

$\text{Ln}_3@C_{80}^+$ (Ln = lanthanide): a new class of stable
metallofullerene cations with multicenter metal-metal
bonding in sub-nanometer confined space

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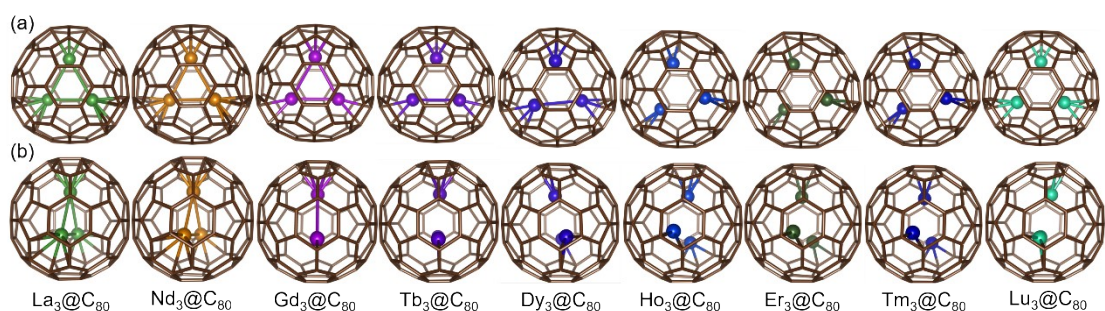


Figure S1. The front view (a) and side view (b) of the optimized geometric structures of $\text{Ln}_3@I_h\text{-C}_{80}$ (Ln = La, Nd, Gd, Tb, Dy, Ho, Er, Tm, Lu) by using PBE0 functional.

Table S1. Relative energies (ΔE , in kcal/mol) of $\text{Ln}_3@C_{80}$ calculated at different theory level

$\text{Ln}_3@C_{80}$	La		Nd		Gd		Tb		Dy		Ho		Er		Lu	
	(Cage spiral number)	PBE	PBE0	PBE	PBE0	PBE	PBE0	PBE	PBE0	PBE	PBE0	PBE	PBE0	PBE	PBE0	
$\text{Ln}_3@I_h(31924)\text{-C}_{80}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$\text{Ln}_3@D_{5h}(31923)\text{-C}_{80}$	15.07	17.37	14.66	16.45	14.44	13.74	13.58	13.94	13.22	14.02	13.31	14.21	13.39	14.23	12.76	16.88
$\text{Ln}_3@C_{2v}(31922)\text{-C}_{80}$	17.85	21.81	13.80	14.11	16.30	16.16	16.80	17.83	17.79	19.50	19.21	21.19	20.53	22.62	23.22	29.21
$\text{Ln}_3@C_{2v}(31920)\text{-C}_{80}$	22.02	24.64	20.94	21.40	25.96	26.35	27.05	28.65	28.71	31.04	30.76	33.35	32.78	35.51	37.42	44.13
$\text{Ln}_3@C_I(28319)\text{-C}_{80}$	33.73	37.73	33.20	33.69	32.56	35.09	32.79	36.59	33.53	38.03	34.64	39.43	35.75	40.67	37.90	46.45
$\text{Ln}_3@C_I(28324)\text{-C}_{80}$	32.29	38.64	31.60	33.46	33.95	35.50	34.35	37.10	35.29	38.72	36.62	40.29	37.93	41.73	40.79	48.43
$\text{Ln}_3@C_I(28325)\text{-C}_{80}$	25.57	28.07	25.30	28.81	14.19	24.15	24.77	25.96	25.81	27.72	27.24	29.40	28.63	30.66	31.48	35.96
$\text{Ln}_3@C_2(29591)\text{-C}_{80}$	30.28	48.73	38.03	30.95	30.74	30.67	31.05	32.03	31.84	33.33	33.09	34.60	34.34	35.74	36.92	41.59
$\text{Ln}_3@C_I(31876)\text{-C}_{80}$	30.28	36.84	13.80	32.05	30.25	32.66	30.24	33.79	30.93	35.14	32.02	36.45	33.13	37.65	35.50	43.84

Table S2. Relative energies (ΔE , in kcal/mol) and HOMO-LUMO gap of the molecules (H-L Gap, in eV) (6-31G* and ECP58MWB basis sets are used for C and Tm atom, respectively)

Tm_3C_{80} (spiral number)	PBE0		PBE	
	ΔE ,	H-L Gap	ΔE	H-L Gap
$\text{Tm}_3@I_h(31924)\text{-C}_{80}$	0.00	1.50 ^{α} /2.70 ^{β}	0.00	0.28 ^{α} /1.43 ^{β}
$\text{Tm}_3@D_{5h}(31923)\text{-C}_{80}$	14.08	0.28 ^{α} /1.43 ^{β}	13.32	0.28 ^{α} /1.38 ^{β}
$\text{Tm}_3@C_{2v}(31922)\text{-C}_{80}$	23.89	1.41 ^{α} /1.59 ^{β}	21.65	0.47 ^{α} /0.59 ^{β}
$\text{Tm}_3@C_{2v}(31920)\text{-C}_{80}$	37.40	0.95 ^{α} /1.54 ^{β}	34.54	0.09 ^{α} /0.52 ^{β}
$\text{Tm}_3@C_I(28319)\text{-C}_{80}$	41.63	1.19 ^{α} /1.81 ^{β}	36.56	0.32 ^{α} /0.78 ^{β}
$\text{Tm}_3@C_I(28324)\text{-C}_{80}$	42.91	1.56 ^{α} /1.44 ^{β}	38.98	0.52 ^{α} /0.40 ^{β}
$\text{Tm}_3@C_I(28325)\text{-C}_{80}$	31.18	1.34 ^{α} /2.30 ^{β}	29.62	0.27 ^{α} /1.16 ^{β}
$\text{Tm}_3@C_2(29591)\text{-C}_{80}$	36.42	1.40 ^{α} /2.49 ^{β}	35.20	0.24 ^{α} /1.38 ^{β}
$\text{Tm}_3@C_I(31876)\text{-C}_{80}$	38.68	1.60 ^{α} /1.25 ^{β}	34.04	0.59 ^{α} /0.30 ^{β}
$\text{Tm}_3\text{C}_2@C_2(22010)\text{-C}_{78}$	75.03	1.93 ^{α} /2.49 ^{β}	69.78	0.55 ^{α} /1.23 ^{β}
$\text{Tm}_3\text{C}_2@C_{2v}(24107)\text{-C}_{78}$	96.77	1.64 ^{α} /1.21 ^{β}	83.02	0.66 ^{α} /0.19 ^{β}
$\text{Tm}_3\text{C}_2@C_I(21975)\text{-C}_{78}$	96.77	1.43 ^{α} /1.57 ^{β}	86.88	0.43 ^{α} /1.17 ^{β}
$\text{Tm}_3\text{C}_2@C_{2v}(24088)\text{-C}_{78}$	100.56	1.77 ^{α} /2.01 ^{β}	92.33	0.35 ^{α} /0.92 ^{β}
$\text{Tm}_3\text{C}_2@D_{3h}(24109)\text{-C}_{78}$	111.09	1.92 ^{α} /2.30 ^{β}	100.36	0.29 ^{α} /0.95 ^{β}

