

SUPPLEMENTARY MATERIAL**C₆₀ as Electron Acceptor and Donor: A Comparative DFT Study of Li@C₆₀ and F@C₆₀**Ambrish Kumar Srivastava¹, Sarvesh Kumar Pandey^{2*}, Anoop Kumar Pandey³,
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CARTESIAN CO-ORDINATES OF EQUILIBRIUM STRUCTURES

(ATOM X Y Z)

C ₆₀			
ATOM	X	Y	Z
C	-0.684651000000	-0.156671000000	-3.478647000000
C	0.765112000000	-0.058382000000	-3.465340000000
C	1.532357000000	-1.125817000000	-2.996956000000
C	0.881654000000	-2.336032000000	-2.523608000000
C	-0.510882000000	-2.430200000000	-2.536527000000
C	-1.309957000000	-1.318604000000	-3.024333000000
C	-1.226642000000	1.145012000000	-3.127649000000
C	-0.111884000000	2.048330000000	-2.897351000000
C	1.119225000000	1.304585000000	-3.105992000000
C	2.227299000000	1.545787000000	-2.292228000000
C	2.685891000000	-0.874625000000	-2.149720000000
C	1.633575000000	-2.832935000000	-1.383266000000
C	0.962607000000	-3.403897000000	-0.300845000000
C	-0.487476000000	-3.501521000000	-0.314260000000

C	-1.209120000000	-3.024798000000	-1.409519000000
C	-2.440112000000	-2.281475000000	-1.200900000000
C	-2.503013000000	-1.227070000000	-2.199225000000
C	-3.023235000000	0.023198000000	-1.861508000000
C	-2.372206000000	1.233368000000	-2.335508000000
C	-0.186566000000	3.003770000000	-1.882649000000
C	-1.378994000000	3.095506000000	-1.056969000000
C	-2.450116000000	2.228528000000	-1.278931000000
C	-3.148462000000	1.633333000000	-0.152008000000
C	-3.502300000000	0.270351000000	-0.511584000000
C	-3.442820000000	-0.742477000000	0.446899000000
C	-2.901087000000	-2.044449000000	0.094965000000
C	-2.149750000000	-2.541051000000	1.235719000000
C	-0.967061000000	-3.254389000000	1.035067000000
C	2.748563000000	-1.929437000000	-1.152006000000
C	1.226687000000	-1.144989000000	3.127672000000
C	2.372277000000	-1.233323000000	2.335538000000
C	3.023205000000	-0.023169000000	1.861512000000
C	2.502891000000	1.227265000000	2.199253000000
C	1.309916000000	1.318720000000	3.024346000000
C	-0.765092000000	0.058342000000	3.465344000000
C	-1.119075000000	-1.304736000000	3.106023000000
C	0.112005000000	-2.048396000000	2.897287000000
C	0.186563000000	-3.003755000000	1.882518000000
C	1.379057000000	-3.095399000000	1.056798000000
C	2.450098000000	-2.228501000000	1.278944000000
C	3.502276000000	-0.270323000000	0.511658000000
C	3.442853000000	0.742501000000	-0.446858000000
C	2.901111000000	2.044455000000	-0.094970000000
C	2.440049000000	2.281576000000	1.200936000000
C	1.209032000000	3.024996000000	1.409448000000
C	0.510706000000	2.430313000000	2.536599000000
C	-0.881717000000	2.336044000000	2.523672000000
C	-1.532372000000	1.125728000000	2.997029000000
C	-2.227139000000	-1.545929000000	2.292242000000
C	-3.026259000000	-0.434436000000	1.804690000000
C	-2.686006000000	0.874549000000	2.149773000000
C	-2.748642000000	1.929343000000	1.152131000000
C	-1.633535000000	2.832753000000	1.383142000000
C	-0.962618000000	3.403728000000	0.300781000000
C	0.487484000000	3.501635000000	0.314213000000
C	0.967135000000	3.254373000000	-1.035142000000
C	2.149778000000	2.541022000000	-1.235731000000
C	3.148415000000	-1.633285000000	0.152011000000
C	3.026309000000	0.434300000000	-1.804627000000
C	0.684659000000	0.156659000000	3.478648000000

