Supporting Information for

An unprecedented C_{80} cage that violates the isolated pentagon rule

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Isolation of $Lu_2O@C_1(31876)$-C_{80} and $Lu_2O@C_{2v}(5)$-C_{80}. Separation and purification of $Lu_2O@C_{2v}(5)$-C_{80} and $Lu_2O@C_1(31876)$-C_{80} were achieved by a multiple-stage HPLC process using toluene as the eluent. The first stage was performed on a Buckyprep column (20 mm × 250 mm, Cosmosil Nacalai Tesque), and one fraction, which is named as Fr7, was collected (Figure S1a). Then, Fr7 was injected into a Buckyprep-M column (20 mm × 250 mm, Cosmosil Nacalai Tesque) for the second stage separation, and a fraction named Fr7-3 was obtained (Figure S1b). After that, Fr7-3 was injected into a 5PBB column (20 mm × 250 mm, Cosmosil Nacalai Tesque), and a fraction named Fr7-3-2 was collected (Figure S1c). Fr7-3-2 was then injected into a Buckyprep column (20 mm × 250 mm, Cosmosil Nacalai Tesque) for recycling separation, and $Lu_2O@C_{2v}(5)$-C_{80} (Fr7-3-2-3) and $Lu_2O@C_1(31876)$-C_{80} (Fr7-3-2-4) were finally obtained (Figure S1d). Their high purity was demonstrated by the analytical HPLC chromatograms and the mass spectra (Figure S2).

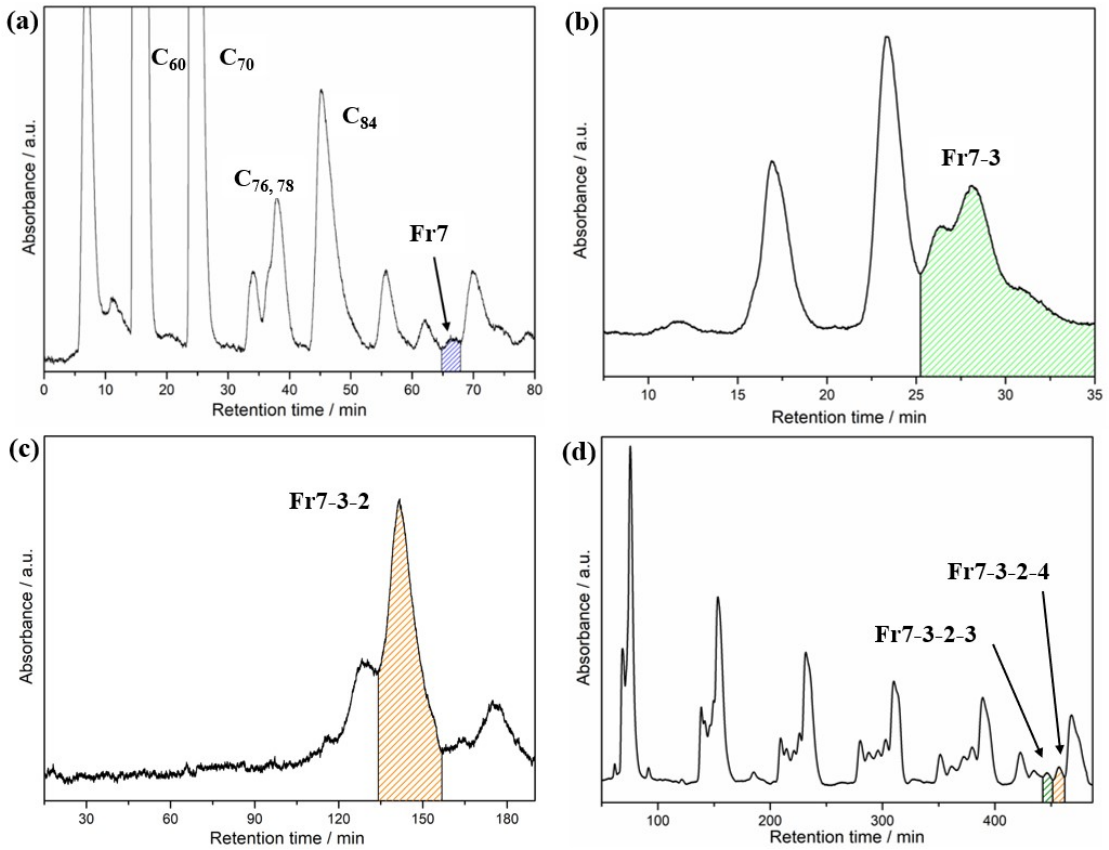

Figure S1. (a) Isolation scheme of fullerene extract on a Buckyprep column. Conditions: 20 mL inject volume; 10 mL/min toluene flow; (b) Isolation scheme of Fr7 on a Buckyprep-M column. Conditions: 15 mL inject volume; 10 mL/min toluene flow; (c) Isolation scheme of Fr7-3 on a 5PBB column. Conditions: 10 mL injection volume; 10 mL/min chlorobenzene flow. (d) Recycling HPLC chromatogram of Fr7-3-2 on a Buckyprep column. Conditions: 5 mL injection volume; 10 mL/min toluene flow. All the detection wavelengths are 330 nm.