Table S3. Calculated relative energies (ΔE , in kcal/mol) of $\text{Ln}_3@C_{80}$ with different spin multiplicities by using PBE0 functional

$\text{Ln}_3@C_{80}$	Doublet	Quartet
La	0	7.81
Nd	0	1.36
Gd	0	10.70
Tb	0	13.45
Dy	0	15.29
Ho	0	17.28
Er	0	20.24
Tm	0	22.62
Lu	0	29.76

Table S4. Calculated Ln-Ln bond length (in Å), the Mayer bond order of the metal moiety in $\text{Ln}_3@I_h-C_{80}^+$ and the ionization energies (IP, in eV) of $\text{Ln}_3@I_h-C_{80}$ by using PBE functional

$\text{Ln}_3@C_{80}$	Ln-Ln				Mayer bond order				IP
	1	2	3	average	1	2	3	Ln_3	
La	3.427	3.427	3.428	3.427	1.678	1.677	1.677	5.032	5.56
Nd	3.473	3.480	3.480	3.478	1.583	1.586	1.582	4.751	5.34
Gd	3.506	3.513	3.474	3.498	1.701	1.632	1.609	4.942	5.34

Tb	3.509	3.510	3.501	3.507	1.627	1.607	1.612	4.846	5.34
Dy	3.507	3.512	3.486	3.502	1.629	1.707	1.568	4.904	5.53
Ho	3.514	3.518	3.513	3.515	1.744	1.737	1.745	5.226	5.42
Er	3.523	3.518	3.514	3.518	1.803	1.819	1.812	5.434	5.46
Tm	3.511	3.529	3.520	3.520	1.686	1.680	1.708	5.074	5.48
Lu	3.568	3.579	3.470	3.539	1.563	1.540	1.966	5.069	5.64

Table S5. Calculated Ln-Ln bond length (in Å), Mayer bond order of the metal moiety in $\text{Ln}_3@C_{80}^+$, ionization energies (IP, in eV) of $\text{Ln}_3@C_{80}$ (PBE0 functional)

$\text{Ln}_3@C_{80}^+$	Ln-Ln				Mayer bond order				IP
	1	2	3	average	Ln(1)	Ln(2)	Ln(3)	Ln_3	
La	3.393	3.393	3.392	3.393	1.419	1.421	1.418	4.258	5.60
Nd	3.449	3.449	3.448	3.449	1.376	1.377	1.380	4.133	5.22
Gd	3.483	3.482	3.464	3.476	1.181	1.685	1.163	4.029	5.50
Tb	3.454	3.492	3.493	3.480	1.314	1.294	1.444	4.052	5.48
Dy	3.481	3.485	3.463	3.476	1.408	1.515	1.317	4.240	5.50
Ho	3.498	3.480	3.498	3.492	1.547	1.521	1.521	4.589	5.35
Er	3.497	3.491	3.507	3.498	1.600	1.592	1.618	4.810	5.43
Tm	3.498	3.495	3.490	3.494	1.492	1.463	1.492	4.447	5.50
Lu	3.542	3.550	3.456	3.516	1.352	1.332	1.821	4.505	5.65

Table S6. The calculated relative energies with different positions of encaged Tm_3 cluster in $Tm_3@I_h-C_{80}^+$. (R_5 and R_6 mean that the metal atom is located toward a hexagon and a pentagon, respectively; B_{65} , B_{66} and V_{665} mean that the metal atom is located toward a 6:5, 6:6 bond and a vertex fused by two hexagons and one pentagon, respectively.)

Metal atom position	$R_6R_6R_6$	$B_{66}R_6R_6$	$B_{56}B_{56}B_{56}$	$R_6R_5R_5$	$B_{66}B_{66}R_6$	$V_{665}V_{665}V_{665}$
Relative energy (in kcal/mol)	0.0	1.51	0.1	1.56	0.01	0.59

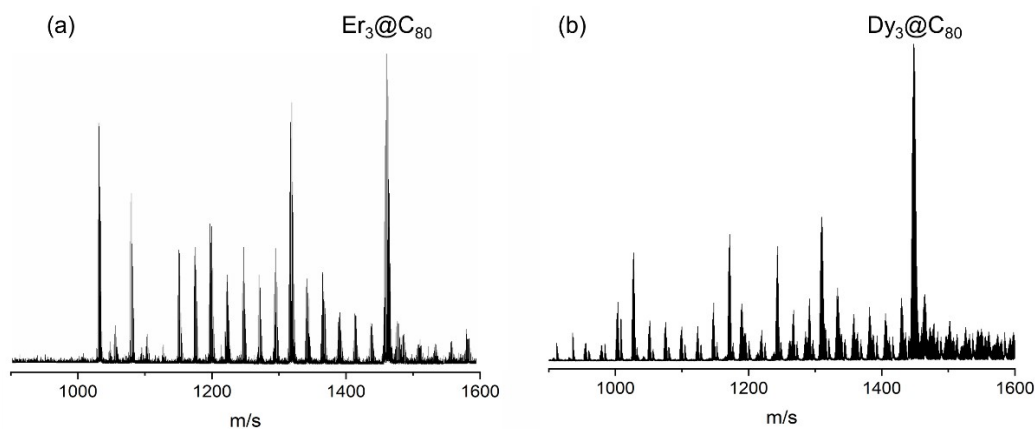


Figure S2. The LDI-TOF mass spectra of samples containing $Er_3@C_{80}^+$ (a) and $Dy_3@C_{80}^+$ (b). The samples were obtained by oxidation of the arc-discharge produced soot by $AgSbF_6$.

