Lu-Lu Bond in $Lu_2@C_{60}$ Metallofullerenes

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Contents

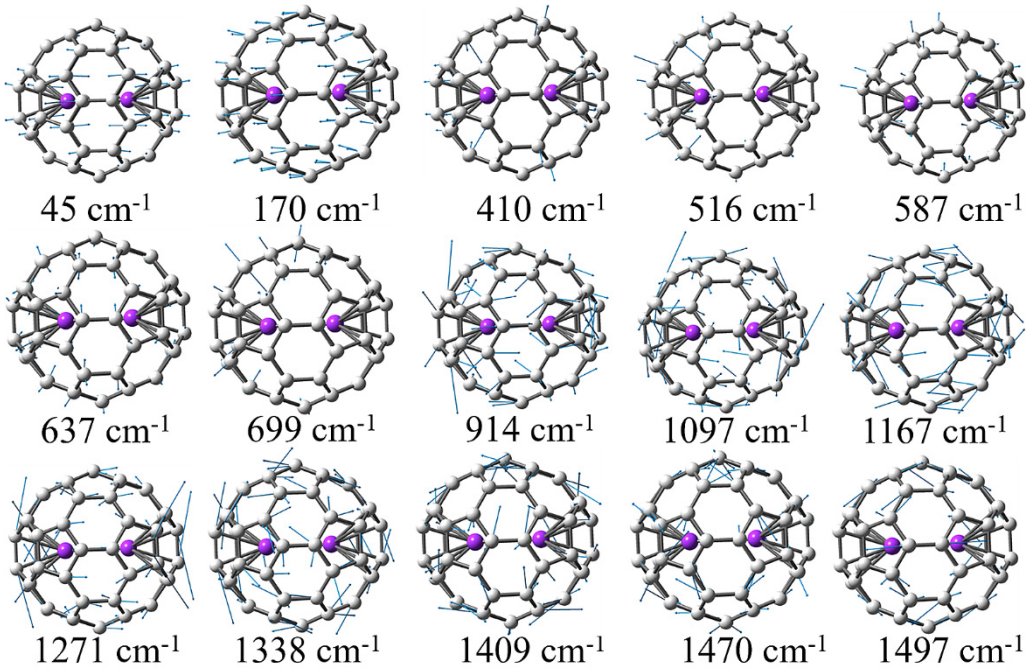

Figure S4 Several selected displacement vectors of $Lu_2@I_h$_C_{60} with vibration frequencies, including the lowest vibration one.

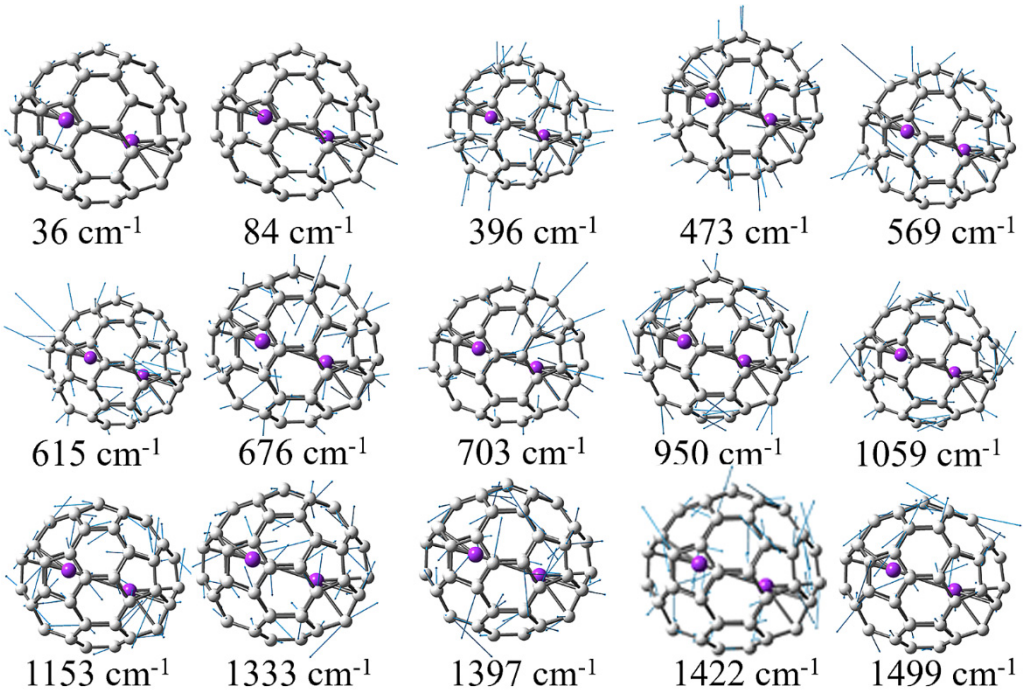

Figure S5 Several selected displacement vectors of $Lu_2@C_{2v}$_C_{60} with vibration frequencies, including the lowest vibration one.