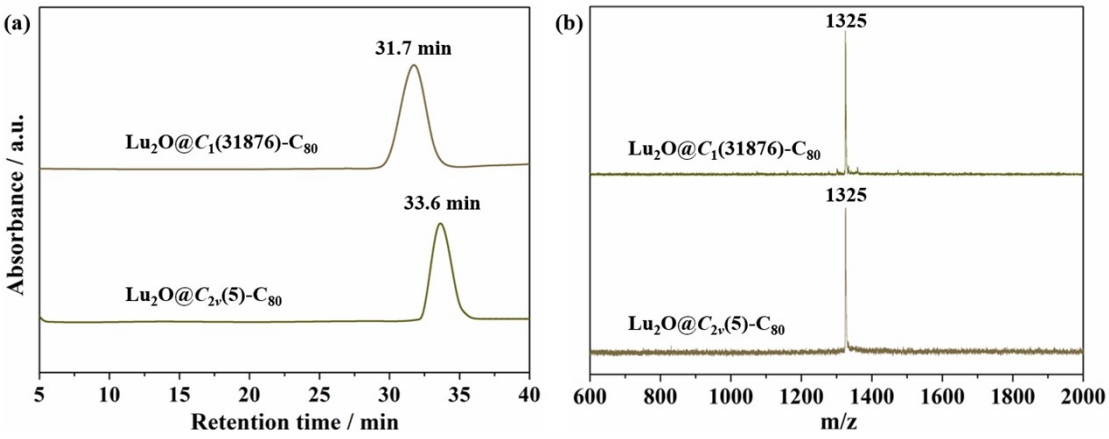

Figure S2. (a) HPLC chromatograms and (b) LDI-TOF mass spectra of $Lu_2O@C_1(31876)$-C_{80} and $Lu_2O@C_{2v}(5)$-C_{80}. HPLC conditions: Buckyprep column (Ø = 4.6 × 250 mm); 20 μL injection volume; 1 mL min^{-1} toluene flow; 330 nm detection wavelength; 40 °C.

Table S1. Crystallographic data of $Lu_2O@C_1(31876)$-C_{80}·Ni^{II}(OEP)·2(C_6H_6) and $Lu_2O@C_{2v}(5)$-C_{80}·Ni^{II}(OEP)·2(C_6H_6).

	$Lu_2O@C_1(31876)$-C_{80}• Ni^{II}(OEP)·2(C_6H_6)	**$Lu_2O@C_{2v}(5)$-C_{80}• Ni^{II}(OEP)·2(C_6H_6)**
***T*, K**	100(2)	100(2)
***λ*, Å**	0.7336	0.7336
color / habit	black / block	black / block
crystal size, mm	0.08×0.06×0.04	0.14×0.10×0.10
empirical formula	$C_{128}H_{56}Lu_2N_4NiO$	$C_{128}H_{56}Lu_2N_4NiO$
fw	2074.42	2074.42
crystal system	monoclinic	monoclinic
space group	*C*2/*m*	*C*2/*m*
***a*, Å**	25.2864(13)	25.2000(3)
***b*, Å**	15.1800(8)	15.1832(18)
***c*, Å**	19.7371(10)	19.6920(3)
***α*, deg**	90	90
***β*, deg**	95.204(2)	94.432(5)
***γ*, deg**	90	90
***V*, Å^3**	7544.8(7)	7511.7(16)
Z	4	4
***ρ*, g/cm^3**	1.826	1.834
***μ*, mm^{-1}**	2.915	3.163
***R*$_1$ (all data)**	0.1316	0.1020
***wR*$_2$ (all data)**	0.2640	0.2526

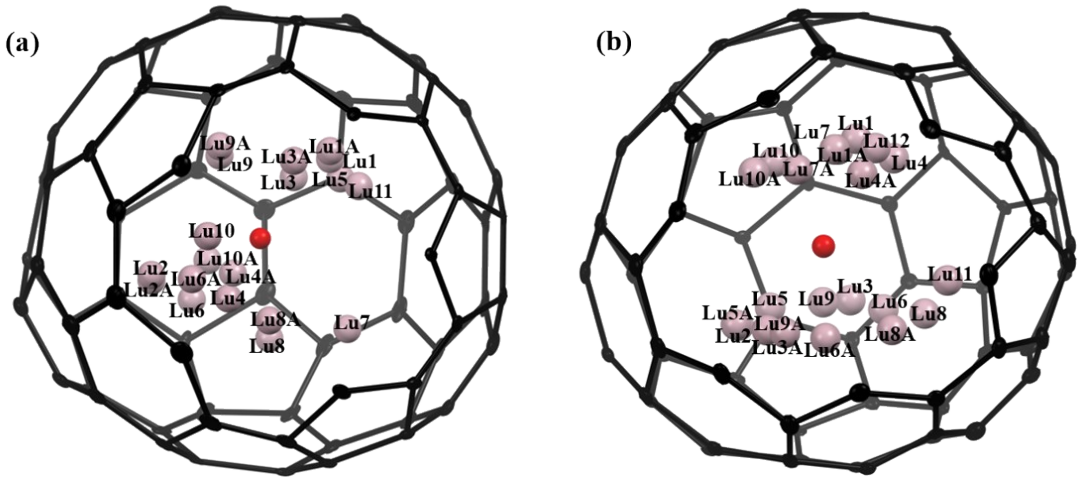

Figure S3. Positions of the disordered lutetium atoms in (a) $Lu_2O@C_1(31876)$-C_{80} and (b) $Lu_2O@C_{2v}(5)$-C_{80} relative to a cage orientation. Those Lu atoms labeled with an "A" are generated by crystallographic operation. Some cage carbon atoms are omitted for clarity.