Cartesian Coordinates (Angstrom) of DFT-Optimized Structures:

La₃@C₈₀ PBE/6-31G*~MWB46

C	-3.42451900	-1.75771100	1.42004100
C	-2.57304400	-1.95745900	2.54777600
C	-2.17712300	-0.85207500	3.38054600
C	-0.84367100	-1.10902000	3.85589200
C	0.08643300	-0.04090900	4.06315300
C	1.47187400	-0.30511100	3.81787900
C	2.34086000	0.71804800	3.29948400
C	3.33753100	0.09068800	2.44200900
C	3.96519800	0.78013400	1.33277000
C	4.26575000	-0.05370500	0.15854600
C	4.06169400	0.46088500	-1.21714800
C	3.54645100	-0.65017300	-2.00862300
C	2.61092800	-0.48302300	-3.09536800
C	1.71261500	-1.56224000	-3.39295300
C	0.38063100	-1.29772200	-3.86876200
C	-0.49193600	-2.31783100	-3.35037300
C	-1.84586600	-2.02804100	-3.01960900
C	-2.41426000	-2.75263000	-1.90715600
C	-3.36739000	-2.09187700	-1.04620100
C	-3.18560700	-2.61411000	0.28414100
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C	0.84772500	1.10703600	-3.85273100
C	2.17817500	0.84442200	-3.37253300
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C	3.54848000	1.81574900	-1.45650600
C	3.30977100	2.67020000	-0.28536900
C	3.51859500	2.16038800	1.09100700
C	2.45000700	2.72461800	1.90947100
C	1.85087700	2.02626300	3.02248200
C	0.48742600	2.32315000	3.35799300
C	-0.38163200	1.29727300	3.87102900
C	-1.71329500	1.55525300	3.39064900
C	-2.60828100	0.48768000	3.09830600
C	-3.53398300	0.69337500	2.01030000
C	-3.59478500	1.92476700	1.23279900

C	-3.97463300	1.54039500	-0.14776600
C	-3.38726200	2.21856200	-1.31345700
C	-3.05744100	1.35640800	-2.43109600
C	-1.89511200	1.57651600	-3.28198900
C	-0.95447600	2.60591300	-2.99204500
C	0.42246100	2.37705700	-3.32709900
C	1.48921000	2.89958300	-2.51373200
C	1.20903300	3.67878700	-1.35208400
C	2.12696800	3.52877500	-0.25026100
C	1.63130500	3.59650400	1.09981000
C	0.24579300	3.84762300	1.39970000
C	-0.30592000	3.21512400	2.55319700
C	-1.68507600	2.75671400	2.57015800
C	-2.61616200	2.98807200	1.48688200
C	-2.07740600	3.71020800	0.32577600
C	-2.45987300	3.33249600	-1.05691900
C	-1.25454100	3.46617400	-1.87091400
C	-0.17112600	3.95935000	-1.05245100
C	-0.65953300	4.06512700	0.29813300
C	-1.48912800	-2.92679300	2.51169300
C	-0.41370200	-2.37508300	3.32511000
C	0.95162300	-2.60552900	2.99422800
C	1.90328300	-1.57161100	3.28848800
C	3.04002900	-1.33388800	2.43783800
C	3.26653400	-2.13373400	1.27758100
C	3.86293500	-1.46051900	0.14975800
C	3.47024300	-1.83373700	-1.18497600
C	2.52734700	-2.88960600	-1.44578600
C	1.66549400	-2.74497300	-2.57379500
C	0.29808400	-3.23898700	-2.54533700
C	-0.25811100	-3.98648400	-1.43708600
C	-1.67841600	-3.75278700	-1.14175000
C	-2.16956500	-3.66548900	0.25511000
C	-1.24998800	-3.81558000	1.39345400
C	0.15684600	-4.11955700	1.09659200
C	1.21147800	-3.47558900	1.87191300
C	2.34327300	-3.20679500	1.01629000
C	1.98261700	-3.60628500	-0.31930900
C	0.64767700	-4.20116800	-0.29998000
La	-0.36802100	-1.85180400	-0.00331000
La	-1.42665700	1.24075300	-0.00211000
La	1.78929900	0.60893400	-0.00422000

Nd₃@C₈₀ PBE/6-31G*~MWB49

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C	1.12540800	-0.82747300	3.87166800
C	0.00801500	0.04772800	4.08592800
C	0.20482300	1.44963900	3.84763800
C	-0.85604000	2.27493700	3.32891000
C	-0.28312800	3.31036800	2.48334800
C	-0.99770900	3.94272200	1.38265200
C	-0.17580200	4.28117500	0.20256500
C	-0.66891100	4.06985400	-1.18479300
C	0.47117400	3.59562800	-1.96991200
C	0.37162300	2.67015100	-3.07687100
C	1.49775200	1.83149000	-3.37707400
C	1.30541100	0.48728000	-3.86046100
C	2.36689700	-0.33500900	-3.33686500
C	2.14906000	-1.71578000	-3.02954700
C	2.89445900	-2.24367500	-1.90764300
C	2.26162200	-3.21894200	-1.05412900
C	2.77662300	-3.03350400	0.27783600
C	0.60238300	-3.86173700	1.13747400
C	0.11448900	-4.12127000	-0.19249700
C	0.93949500	-3.73771600	-1.31558900
C	0.26238200	-3.28357700	-2.48449800
C	0.86127700	-2.27698900	-3.32729900
C	-0.20330700	-1.44898900	-3.83597700
C	-0.00815700	-0.04801400	-4.07736800
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C	-2.07826500	2.52725000	-2.53491200
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C	-2.36073500	3.41897200	1.11514100
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C	-2.04616900	-3.51997500	-1.37205500