Li@C₆₀

C	-0.071431000000	-1.550110000000	3.177916000000
C	1.106731000000	-2.167218000000	2.585040000000
C	2.267080000000	-1.395912000000	2.364072000000
C	2.284771000000	0.001577000000	2.730885000000
C	1.151012000000	0.594512000000	3.309604000000
C	-0.048381000000	-0.198711000000	3.529793000000
C	-1.258229000000	-2.118985000000	2.555305000000
C	-0.817852000000	-3.073419000000	1.561644000000
C	0.653488000000	-3.103638000000	1.580520000000
C	1.363416000000	-3.256283000000	0.371854000000
C	2.996613000000	-1.543035000000	1.117630000000
C	3.034955000000	0.726530000000	1.717253000000
C	2.628211000000	2.001123000000	1.322502000000
C	1.453082000000	2.615127000000	1.925318000000
C	0.732005000000	1.917659000000	2.899861000000
C	-0.726473000000	1.947152000000	2.881407000000
C	-1.208922000000	0.642120000000	3.279870000000
C	-2.350947000000	0.095490000000	2.673052000000
C	-2.380550000000	-1.301885000000	2.305678000000
C	-1.503053000000	-3.198162000000	0.336073000000
C	-2.665597000000	-2.345148000000	0.076968000000
C	-3.084438000000	-1.420307000000	1.041777000000
C	-3.504805000000	-0.089081000000	0.630393000000
C	-3.045708000000	0.849636000000	1.641371000000
C	-2.577843000000	2.106474000000	1.257378000000
C	-1.394121000000	2.672540000000	1.889572000000
C	-0.645231000000	3.395847000000	0.882365000000
C	0.759646000000	3.367449000000	0.900096000000
C	3.480924000000	-0.230283000000	0.717605000000
C	1.255564000000	2.141282000000	-2.550415000000
C	2.373514000000	1.332755000000	-2.303403000000
C	2.354308000000	-0.066327000000	-2.674427000000
C	1.210362000000	-0.616047000000	-3.281448000000
C	0.048954000000	0.223458000000	-3.533836000000
C	-1.103170000000	2.188753000000	-2.579503000000
C	-0.646324000000	3.123772000000	-1.572744000000
C	0.811517000000	3.094439000000	-1.554546000000
C	1.493784000000	3.213467000000	-0.340322000000
C	2.654059000000	2.373129000000	-0.081358000000
C	3.084360000000	1.456304000000	-1.041442000000
C	3.047035000000	-0.814003000000	-1.644106000000
C	2.588050000000	-2.079823000000	-1.258800000000
C	1.401437000000	-2.648757000000	-1.890042000000
C	0.730454000000	-1.917519000000	-2.880243000000

C	-0.734889000000	-1.888026000000	-2.898991000000
C	-1.151417000000	-0.568590000000	-3.311276000000
C	-2.287025000000	0.027360000000	-2.732426000000
C	-2.258851000000	1.426052000000	-2.361281000000
C	-1.353415000000	3.270894000000	-0.375808000000
C	-2.552896000000	2.478191000000	-0.146494000000
C	-2.995685000000	1.579047000000	-1.117417000000
C	-3.478508000000	0.266696000000	-0.718678000000
C	-3.034610000000	-0.691240000000	-1.719832000000
C	-2.637291000000	-1.974395000000	-1.323975000000
C	-1.459372000000	-2.591550000000	-1.925951000000
C	-0.772097000000	-3.369513000000	-0.908207000000
C	0.657910000000	-3.398340000000	-0.889894000000
C	3.503627000000	0.125628000000	-0.631519000000
C	2.565345000000	-2.450411000000	0.142318000000
C	0.071748000000	1.571414000000	-3.175525000000
Li	-0.029664000000	-1.518320000000	0.037581000000