Table S2. Fractional occupancies of the Lu positions in $Lu_2O@C_1(31876)$-C_{80} and $Lu_2O@C_{2v}(5)$-C_{80}.

EMFs	Fractional occupancy of the Lu positions					
$Lu_2O@C_1(31876)$-C_{80}	Lu1/Lu1A	Lu2/Lu2A	Lu3/Lu3A	Lu4/Lu4A	Lu5/Lu5A	Lu6/Lu6A
	0.24	0.24	0.11	0.10	0.09	0.06
	Lu7	Lu8/Lu8A	Lu9/Lu9A	Lu10/Lu10A	Lu11	
	0.06	0.04	0.04	0.02	0.02	
$Lu_2O@C_{2v}(5)$-C_{80}	Lu1/Lu1A	Lu2	Lu3/Lu3A	Lu4/Lu4A	Lu5/Lu5A	Lu6/Lu6A
	0.21	0.25	0.16	0.10	0.06	0.06
	Lu7/Lu7A	Lu8/Lu8A	Lu9/Lu9A	Lu10/Lu10A	Lu11	Lu12
	0.06	0.05	0.05	0.05	0.04	0.03

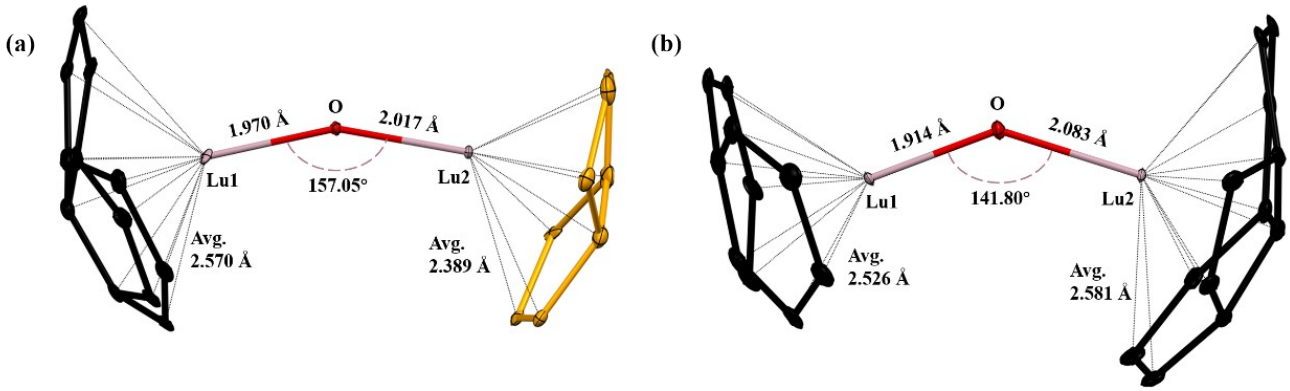

Figure S4. Structures of the major Lu_2O sites with respect to the nearest carbon atoms in the (a) C_1(31876)-C_{80} and (b) C_{2v}(5)-C_{80} cages. C, O, and Lu atoms are shown in black, red, and purple, respectively.

Table S3. Details of the oxide clusters at the major sites for $Lu_2O@C_1$(31876)-C_{80}, $Lu_2O@C_{2v}$(5)-C_{80} and $Sc_2O@C_{2v}$(5)-C_{80}.

$Lu_2O@C_1$(31876)-C_{80}		**$Lu_2O@C_{2v}$(5)-C_{80}**		**$Sc_2O@C_{2v}$(5)-C_{80}**[S1]	
Lu1-cage	2.570 Å (avg.)	Lu1-cage	2.526 Å (avg.)	Sc1-cage	2.519 Å (avg.)
Lu2-cage	2.389 Å (avg.)	Lu2-cage	2.581 Å (avg.)	Sc2-cage	2.503 Å (avg.)
Lu1-O	1.970 Å	Lu1-O	1.914 Å	Sc1-O	1.861 Å
Lu2-O	2.017 Å	Lu2-O	2.083 Å	Sc2-O	2.017 Å
Lu1-O-Lu2	157.05°	Lu1-O-Lu2	141.80°	Sc1-O-Sc2	160.79°

Table S4. Relative energy (ΔE / kcal·mol^{-1}) and the energy gaps (Gap / eV) between HOMO and LUMO of $Lu_2O@C_{80}$ isomers on the PBE/6-31G(d)-SDD level.