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C	-3.82949700	0.02566200	1.37279200
C	-3.21646400	-0.50078700	2.54454900
C	-2.69143900	-1.85917600	2.54756700
C	-2.89215100	-2.80754300	1.46206500
C	-3.61643300	-2.28932100	0.28453200
C	-3.21020800	-2.63718000	-1.10444500
C	-3.37738300	-1.42270000	-1.90555900
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C	-4.01538400	-0.88239900	0.26658700
C	2.99069000	-1.36140900	2.53052800
C	2.37464200	-0.33154500	3.35199400
C	2.53762500	1.05517100	3.03415400
C	1.45493400	1.94989100	3.33356000
C	1.15620200	3.08362000	2.49283200
C	1.92863900	3.33023000	1.32260600
C	1.24299400	3.92451200	0.20051000
C	1.64327300	3.54954700	-1.13102000
C	2.75005600	2.66012000	-1.39323800
C	2.67945400	1.82877600	-2.54847800
C	3.24782100	0.48787500	-2.52231500
C	4.04962900	-0.03439500	-1.42274700
C	3.87090400	-1.47834600	-1.13063600
C	3.79520000	-1.98364800	0.26680500
C	3.90183400	-1.07950000	1.43008800
C	4.13141300	0.35635700	1.13635500
C	3.39986300	1.35907200	1.91369700
C	3.05918300	2.46938100	1.05979100
C	3.50956700	2.15511500	-0.27173200
C	4.21087600	0.86834600	-0.26038800
Nd	-1.22045200	-1.60807500	-0.01127300
Nd	2.00479200	-0.25023000	-0.01150000
Nd	-0.78681800	1.85894300	-0.01446600

Gd₃@C₈₀ PBE/6-31G*~MWB53

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C	3.52661000	-2.10015300	-0.48833600
C	2.83847300	-2.84862700	0.53030400
C	2.98565800	-2.14855700	1.77433600
C	0.82063300	-3.08167500	2.48403600
C	0.69967200	-3.84270400	1.27030500
C	1.69114300	-3.67652000	0.24509500
C	1.26257000	-3.78748900	-1.10792400
C	1.90410400	-2.99696000	-2.13050300
C	0.89400800	-2.61417300	-3.08110900
C	0.96041500	-1.35263800	-3.75737700
C	-0.27409900	-0.69883600	-4.05107000
C	-0.38318800	0.73663700	-4.03700500
C	-1.71457700	1.08487300	-3.60459200
C	-1.95186500	2.26301100	-2.82858600
C	-2.99961000	2.23890300	-1.82818700
C	-2.98597100	3.05766500	-0.60606400
C	-3.57549100	2.20293400	0.45442600
C	-3.06480700	2.16346000	1.81781900
C	-3.13510900	0.91831700	2.53913400
C	-2.12040600	0.52449200	3.48926100
C	-2.01203400	-0.90871900	3.47501600
C	-0.74525400	-1.54226900	3.66717900
C	-0.50131800	-2.75927200	2.93988000
C	-1.46120600	-3.34725500	2.03177600
C	-0.71852700	-4.07084600	0.98104400
C	-1.19149100	-4.12418600	-0.41134700
C	-0.15428100	-3.93321800	-1.42495500
C	-0.36302100	-3.17236800	-2.65103800

C	-1.59097300	-2.46722100	-2.87654000
C	-1.53685000	-1.25256800	-3.62940400
C	-2.42137800	-0.14737200	-3.34891100
C	-3.34094400	-0.22841400	-2.27486000
C	-3.62562700	0.97314700	-1.53822900
C	-3.96502900	0.94017600	-0.14306300
C	-4.01351700	-0.30948100	0.57902200
C	-3.66260000	-0.29786200	1.95263500
C	-2.95718500	-1.43261600	2.51538500
C	-2.70229200	-2.63911200	1.76967200
C	-3.19964800	-2.72180400	0.40379800
C	-2.48643800	-3.45257200	-0.67272000
C	-2.62565000	-2.62031400	-1.87629100
C	-3.43917100	-1.47326900	-1.56298600
C	-3.77794400	-1.52144400	-0.16842800
C	2.44432500	0.15223300	3.29691800
C	1.53756300	1.24540700	3.58216100
C	1.58662400	2.43291100	2.80714500
C	0.35066900	3.12214800	2.55161300
C	0.11495000	3.87738100	1.35166600
C	1.11709900	3.88609400	0.32541300
C	0.67317400	3.95934400	-1.02565600
C	1.42509200	3.29553700	-2.06304300
C	2.64190800	2.58827800	-1.78176200
C	2.93941300	1.41814900	-2.54534700
C	3.67253700	0.30102700	-1.96116500
C	4.26163700	0.33173800	-0.62732100
C	4.17938900	-0.93802700	0.12015200
C	3.80077400	-0.96836900	1.55429300
C	3.48076800	0.24164300	2.29892300
C	3.61354400	1.50144100	1.58043200
C	2.62979300	2.54007100	1.82367200
C	2.37757200	3.23617600	0.59467500
C	3.16897300	2.62124800	-0.43842600
C	3.99084700	1.55839900	0.14675900
Gd	-0.86339900	-1.79583500	0.01673300
Gd	1.99413200	0.15253800	0.13934500
Gd	-1.14207500	1.63134300	0.01606400