F@C₆₀

C	-3.035946000000	-1.293104000000	1.306798000000
C	-3.485737000000	-0.050014000000	0.703165000000
C	-3.488651000000	0.090081000000	-0.684245000000
C	-3.042614000000	-1.006930000000	-1.526467000000
C	-2.614477000000	-2.199816000000	-0.948690000000
C	-2.611510000000	-2.346248000000	0.500072000000
C	-2.299815000000	-0.965131000000	2.515473000000
C	-2.299489000000	0.478111000000	2.661103000000
C	-3.030993000000	1.045117000000	1.541335000000
C	-2.602784000000	2.239610000000	0.961876000000
C	-3.037962000000	1.331412000000	-1.288686000000
C	-2.311670000000	-0.443190000000	-2.648320000000
C	-1.183528000000	-1.094167000000	-3.153844000000
C	-0.734811000000	-2.332937000000	-2.553960000000
C	-1.438309000000	-2.866992000000	-1.474228000000
C	-0.703944000000	-3.383452000000	-0.340605000000
C	-1.433612000000	-3.104948000000	0.876557000000
C	-0.724675000000	-2.797325000000	2.037947000000
C	-1.170063000000	-1.703842000000	2.875709000000
C	-1.169295000000	1.129103000000	3.158308000000
C	0.007484000000	0.360555000000	3.529876000000
C	0.007682000000	-1.024514000000	3.390795000000
C	1.183661000000	-1.702984000000	2.870573000000
C	0.735428000000	-2.796806000000	2.034796000000
C	1.439515000000	-3.104012000000	0.870382000000
C	0.704593000000	-3.382828000000	-0.343609000000
C	1.433729000000	-2.865972000000	-1.480400000000

C	0.725250000000	-2.332438000000	-2.557099000000
C	-2.310894000000	1.000048000000	-2.502080000000
C	2.299327000000	1.001590000000	-2.512013000000
C	1.168901000000	1.738580000000	-2.868599000000
C	0.722379000000	2.833269000000	-2.029482000000
C	1.424094000000	3.152159000000	-0.865637000000
C	2.602498000000	2.387375000000	-0.494648000000
C	3.485625000000	0.092421000000	-0.699268000000
C	3.036536000000	-1.004871000000	-1.539510000000
C	2.300511000000	-0.441601000000	-2.658253000000
C	1.170618000000	-1.093349000000	-3.158895000000
C	-0.007499000000	-0.325042000000	-3.527589000000
C	-0.007693000000	1.059673000000	-3.386123000000
C	-0.733069000000	2.832735000000	-2.026327000000
C	-1.429997000000	3.151183000000	-0.859484000000
C	-0.699668000000	3.475035000000	0.352463000000
C	0.698806000000	3.475506000000	0.349449000000
C	1.428806000000	2.915636000000	1.472121000000
C	2.605365000000	2.241356000000	0.950612000000
C	3.036980000000	1.047213000000	1.528274000000
C	3.488693000000	-0.047634000000	0.688118000000
C	2.611730000000	-2.198035000000	-0.959938000000
C	2.615237000000	-2.344463000000	0.488824000000
C	3.042469000000	-1.291047000000	1.293730000000
C	2.311406000000	-0.963524000000	2.505591000000
C	2.310667000000	0.479774000000	2.651229000000
C	1.182113000000	1.129928000000	3.153187000000
C	0.732362000000	2.370374000000	2.552166000000
C	-0.722992000000	2.369903000000	2.555340000000
C	-1.424436000000	2.914683000000	1.478292000000
C	-1.182510000000	1.737789000000	-2.863512000000
C	-2.606348000000	2.385681000000	-0.483418000000
C	3.031355000000	1.333393000000	-1.301745000000
F	0.000777000000	-0.861385000000	-0.078328000000