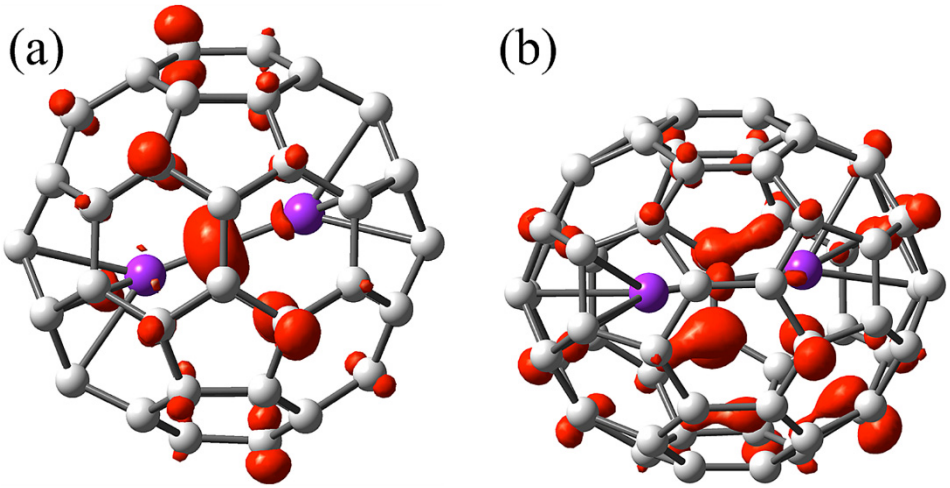

Figure S6 Lowest unoccupied molecular orbitals (LUMO) with localization of $Lu_2@I_h$_C_{60} (a) and $Lu_2@C_{2v}$_C_{60} (b) with isovalue of 0.03 a.u. for the surface.

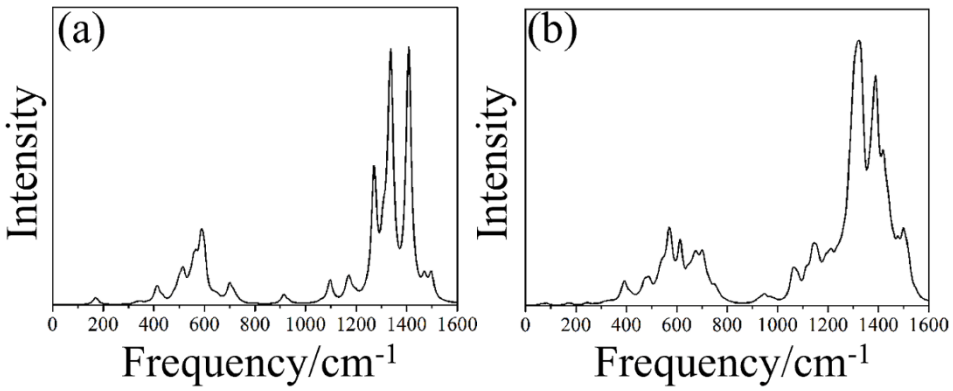

Figure S4 IR vibration spectra for $Lu_2@I_h$_C_{60} (a) and $Lu_2@C_{2v}$_C_{60} (b). The broadening function is Gaussian function and full width at half maximum is 12 cm^{-1}.

Coordinates for optimized geometries

$Lu_2@I_h$_C_{60}

C	0.66745000	-3.63957500	0.21508200
C	0.28693300	-3.49792200	-1.19594000
C	1.15135000	-2.66834800	-2.04874800
C	0.31494100	-1.87493400	-2.94205000
C	0.72771100	-0.60826900	-3.43454300
C	-0.24895500	0.46191100	-3.54300100
C	0.38872700	1.68032800	-3.10339800
C	-0.31156800	2.67779300	-2.35359700
C	0.31390400	3.46116900	-1.28287900
C	-0.71292800	3.63636300	-0.21053600
C	-0.33108000	3.49425500	1.20504000
C	-1.19214800	2.67893900	2.06856300
C	-0.35585300	1.89430100	2.96708600
C	-0.75671800	0.60024400	3.38899900
C	0.21241100	-0.47690500	3.53096000
C	-0.43812500	-1.70050100	3.13863800
C	0.26342300	-2.66494700	2.35126900
C	-0.35659900	-3.46481100	1.28454700
C	1.88207900	-2.94064300	0.66088400
C	1.64294800	-2.37013700	1.98161900
C	2.30970600	-1.19854100	2.42935600
C	1.57170700	-0.21737100	3.20641600
C	1.96570000	1.09208500	2.74257800
C	1.03599100	2.17541700	2.64202100
C	1.08338200	3.17475000	1.56927500
C	2.09515200	3.00236800	0.51264100
C	1.70735100	3.14660000	-0.92402500
C	2.37852400	2.07057000	-1.66086100
C	1.76759000	1.36904800	-2.74828000
C	1.98195500	-0.04162200	-2.96869600
C	2.78115500	-0.78996900	-2.06185400
C	2.39371000	-2.10561700	-1.62173500
C	2.77297000	-2.24706500	-0.21508100
C	3.39320000	-1.01842000	0.20947500
C	3.19107100	-0.49295200	1.51482400
C	2.96652800	0.92166700	1.69697500
C	2.98924100	1.84298500	0.60219200
C	3.18556700	1.29124700	-0.73167600
C	3.37134400	-0.10260200	-0.92203300
C	-1.12374000	-3.17917800	-1.55915400
C	-1.07815300	-2.16468500	-2.62262000