Tb₃@C₈₀ PBE/6-31G*~MWB54

C	3.22873300	0.25246400	-2.42885000
C	2.25315000	0.24328400	-3.45521600
C	1.38624200	1.38187600	-3.64177400

C	0.08997400	0.87974600	-4.02830200
C	-1.10926700	1.54988800	-3.64202700
C	-2.26382200	0.73818700	-3.38178700
C	-3.21872000	1.09811500	-2.36792100
C	-3.78242800	-0.11814700	-1.78839300
C	-4.30769400	-0.19558900	-0.42648800
C	-4.00406900	-1.45680300	0.27441300
C	-3.54866500	-1.47535200	1.68169200
C	-2.59809800	-2.55577100	1.83563500
C	-1.51009100	-2.51814200	2.77149400
C	-0.30499800	-3.21972400	2.41862200
C	0.98726400	-2.74889400	2.82779800
C	1.97179400	-3.19846800	1.86613500
C	3.09866800	-2.32544500	1.56840000
C	3.52459000	-2.30004900	0.17799100
C	3.92778300	-1.02592700	-0.38450400
C	3.51646700	-0.98503800	-1.75961200
C	3.39632700	1.46090200	-1.66828100
C	3.80549600	1.43556300	-0.29138800
C	4.04611100	0.18434800	0.38911400
C	3.76304100	0.11563900	1.77695000
C	3.23245300	-1.11278000	2.33620600
C	2.27884400	-0.73582200	3.35554500
C	1.11162500	-1.52961100	3.58355100
C	-0.09302400	-0.87856700	3.99363500
C	-1.38978900	-1.37108700	3.59722300
C	-2.27600700	-0.24311300	3.40720500
C	-3.34659800	-0.25872300	2.44582000
C	-3.68070100	0.98822700	1.77885500
C	-4.14613800	1.03662100	0.37247800
C	-3.49582800	2.21355900	-0.21555800
C	-3.03210800	2.27847700	-1.58174900
C	-1.92666800	3.13787500	-1.89485000
C	-0.97611200	2.77615700	-2.91390100
C	0.31510200	3.28204700	-2.52312200
C	1.51247300	2.55972300	-2.84188300
C	2.60217300	2.64274400	-1.89032000
C	2.54646600	3.42119800	-0.64382900
C	3.29095400	2.62333500	0.36222900
C	2.85463400	2.48265000	1.74482800
C	3.11688800	1.23989500	2.42482600
C	2.20790100	0.69818400	3.40898500
C	0.96872300	1.35360800	3.69291000
C	-0.16360900	0.55630300	4.04786800

C	-1.50317600	0.94822500	3.68477500
C	-1.73999000	2.13939900	2.95137400
C	-2.83041400	2.13734700	2.01408200
C	-2.73449000	2.89472200	0.79951600
C	-1.57843100	3.70334300	0.49571600
C	-1.21273600	3.86192800	-0.87061900
C	0.18794900	3.98370600	-1.25305900
C	1.27788500	4.09705100	-0.28656400
C	0.87126900	3.97999100	1.11775600
C	1.64503800	3.20021600	2.09760500
C	0.71897100	2.60647300	3.03449200
C	-0.61443600	2.98443200	2.66241200
C	-0.53467000	3.78945400	1.47475300
C	1.50223500	-0.95645800	-3.73469300
C	0.16117300	-0.55731200	-4.08199100
C	-0.96515200	-1.36946600	-3.75000600
C	-2.19238400	-0.69694400	-3.43434200
C	-3.10343400	-1.22525700	-2.45488800
C	-2.79760600	-2.43914200	-1.76208600
C	-3.25268800	-2.52100100	-0.39717300
C	-2.43231200	-3.20611600	0.56698700
C	-1.20571000	-3.87210000	0.20505200
C	-0.14933800	-3.93344100	1.17988100
C	1.27133100	-3.98257500	0.82639800
C	1.66979000	-3.91939400	-0.58917000
C	2.84607400	-3.07747400	-0.88484900
C	2.82613800	-2.20948700	-2.06620100
C	1.74193300	-2.16945000	-3.01876100
C	0.62562600	-3.02995500	-2.75971900
C	-0.70980500	-2.63009500	-3.11949500
C	-1.61843300	-3.16402700	-2.13890600
C	-0.83389400	-3.88747700	-1.16761200
C	0.57271700	-3.83476600	-1.54800700
Tb	0.95783800	1.74633800	0.01118300
Tb	1.06556400	-1.68545800	0.01223800
Tb	-2.00203000	-0.06290200	0.14612000

Dy₃@C₈₀ PBE/6-31G*~MWB55

C	3.24629900	0.24276700	-2.41263000
C	2.27364200	0.25391200	-3.44205100
C	1.41949200	1.40334900	-3.62146600
C	0.12003000	0.91955900	-4.02122500
C	-1.07396400	1.59773200	-3.63269700

C	-2.23850600	0.79616400	-3.38695100
C	-3.19205400	1.15598200	-2.37187300
C	-3.76771000	-0.06032200	-1.80512300
C	-4.29889600	-0.14484100	-0.44742000
C	-4.00681800	-1.41278400	0.24033700
C	-3.56375200	-1.45257200	1.64896700
C	-2.63236700	-2.54889400	1.79957700
C	-1.55039200	-2.53094200	2.74141300
C	-0.35073800	-3.24043700	2.38604200
C	0.94386500	-2.78564800	2.80523000
C	1.92756200	-3.23600600	1.84382800
C	3.06078000	-2.36784400	1.55923000
C	3.48979300	-2.33031600	0.17339400
C	3.91920700	-1.06065900	-0.37625100
C	3.51754600	-1.00294600	-1.75366000
C	3.42202400	1.44171200	-1.63799200
C	3.82343000	1.39796400	-0.25866300
C	4.04895800	0.13785100	0.41113300
C	3.75595600	0.05780000	1.79678900
C	3.20985100	-1.16863900	2.34323900
C	2.25502300	-0.79255000	3.36160200
C	1.07869000	-1.57647800	3.57584800
C	-0.12137400	-0.91742600	3.98648300
C	-1.42084600	-1.39265000	3.57824200
C	-2.29329600	-0.25304100	3.39520900
C	-3.35658700	-0.24751200	2.42684500
C	-3.67740900	1.00945200	1.77213500
C	-4.13654300	1.07750200	0.36454200
C	-3.47116300	2.25313500	-0.20916600
C	-2.99929300	2.32630100	-1.57292000
C	-1.88331400	3.17621300	-1.87182500
C	-0.93217200	2.81426100	-2.89059400
C	0.36251700	3.30101300	-2.48760100
C	1.55444000	2.57145500	-2.80912800
C	2.64163400	2.63409400	-1.85215500
C	2.58665600	3.39942700	-0.59717300
C	3.31745600	2.58372000	0.40405400
C	2.86844800	2.43078800	1.78152000
C	3.11695500	1.18147500	2.45240100
C	2.19809100	0.64134600	3.42818800
C	0.96462300	1.30698700	3.71412500
C	-0.17733400	0.51765500	4.05618800
C	-1.51035700	0.92751900	3.68960500
C	-1.73163000	2.12910600	2.96791400