Isomer[a]	APP[b]	Multiplicity	ΔE	Gap
$Lu_2O@I_h(7)$-C_{80}	0	Singlet	0.0	0.13
$Lu_2O@D_{5h}(6)$-C_{80}	0	Singlet	3.4	0.20
$Lu_2O@C_1(31876)$-C_{80}	**1**	**Singlet**	**6.3**	**0.77**
$Lu_2O@C_{2v}(5)$-C_{80}	**0**	**Singlet**	**6.9**	**0.73**
$Lu_2O@C_1(28324)$-C_{80}	1	Singlet	15.5	0.86
$Lu_2O@C_{2v}(3)$-C_{80}	0	Singlet	16.4	0.35
$Lu_2O@C_1(31891)$-C_{80}	1	Singlet	19.1	0.17

[a]Isomer number according to the spiral algorithm of Fowler and Manolopoulos.[S2] The simplified number is used for the IPR isomers. [b]APP: number of adjacent pentagon pairs.

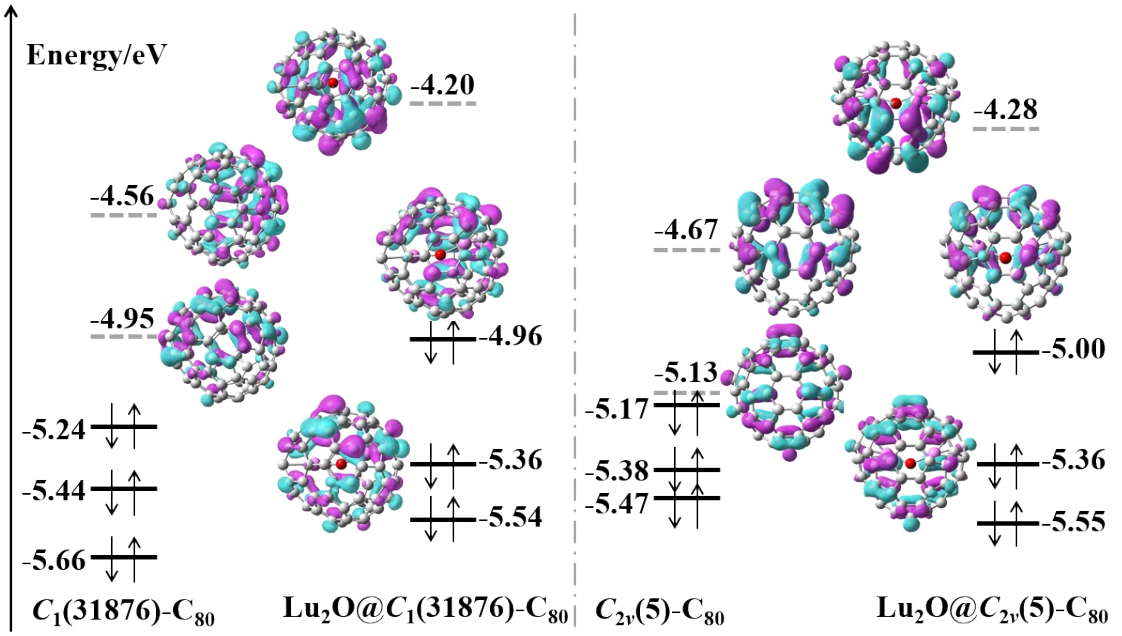

Figure S5. Energies of frontier molecular orbitals of $C_1(31876)$-C_{80}, $C_{2v}(5)$-C_{80}, $Lu_2O@C_1(31876)$-C_{80}, and $Lu_2O@C_{2v}(5)$-C_{80}, maps of LUMO and LUMO+1 of $C_1(31876)$-C_{80} and $C_{2v}(5)$-C_{80}, and LUMO, HOMO and HOMO-1 of $Lu_2O@C_1(31876)$-C_{80} and $Lu_2O@C_{2v}(5)$-C_{80} on the PBE/6-311G(d,p)~def2-TZVP//6-31G(d)~SDD.

Frontier molecular orbital analyses. Based on the frontier molecular orbital analyses, it can be clearly confirmed that the LUMO and LUMO+1 of C_{80} clearly become the HOMO-1 and HOMO of $Lu_2O@C_{80}$, respectively, indicating the four-electron transfer

from Lu_2O to C_{80}, *i.e.*, $(Lu_2O)^{4+}@(C_{80})^{4-}$. Furthermore, the HOMO and LUMO orbitals of $Lu_2O@C_1(31876)$-C_{80} and $Lu_2O@C_{2v}(5)$-C_{80} are mainly located on the cage frameworks, and their the HOMO-LUMO gaps are 0.76 eV and 0.72 eV, respectively.

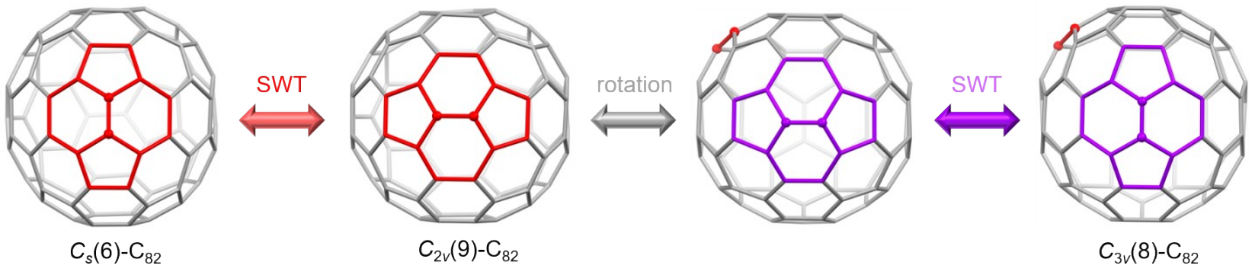

Figure S6. Transformation between $C_s(6)$-C_{82}, $C_{2v}(9)$-C_{82} and $C_{3v}(8)$-C_{82}.