C	-2.02914000	-1.10677600	-2.76030700
C	-1.60069000	0.19948900	-3.19003400
C	-2.31516400	1.18159700	-2.38683600
C	-1.69253900	2.39267400	-1.98791400
C	-1.92922500	2.95366800	-0.66435800
C	-2.78802500	2.22100500	0.21493300
C	-2.41058000	2.08039000	1.61568700
C	-2.84232000	0.77942700	2.06957800
C	-2.02336700	0.02776000	2.95569600
C	-1.82276200	-1.38790500	2.78212400
C	-2.40391400	-2.06265500	1.66442600
C	-1.74527700	-3.15099300	0.92676700
C	-2.13190600	-3.00708500	-0.50588100
C	-3.01499100	-1.83486500	-0.60004700
C	-3.03435200	-0.93566400	-1.71045000
C	-3.22383900	0.47573100	-1.49477500
C	-3.45298100	1.00728800	-0.19643500
C	-3.46327300	0.10519300	0.94228000
C	-3.20447900	-1.27571300	0.73355600
Lu	0.30151900	1.49915300	0.06882700
Lu	-0.33568600	-1.47489800	-0.06186500

$Lu_2@C_{2v}$_C_{60}

C	-3.01030800	-1.15708900	-1.00845500
C	-2.75731100	-1.81671700	0.26428300
C	-2.76918400	-1.02512500	1.50932900
C	-1.97805100	-1.46161100	2.62712400
C	-1.40768300	-0.46696800	3.51533000
C	-0.01990300	-0.78163300	3.72068200
C	0.73643000	0.43559000	3.65920200
C	1.95938000	0.36595600	2.93835800
C	2.36106400	1.51524700	2.14064500
C	3.16223100	1.01907900	1.03583600
C	3.11067000	1.65890600	-0.22366300
C	3.14498000	0.88551100	-1.44410800
C	2.22016200	1.49285400	-2.38132100
C	1.43297000	0.69118800	-3.23342700
C	0.02859600	1.01629500	-3.43367700
C	-0.69995100	-0.24163600	-3.54988900
C	-2.00480400	-0.34020400	-2.98016100
C	-2.34584400	-1.56997800	-2.24741300
C	-3.17902800	0.27851500	-1.06431700
C	-2.56474100	0.78539200	-2.27886000

C	-1.86404600	2.02920300	-2.20668600
C	-0.54898900	2.14946500	-2.81803000
C	0.26618900	2.99389900	-1.95903100
C	1.61173400	2.64636800	-1.72556700
C	2.17436600	2.75993600	-0.39433800
C	1.39344800	3.25605900	0.69255000
C	1.51449000	2.67424700	2.02491500
C	0.19485000	2.72723200	2.69674800
C	-0.17865000	1.57289200	3.51384000
C	-1.52025700	0.94805500	3.32695100
C	-2.41245000	1.41256300	2.30720100
C	-3.01325300	0.41675500	1.41604900
C	-3.16955700	1.04351200	0.12709700
C	-2.57420400	2.37344200	0.17769900
C	-1.86556900	2.80303100	-0.99470100
C	-0.55472400	3.41112300	-0.82564000
C	-0.01155300	3.60365300	0.48011200
C	-0.77646500	3.27482100	1.71376700
C	-2.09747100	2.63555700	1.52537300
C	-0.93986500	-2.44746400	2.40201600
C	0.31039300	-1.94434900	2.94686100
C	1.53832000	-2.01691600	2.17411900
C	2.40004100	-0.84935600	2.26772100
C	3.18311800	-0.43495400	1.12501000
C	3.16618900	-1.19366300	-0.06244000
C	3.17244800	-0.53341800	-1.35875400
C	2.42255000	-1.36433500	-2.27350600
C	1.55118100	-0.76366900	-3.22521000
C	0.24592900	-1.35140700	-3.50410400
C	-0.13276000	-2.61638100	-2.89101400
C	-1.49327400	-2.72585600	-2.29460600
C	-1.38488900	-3.50347400	-1.06416400
C	-1.94450500	-3.02187800	0.19383200
C	-0.91275000	-3.19427000	1.20942000
C	0.33917200	-3.54238700	0.55485000
C	1.55258000	-2.82934800	0.94808600
C	2.41037700	-2.42749900	-0.16202400
C	2.01294000	-2.59111500	-1.56758300
C	0.80879100	-3.28543300	-1.95103700
C	0.01999600	-3.83117100	-0.84646100
Lu	-0.14119600	-1.42520800	-0.81394900
Lu	-0.26359900	1.09694000	1.05098700