C	-2.81601200	2.14679000	2.02306500
C	-2.70774100	2.91591800	0.81678700
C	-1.54182600	3.71495600	0.52719600
C	-1.16668300	3.88065200	-0.83594400
C	0.23586600	3.98905400	-1.21073100
C	1.32094400	4.07661600	-0.23816500
C	0.90455100	3.94547500	1.15900200
C	1.66475400	3.15340900	2.13547200
C	0.73009000	2.56811600	3.06789800
C	-0.59733600	2.96615600	2.69442300
C	-0.50378100	3.77688500	1.51191200
C	1.51111100	-0.93433100	-3.73916000
C	0.17622600	-0.51785400	-4.09004400
C	-0.96007400	-1.32119900	-3.76945300
C	-2.18130400	-0.63924400	-3.45234300
C	-3.10017500	-1.16755800	-2.48035200
C	-2.81266800	-2.39247900	-1.79962000
C	-3.27080300	-2.48149300	-0.43761100
C	-2.46838200	-3.18915100	0.52484200
C	-1.24747900	-3.86280100	0.16134900
C	-0.19645200	-3.94505600	1.14135000
C	1.22584900	-4.00560000	0.79445000
C	1.62956000	-3.92843000	-0.61882000
C	2.80770300	-3.08837800	-0.89828000
C	2.80943200	-2.21326200	-2.07298900
C	1.73335400	-2.15502100	-3.03125900
C	0.60747400	-3.00689000	-2.78558200
C	-0.72147000	-2.59036200	-3.14873500
C	-1.64074300	-3.12613700	-2.17900800
C	-0.86932000	-3.86636300	-1.21004900
C	0.53949700	-3.82306700	-1.58241300
Dy	1.00059800	1.72201300	0.00855800
Dy	1.01736300	-1.71459400	0.01294400
Dy	-2.00256200	-0.01133600	0.14007000

Ho₃@C₈₀ PBE/6-31G*~MWB56

C	-3.65804100	1.14369800	1.39529200
C	-3.21854200	0.44058000	2.54935300
C	-2.17333700	0.96958900	3.38753800
C	-1.41207500	-0.13973300	3.90281700
C	-0.00067800	-0.02636500	4.11832400
C	0.80503400	-1.19036100	3.89936000
C	2.14531800	-1.07787500	3.39075000

C	2.40905100	-2.21357700	2.53739800
C	3.29070300	-2.13888000	1.40498100
C	2.92181500	-2.92397500	0.25130500
C	3.16244000	-2.45510200	-1.11011400
C	2.07165900	-2.95542100	-1.92891900
C	1.55408400	-2.22539800	-3.04593200
C	0.16358000	-2.36913100	-3.35232700
C	-0.60308200	-1.25386700	-3.84019300
C	-1.94332000	-1.36677900	-3.33023100
C	-2.71963300	-0.20303900	-3.03664500
C	-3.60406400	-0.29785400	-1.91574600
C	-3.84140300	0.84581600	-1.07185100
C	-4.07310300	0.36981400	0.26735300
C	-3.08540500	2.44457800	1.13183700
C	-2.92510300	2.98807200	-0.20216400
C	-3.23198900	2.12015600	-1.32969500
C	-2.40310100	2.21818300	-2.48874100
C	-2.15150600	1.07668200	-3.33322000
C	-0.80381100	1.18706100	-3.82448100
C	0.00155000	0.02585200	-4.05594600
C	1.41160000	0.13966900	-3.83050200
C	2.17681800	-0.96908100	-3.32563400
C	3.24911300	-0.45090600	-2.49600600
C	3.82312600	-1.18665600	-1.38652400
C	4.30382300	-0.40833600	-0.22250500
C	4.00531400	-0.88639500	1.15263800
C	3.62361300	0.26476800	1.95853400
C	2.70855900	0.19891500	3.07823600
C	1.94461900	1.36523400	3.39151600
C	0.60570500	1.25448900	3.91103300
C	-0.15782200	2.36348300	3.40876600
C	-1.54248700	2.21641700	3.08735700
C	-2.05035700	2.98698200	1.97267600
C	-1.23992300	3.90001500	1.18015600
C	-1.79598600	3.93356200	-0.19613800
C	-0.87586300	3.91707000	-1.35578600
C	-1.21951300	3.06149300	-2.47488700
C	-0.22939200	2.39853800	-3.30394400
C	1.16810200	2.48495200	-3.01613900
C	1.99143600	1.35733900	-3.32959600
C	3.11022200	0.99640800	-2.49492500
C	3.44492700	1.75155500	-1.32972700
C	4.04882600	1.04176700	-0.21242700
C	3.66561800	1.43953700	1.12805600

