	-1.70831700
C	-0.79416600	3.74564700	0.93585500
O	0.32751200	3.47829800	0.80556900
O	-1.90059000	4.06544300	1.07952700

**DCIBDC-2 – Side**

C	0.11743600	-0.02564900	-0.03835300
C	0.12373400	0.18402400	1.34506800
C	1.32465200	0.09581300	2.06651500
C	2.52340500	-0.18457300	1.40270600
C	2.50318600	-0.37743200	0.02281700
C	1.31686000	-0.32466500	-0.68076800
H	3.43816100	-0.56615300	-0.48283200
C	3.85795400	-0.31114000	2.08447000
O	3.96915100	-0.92600900	3.18065200
O	4.86983900	0.18754400	1.49283800
C	-1.10564500	0.08500500	-0.91006500
O	-1.21936500	-0.73542600	-1.87387600
O	-1.95567000	0.99903700	-0.71013100
Cl	1.31981000	0.40499800	3.77970900
H	1.29500800	-0.50647400	-1.74476300
Cl	-1.36290600	0.49335500	2.19760000
Li	5.73643700	-0.40836800	3.01958500
Li	-2.78728100	0.20798000	-2.15800100
C	4.09484200	2.59891700	0.14623300

O	3.76557600	3.01703700	1.17753300
O	4.41462400	2.21985500	-0.90276400

**NDC – Center**

C	0.10165800	-0.33235000	-0.16747600
C	0.14420900	0.05569900	1.15205400
C	1.40707900	0.20060200	1.80674900
C	2.61481500	-0.04253200	1.06234600
C	2.51666600	-0.41793900	-0.31680900
C	1.27398300	-0.54950000	-0.89654100
H	0.61533100	0.71996300	3.74146500
H	-0.86102800	-0.45473100	-0.64081800
C	1.51644300	0.54852100	3.17821600
C	3.85779300	0.12576900	1.72742400
H	1.21903100	-0.82434500	-1.93882300
C	3.91749100	0.48784700	3.04707700
C	2.73702300	0.69178300	3.78234300
H	4.76173800	-0.05418400	1.17253900
H	4.88016700	0.60970000	3.52641200
H	2.78888200	0.96534800	4.82803300
C	3.69194900	-0.70930000	-1.21169100
O	4.84321400	-0.97471100	-0.73707600
O	3.50472000	-0.71176100	-2.47135700
C	-1.18020100	0.34145000	1.79829300
O	-1.27996000	1.18583700	2.74966200

O	-2.21582600	-0.24544800	1.35354700
Li	5.28636600	-1.14883100	-2.51623400
Li	-3.06987600	0.75875600	2.63781900
C	0.30125300	3.53283700	2.81438600
O	0.18991300	3.60307600	3.96788500
O	0.42651800	3.51095800	1.66138200

**NDC – Side**

C	0.06118800	0.00965100	-0.02647500
C	0.08371200	-0.04861000	1.34967800
C	1.34201600	-0.04000200	2.03485500
C	2.55585500	0.01687700	1.26337700
C	2.47298800	0.06833900	-0.16309000
C	1.23987600	0.08450500	-0.77357000
H	0.54303500	-0.15387600	4.02734200
H	-0.89522000	-0.00648300	-0.52641000
C	1.44899600	-0.10976300	3.44884200
C	3.79523500	0.04929100	1.95385000
H	1.19562100	0.14238100	-1.85083300
C	3.85176400	-0.01133300	3.32074500
C	2.66805300	-0.10140800	4.07335000
H	4.70488500	0.10326400	1.38090900
H	4.81212900	0.00770700	3.81906800
H	2.71750300	-0.15701100	5.15308200
C	3.66237800	0.06451300	-1.07893400

O	4.76078500	-0.48239900	-0.72903600
O	3.54585500	0.58305400	-2.23315500
C	-1.26059300	-0.09847000	2.02598400
O	-1.40089800	0.19781300	3.25629300
O	-2.27527000	-0.42215600	1.32775200
Li	5.29043600	0.02679400	-2.41963500
Li	-3.17486100	-0.14930300	2.90351400
C	4.81261500	-2.82551800	0.85819300
O	5.87846300	-2.56916500	1.24050800
O	3.75485900	-3.12895400	0.49124800