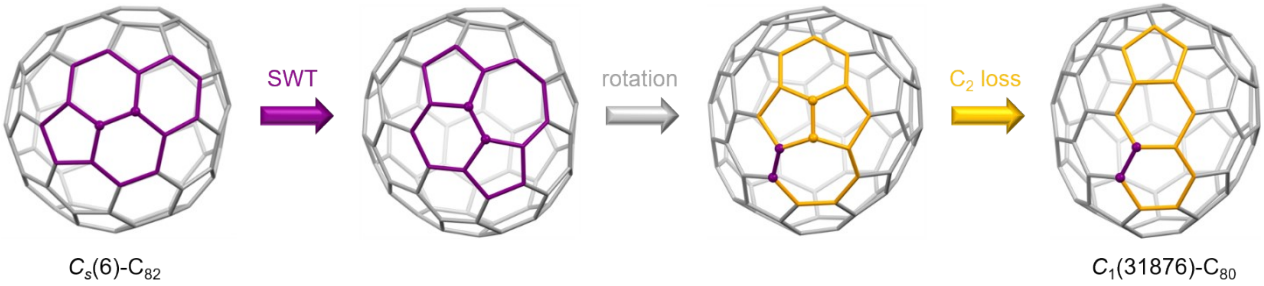

Figure S7. Transformation from $C_s(6)$-C_{82} to $C_1(31876)$-C_{80}.

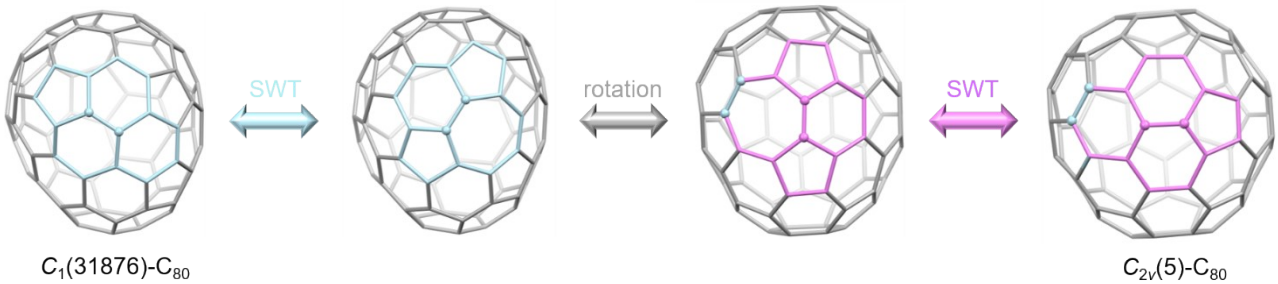

Figure S8. Transformation between $C_1(31876)$-C_{80} and $C_{2v}(5)$-C_{80}.

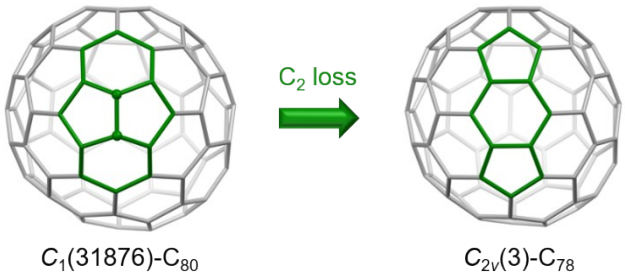

Figure S9. Transformation from $C_1(31876)$-C_{80} to $C_{2v}(3)$-C_{78}.

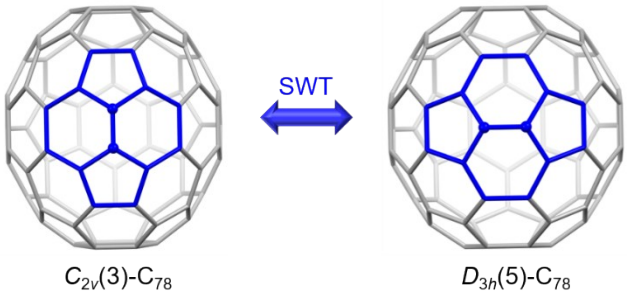

Figure S10. Transformation between C_{2v}(3)-C_{78} and D_{3h}(5)-C_{78}.

Table S5. Cartesian coordinates of the four low-energy $Lu_2O@C_{80}$ isomers.