C	2.82673400	2.58342400	1.40610800
C	2.00441100	2.54291700	2.56414600
C	0.69879700	3.16811900	2.56864000
C	0.20018200	3.90451300	1.44060200
C	1.07039800	3.98876000	0.29323700
C	0.55118200	3.97532200	-1.07083000
C	1.53448700	3.28818600	-1.88998400
C	2.64834700	2.91492300	-1.05639500
C	2.35867200	3.34036800	0.28812100
C	-3.10662100	-1.00367400	2.54043600
C	-1.98699200	-1.35125100	3.38504800
C	-1.16515300	-2.47446700	3.05905700
C	0.22841400	-2.39970700	3.36884500
C	1.21439900	-3.03323500	2.53140400
C	0.83090700	-3.75289400	1.36681600
C	1.71517800	-3.71458000	0.24417400
C	1.19479000	-3.73980400	-1.09818000
C	-0.21218400	-3.84497100	-1.36581200
C	-0.70411200	-3.16501800	-2.52113100
C	-2.02561500	-2.56120300	-2.50978600
C	-2.94348500	-2.70180600	-1.39734100
C	-3.71234500	-1.50003400	-1.10776500
C	-3.99166200	-1.07068400	0.25951000
C	-3.49147600	-1.79451800	1.40384600
C	-2.76648400	-3.03830400	1.13768100
C	-1.57372100	-3.29104700	1.93508500
C	-0.58065800	-3.90592600	1.09381400
C	-1.12318400	-4.02359300	-0.24562700
C	-2.50639000	-3.51971300	-0.24417700
Ho	-0.66219400	1.87856900	-0.05769100
Ho	-1.29995300	-1.51024800	-0.06093600
Ho	1.95910800	-0.36685700	-0.06440700

Er₃@C₈₀ PBE/6-31G*~MWB57

C	-2.17008900	2.80975800	1.98369800
C	-2.10805300	1.83167300	3.01209200
C	-0.87591000	1.55502100	3.70696500
C	-0.85182000	0.15409000	4.03436300
C	0.37831400	-0.57757400	4.03023000
C	0.33243100	-1.94575400	3.61331900
C	1.43534500	-2.53562400	2.90552400
C	0.91239300	-3.50101600	1.96248500
C	1.57897400	-3.81745200	0.72329300

C	0.69595800	-4.07330000	-0.39779700
C	1.01818400	-3.61798700	-1.73895700
C	-0.22302800	-3.31659900	-2.41849100
C	-0.31592400	-2.27042900	-3.38821200
C	-1.55389100	-1.55754500	-3.48422600
C	-1.57674900	-0.15133000	-3.78615000
C	-2.67870300	0.44532900	-3.08033900
C	-2.60823800	1.79200900	-2.60697000
C	-3.27343400	2.06044900	-1.36867900
C	-2.72724400	3.01100500	-0.43395100
C	-3.06472200	2.57328800	0.89512500
C	-0.97523400	3.56966800	1.70595300
C	-0.65601700	4.10343100	0.40005400
C	-1.51412900	3.73328500	-0.71123700
C	-0.89724700	3.51584200	-1.98034800
C	-1.43349800	2.55322200	-2.91344500
C	-0.32420800	1.94751900	-3.59935800
C	-0.36582600	0.57726700	-4.01866200
C	0.86182000	-0.15695900	-4.01187100
C	0.88462400	-1.55895500	-3.68912100
C	2.11938800	-1.84323700	-2.99221100
C	2.23160800	-2.88120700	-2.00508100
C	3.19567400	-2.70575800	-0.91036100
C	2.87881200	-3.17980600	0.45832400
C	3.32839300	-2.13079900	1.38610300
C	2.62199000	-1.78976900	2.61003900
C	2.70011300	-0.44949800	3.10466800
C	1.59410700	0.14551700	3.81398600
C	1.57187800	1.54868100	3.50407800
C	0.33126000	2.24889200	3.38672500
C	0.25477900	3.29707900	2.39758100
C	1.35960000	3.67597700	1.54084300
C	0.80709900	4.22549800	0.28277200
C	1.44339400	3.88707800	-1.00651200
C	0.55629600	3.53598400	-2.10390600
C	0.89173500	2.53888200	-3.10570000
C	2.09602100	1.76903800	-3.01902900
C	2.08428000	0.43528200	-3.53290800
C	2.85512600	-0.60019000	-2.89498800
C	3.66706600	-0.33475200	-1.75733100
C	3.83158000	-1.39595800	-0.78221000
C	3.92770900	-1.05763100	0.62271900
C	3.93242900	0.31437300	1.08590000
C	3.36372500	0.59358200	2.36053800

C	2.66162500	1.83446800	2.60137400
C	2.55773300	2.84818100	1.58967200
C	3.21262500	2.59876400	0.33470500
C	2.65204800	3.07599900	-0.93068500
C	2.97409100	2.06742100	-1.92908700
C	3.74248300	1.02422400	-1.30146300
C	3.88742600	1.34713200	0.09235100
C	-2.85473400	0.59614400	2.89974700
C	-2.06393100	-0.43749400	3.53186500
C	-2.08812900	-1.77048300	3.02793800
C	-0.88293800	-2.53653900	3.11556100
C	-0.53193500	-3.49014900	2.09810700
C	-1.37535800	-3.70986300	0.97292500
C	-0.74429400	-4.03842400	-0.26594300
C	-1.31078600	-3.58690600	-1.51279400
C	-2.52804500	-2.82952900	-1.56036800
C	-2.63588600	-1.82958400	-2.57489500
C	-3.35839400	-0.59242300	-2.32570600
C	-4.08932200	-0.33992200	-1.10012300
C	-3.98315200	1.03305300	-0.62442000
C	-3.83569500	1.35621800	0.79284000
C	-3.73630300	0.32603500	1.79890700
C	-3.89442200	-1.05920500	1.35373000
C	-2.99842000	-2.04858800	1.93746700
C	-2.63095600	-2.99694000	0.91914400
C	-3.25802000	-2.59782800	-0.32298900
C	-4.08901000	-1.40773800	-0.07930000
Er	0.55783600	1.89910000	-0.01956700
Er	-1.95408400	-0.44631800	0.03135200
Er	1.36567900	-1.43827700	-0.04071600