$Lu_2O@I_h$(7)-C_{80}				**$Lu_2O@D_{5h}$(6)-C_{80}**			
C	-0.03901400	-0.01862200	0.05269100	C	-0.04448500	-0.03361000	0.11727000
C	1.40502100	-0.02732000	0.06776600	C	1.40269300	-0.02396000	0.11882800
C	2.16884500	1.21580800	0.07166900	C	2.14258200	1.20690600	0.08707400
C	3.39931500	1.00570500	-0.66291500	C	3.41239000	1.16018900	-0.57199500
C	4.05020200	2.06183700	-1.39902200	C	3.94367100	2.32438500	-1.25325400
C	4.69657500	1.67831000	-2.63372600	C	4.64758700	1.90644800	-2.45646100
C	4.70036300	2.55549500	-3.80457700	C	4.59859000	2.68761600	-3.65772500
C	4.62280800	1.69080300	-4.97381400	C	4.68671900	1.95740100	-4.88849100
C	3.93249700	2.07323800	-6.17678400	C	4.02101200	2.42565100	-6.09485500
C	3.32741600	1.04383600	-6.96451400	C	3.51246700	1.29128200	-6.84071000
C	2.08623900	1.28077600	-7.64895900	C	2.26449700	1.36639200	-7.53771000
C	1.31922000	0.04129900	-7.62544400	C	1.52678100	0.13828900	-7.64423800
C	-0.12460500	0.04885300	-7.56905500	C	0.08030100	0.12944100	-7.68930500
C	-0.77452600	-1.01895500	-6.86118300	C	-0.41220400	-1.00382500	-6.95763800
C	-2.02309300	-0.81863900	-6.15248100	C	-1.60737900	-0.91445000	-6.17800400
C	-2.02550900	-1.69678800	-4.98293700	C	-1.66502100	-1.76013200	-5.01906400
C	-2.68204200	-1.31968900	-3.74326900	C	-2.40532700	-1.37624700	-3.85465100
C	-1.95641400	-1.67050800	-2.54378900	C	-1.70208500	-1.80854600	-2.68427700
C	-1.92746200	-0.83669400	-1.35338600	C	-1.68206500	-1.01243500	-1.48956000
C	-0.69681800	-1.08351900	-0.64253700	C	-0.51256400	-1.13518000	-0.67640200

C	-0.68899500	1.24680800	0.11368300	C	-0.75223700	1.17634800	0.13124700
C	-1.93062500	1.48501500	-0.57552700	C	-1.94981900	1.32202100	-0.64783700
C	-2.54091500	0.45355800	-1.35641400	C	-2.42446400	0.25662300	-1.47474300
C	-3.24725600	0.82571200	-2.56720100	C	-3.14008200	0.65016100	-2.65579100
C	-3.41197400	-0.04634100	-3.73188200	C	-3.11960700	-0.15467500	-3.84043900
C	-3.38591000	0.84093300	-4.91811300	C	-3.10331000	0.69881900	-4.99047800
C	-2.66081100	0.47778100	-6.12987600	C	-2.34988000	0.35457100	-6.16352300
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C	-0.00892100	2.54956800	-7.59380500	C	0.08985100	2.59487700	-7.61592300
C	1.43613200	2.54471000	-7.58492200	C	1.52293700	2.63403600	-7.52303000
C	2.09265500	3.61070800	-6.88776500	C	2.07631900	3.74612900	-6.81195300
C	3.32049700	3.36470500	-6.17356400	C	3.32186100	3.62056400	-6.08084300
C	3.34667100	4.20703300	-4.98753600	C	3.25232600	4.40947000	-4.86000500
C	4.06786200	3.86339900	-3.78324600	C	3.85810600	3.95390800	-3.64304700
C	3.48549600	4.30522900	-2.51064800	C	3.21346400	4.35851000	-2.42804200
C	3.47453900	3.39990600	-1.33800400	C	3.24459900	3.51934700	-1.23962600
C	2.18129300	3.53682900	-0.68569600	C	1.97631000	3.61527300	-0.54392100
C	1.52026300	2.47042600	0.03725100	C	1.40113600	2.47461900	0.10158500
C	0.07744000	2.48159100	0.08930000	C	-0.03411300	2.43265200	0.14689300
C	-0.68430200	3.47218400	-0.59857000	C	-0.83318100	3.38416400	-0.57179700
C	-1.92979800	2.86331100	-1.02064900	C	-2.02670000	2.71106500	-1.07338300
C	-2.51661200	3.22985600	-2.25716900	C	-2.69053000	3.12095700	-2.27694300
C	-3.18519800	2.19587700	-3.00920400	C	-3.23553000	2.04529600	-3.06936000
C	-3.24085400	2.20882200	-4.44447900	C	-3.21222300	2.07543900	-4.52208700
C	-2.56485600	3.25602500	-5.18198100	C	-2.64194200	3.18235100	-5.25071300
C	-1.98540900	2.90188200	-6.42063400	C	-1.94083200	2.82327200	-6.44926800
C	-0.74934900	3.52626800	-6.87968400	C	-0.73249700	3.51588600	-6.88379300

C	-0.08901700	4.54406800	-6.09607400	C	-0.16510800	4.54392100	-6.06989700
C	1.34039400	4.59813400	-6.15697900	C	1.25317600	4.66395800	-6.07553400
C	2.10465300	4.96213000	-4.98899600	C	1.98429400	5.06710100	-4.86807400
C	1.46629900	5.31142500	-3.75940600	C	1.28807700	5.33849900	-3.65505700
C	2.16836000	4.94342900	-2.54523600	C	1.94542900	5.01613500	-2.43295000
C	1.39983100	4.50040500	-1.40964200	C	1.17650800	4.56382300	-1.26718300
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C	4.64479600	0.30697200	-3.10134300	C	4.63809300	0.53009700	-4.92069100
C	4.61829800	0.31981300	-4.53809200	C	3.91619300	0.11132700	-6.12832400
C	3.92673100	-0.69820500	-5.28210300	C	3.11650700	-1.06634200	-6.13490800
C	3.32618400	-0.33147300	-6.51247600	C	1.93376100	-1.04236800	-6.93632800
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C	-0.00590300	-2.00505700	-6.15244700	C	-0.51346100	-2.53701600	-4.57558900
C	-0.75212200	-2.40287500	-4.98851200	C	-0.53663900	-2.56649700	-3.12307000
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C	-0.71194000	-2.42381600	-2.55216400	C	0.65594500	-1.87571500	-1.12585100
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C	2.12260200	-2.43611200	-2.64470200	C	3.06177900	-1.95745100	-2.61134400

C	3.34261600	-1.79048200	-3.11257300	C	3.77525800	-1.45575700	-3.75791400
C	3.32838800	-1.78172600	-4.53418200	C	3.10049700	-1.91064200	-4.94687100
C	2.10006700	-2.41902900	-4.97475900	C	1.97139900	-2.74793300	-4.55496600
C	1.36063600	-2.82701400	-3.79899700	C	1.94701600	-2.77668300	-3.07377700
Lu	2.25373200	2.37955600	-3.16161100	Lu	-0.72597600	2.61689000	-3.74068100
Lu	-1.13316500	0.51253300	-4.09952500	Lu	1.19340600	-0.64712500	-3.78985600
O	0.62610200	1.35953600	-3.69597800	O	0.76906200	1.29971000	-3.75071000

$Lu_2O@C_1(31876)$-C_{80}				$Lu_2O@C_{2v}(5)$-C_{80}			
C	12.75074800	9.23706500	13.83271500	C	16.56554100	7.58461400	-0.21818300
C	12.17940700	7.97204700	13.45741500	C	15.22292100	7.47033100	0.29475600
C	12.29174100	7.81831400	12.01905300	C	17.48257800	6.49491400	-0.13714200
C	12.95793600	8.98493900	11.48460200	C	18.87538300	6.82479800	0.09507500
C	13.16777200	9.90987400	12.59910200	C	19.65132700	5.99300900	0.97849800
C	14.24878100	10.86066500	12.60194200	C	19.13923700	4.78284400	1.57373000
C	14.80530800	11.20756600	13.86974100	C	17.84247500	4.37381000	1.14450600
C	14.46933900	10.44871600	15.06565500	C	16.99826800	5.25625400	0.35306400
C	13.57166800	9.33625700	15.01841800	C	15.63318000	5.12765600	0.83358000
C	13.90458400	8.11604400	15.78955500	C	15.62098200	4.09781100	1.83960000
C	13.47920300	6.80792900	15.26523200	C	19.63446200	4.40948800	2.89803800
C	12.62878900	6.75989600	14.09606600	C	17.44058800	3.24572700	3.28261700
C	12.93731600	5.80957200	13.03077400	C	16.55802600	3.35474400	4.43182600
C	12.80374000	6.50036100	11.74699300	C	15.25031700	3.82827000	4.26532100
C	13.80895500	6.30060000	10.72300300	C	14.76493100	4.19876300	2.94972700
C	14.39092200	7.48501300	10.04222100	C	16.97957500	3.61985300	2.01575000
C	13.99230000	8.84600500	10.47603600	C	13.89921800	5.33871600	3.09102100
C	14.96401200	9.90578600	10.40309000	C	18.77707100	3.59640300	3.69972100
C	15.08777700	10.91724700	11.44321300	C	20.68091000	5.23995600	5.00116900
C	16.47681300	11.28011100	11.56191100	C	21.09086600	6.38230500	5.78030500

C	17.03935400	11.58974000	12.83378900	C	21.54897500	7.54017700	5.13877100
C	16.18046700	11.61354000	13.98255800	C	21.14185700	6.47727300	2.91579000
C	16.66441700	11.18825500	15.26888200	C	20.63212000	5.26581200	3.57413200
C	15.61173300	10.44634400	15.91896500	C	21.59183700	7.57832600	3.70318000
C	15.89047300	9.35744200	16.79367300	C	20.66246900	6.80816600	1.58914000
C	15.01949300	8.17568600	16.73612000	C	13.81184900	5.65736600	4.51087600
C	15.53993100	6.94787600	17.23340600	C	19.64888700	4.57156400	5.76595400
C	15.17153400	5.67765500	16.64133500	C	14.84579500	8.76613300	0.78780900
C	14.24558700	5.59443300	15.57591800	C	13.51453200	7.67908300	2.56808500
C	14.44168800	4.54689500	14.55477300	C	13.87914800	6.36974000	2.10134400
C	13.86501000	4.73660000	13.22009400	C	18.72302600	3.77647800	5.13402900
C	14.56617000	4.29914000	12.06063900	C	17.34090700	3.78055600	5.56578400
C	14.58992200	5.10800800	10.84661400	C	19.25015400	5.41366000	6.87249000
C	15.92011400	5.02506500	10.30821500	C	17.86825900	5.60786500	7.17549700
C	16.45871100	6.11658000	9.62561800	C	16.86924000	4.75430400	6.49787600
C	15.68866400	7.32941700	9.45837300	C	14.70854900	4.74889800	5.22617000
C	16.64006100	8.41387000	9.40356600	C	19.81620000	7.75553400	7.38499600
C	16.28030400	9.68111300	9.87926800	C	18.44772500	7.97244000	7.77536900
C	17.22995300	10.49221600	10.59887200	C	17.47964200	6.93207600	7.65919000
C	18.54536400	10.00532800	10.86427100	C	20.20768500	6.49217400	6.92898500
C	19.20850400	10.49598000	12.06382900	C	16.11693600	7.35523100	7.44615000
C	18.41572300	11.21565600	13.04860300	C	15.94605700	9.67023800	0.63962700
C	18.91727500	10.87726400	14.34725200	C	16.21448800	10.67626500	1.61694800
C	18.02974500	10.83195300	15.48276700	C	13.33063300	7.98566700	3.98068700
C	18.31797500	9.89621800	16.50467100	C	15.48579400	5.22073700	6.32540200
C	17.25422500	9.21187900	17.20792600	C	13.49712400	6.96672100	4.99702700
C	17.76375800	7.93735300	17.63334400	C	17.59149600	11.06218600	1.75727200
C	16.90346000	6.83242700	17.70257500	C	18.09390700	11.53086600	3.01254500

C	17.40011400	5.51723200	17.35300700	C	17.23566600	11.66392100	4.12830000
C	16.30773400	4.78568900	16.74720800	C	15.85760900	11.29359200	4.01214600
C	16.55120900	3.87282100	15.71957800	C	15.32661600	10.79219500	2.78504000
C	15.60131300	3.72787800	14.64869800	C	19.24372600	9.93315700	6.74188500
C	16.36051500	3.39792100	13.45625400	C	20.98054500	9.71681200	4.48707700
C	15.86705800	3.70058000	12.19868400	C	19.94887100	10.70594800	4.47632400
C	16.74591300	4.22805400	11.18414900	C	19.05295600	10.82548700	5.64191600
C	18.08548500	4.60646800	11.49507600	C	17.71542400	11.31389500	5.43654100
C	18.63683900	5.74634800	10.75304700	C	19.44283900	11.06909100	3.18114600
C	17.84304800	6.45131300	9.80488900	C	14.22456500	9.87825400	2.90615500
C	17.96273300	7.90056300	9.64198500	C	14.00656700	8.86293900	1.92165700
C	18.91308000	8.66482700	10.37997200	C	14.76878400	6.26174100	0.92966500
C	19.89904600	7.92208800	11.14274600	C	15.11520400	6.52188600	6.84424500
C	20.62991900	8.46023600	12.27935700	C	14.06437000	7.37582500	6.28595300
C	20.27699300	9.78868600	12.75882300	C	15.74402800	8.73055300	7.23633900
C	20.04844600	9.97255900	14.18984900	C	14.47693400	8.77938600	6.51645400
C	20.21715400	8.90221500	15.16883500	C	20.56179500	8.16665500	1.05119300
C	19.43666100	8.97167800	16.37056700	C	19.41144300	8.18058700	0.11830900
C	19.11173100	7.78605400	17.12280400	C	16.78652400	9.73345200	7.13469400
C	19.55875300	6.52386000	16.69382800	C	18.11502700	9.35071500	7.44739600
C	18.70800000	5.36457500	16.85256500	C	14.37386300	9.78016400	5.43773400
C	18.93372500	4.50206300	15.70300800	C	13.76611900	9.36063900	4.19618300
C	17.89203300	3.74089500	15.16879200	C	15.43721100	10.74111700	5.29868700
C	17.76681100	3.56492600	13.73876400	C	16.59994400	10.76378600	6.16575600
C	18.61903300	4.25931600	12.82275900	C	20.76958000	9.26777800	1.99730300
C	19.70388300	5.05861600	13.40417300	C	21.30069100	8.95113800	3.28865700
C	20.21748100	6.16469700	12.64416900	C	17.03337700	8.94232900	-0.01247200
C	19.69717700	6.49593400	11.36014200	C	18.42385500	9.27569500	0.15855000

C	20.75916500	7.37781300	13.24432300	C	21.15907100	8.85100100	5.62169100
C	20.61560100	7.56609400	14.67883000	C	20.30082900	8.95598100	6.72976500
C	20.27236200	6.40826500	15.44457900	C	19.83140800	10.37143900	1.96219300
C	19.86398000	5.15205600	14.81390000	C	18.68056900	10.37047200	1.06589600
Lu	14.56081500	7.79965700	12.95321800	Lu	15.79323300	7.87619800	4.76012000
Lu	18.43506900	8.35602500	13.19613600	Lu	18.58899000	8.14130900	2.34438600
O	16.54347700	7.71319400	13.23096200	O	17.49784300	7.43617200	3.84443500

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