Tm₃@C₈₀ PBE/6-31G*~MWB58

C	-3.34019400	1.75426800	1.54144800
C	-2.99523200	0.96069400	2.66842500
C	-1.84495700	1.27374100	3.47641400
C	-1.28082100	0.03572900	3.94799500
C	0.13432300	-0.11077400	4.11422400
C	0.70703100	-1.39633700	3.84778500
C	2.02642600	-1.51517200	3.29093300
C	2.05078500	-2.66079600	2.41081500
C	2.89262600	-2.72257700	1.24823600
C	2.34749300	-3.40422900	0.09959800
C	2.61845300	-2.95654000	-1.25924900

C	1.43697600	-3.24227100	-2.04985000
C	1.02540100	-2.40685800	-3.13574700
C	-0.37695400	-2.29092000	-3.39505400
C	-0.94542000	-1.04562300	-3.83923700
C	-2.26535400	-0.92461500	-3.28056300
C	-2.80864700	0.35343400	-2.94286000
C	-3.65424500	0.39743100	-1.78966300
C	-3.65603200	1.54727700	-0.92205000
C	-3.92380100	1.09281800	0.41813200
C	-2.54969300	2.93300600	1.27444700
C	-2.34056000	3.46961200	-0.05550400
C	-2.83508700	2.69610400	-1.18394400
C	-2.04184900	2.66732000	-2.37207500
C	-2.02830700	1.51575200	-3.24112700
C	-0.70057500	1.39218900	-3.78044200
C	-0.12689900	0.10901600	-4.06019400
C	1.28642400	-0.03789600	-3.88220400
C	1.85231100	-1.27626400	-3.41794500
C	3.01854000	-0.97322100	-2.61249300
C	3.47454700	-1.81588900	-1.53078800
C	4.13811900	-1.16889900	-0.38189900
C	3.81936700	-1.61853800	0.99549400
C	3.68221400	-0.43334700	1.83337500
C	2.80335400	-0.35527600	2.98177400
C	2.27466300	0.92258600	3.34111400
C	0.95554700	1.04381100	3.90772300
C	0.38951000	2.28371300	3.45057800
C	-1.00830100	2.39106300	3.17306700
C	-1.40355400	3.25357100	2.08204400
C	-0.46790700	4.01365000	1.27248600
C	-1.05513900	4.18762800	-0.07745700
C	-0.19410500	4.03616800	-1.26895600
C	-0.72476300	3.28280800	-2.38884900
C	0.10067700	2.46970000	-3.26244200
C	1.49847900	2.29365800	-3.01786900
C	2.09269300	1.04418100	-3.38119900
C	3.15005000	0.47176600	-2.58801200
C	3.65620200	1.12880500	-1.42713200
C	4.15544900	0.29999100	-0.34195100
C	3.90437600	0.73333800	1.01887400
C	3.29646400	2.00372600	1.34371200
C	2.52196300	2.08962600	2.53326300
C	1.35065800	2.93734200	2.59463600
C	0.95308400	3.75797100	1.48641400

C	1.78564500	3.71674900	0.31308000
C	1.22501600	3.82373600	-1.02945300
C	2.04352700	2.99435900	-1.89620900
C	3.09871100	2.41271900	-1.10901600
C	2.93779200	2.85487100	0.25188500
C	-3.14654200	-0.47888000	2.63438900
C	-2.08127800	-1.04101500	3.43302200
C	-1.48905100	-2.28740600	3.06279600
C	-0.09561900	-2.47107600	3.32158200
C	0.72958500	-3.25175500	2.43681100
C	0.18539300	-3.86976700	1.27762300
C	1.02217700	-3.97139400	0.12431600
C	0.46333900	-3.87931400	-1.20031700
C	-0.94559900	-3.71846000	-1.41659000
C	-1.34390200	-2.93273200	-2.54117900
C	-2.53174300	-2.10012600	-2.47255400
C	-3.42004000	-2.09476000	-1.32915700
C	-3.94594700	-0.78057500	-0.99387300
C	-4.10076600	-0.33742200	0.38686400
C	-3.70081500	-1.16128100	1.49984400
C	-3.22247200	-2.50768100	1.18887300
C	-2.07228100	-2.98958300	1.93994100
C	-1.23708900	-3.75766100	1.05438400
C	-1.83447600	-3.74681800	-0.26495700
C	-3.10009400	-2.99927900	-0.20598900
Tm	-0.34199500	1.96305200	-0.05736100
Tm	-1.55022800	-1.26083000	-0.04227200
Tm	1.86880700	-0.69464700	-0.06840000

Lu₃@C₈₀ PBE/6-31G*~MWB60

C	-3.68724800	0.04071200	-1.61787100
C	-2.96787300	0.03046300	-2.83724400
C	-2.24434900	-1.15143400	-3.24501400
C	-1.04220100	-0.71429000	-3.90874300
C	0.16855800	-1.46620600	-3.81480600
C	1.40366300	-0.74302400	-3.81903800
C	2.52119700	-1.20022600	-3.03928200
C	3.25056700	-0.04325400	-2.55450600
C	4.04023000	-0.05082800	-1.34536700
C	4.04991800	1.19521800	-0.58240000
C	3.97922100	1.19536600	0.89240600
C	3.15471000	2.32680800	1.28227200
C	2.31286000	2.33037100	2.44832500

C	1.12843100	3.13503700	2.41774200
C	-0.06699700	2.69743500	3.08589500
C	-1.19936900	3.17554500	2.33564400
C	-2.41670400	2.41249900	2.27730500
C	-3.18358600	2.49858400	1.04514400
C	-3.79436200	1.27767100	0.56308100
C	-3.73158500	1.27348900	-0.87259200
C	-3.76003300	-1.18848100	-0.86951200
C	-3.82221200	-1.18712500	0.56594000
C	-3.81059000	0.04596300	1.31391100
C	-3.19928400	0.04011600	2.59230700
C	-2.47858300	1.20573900	3.05237200
C	-1.34384200	0.74010000	3.81020000
C	-0.10915100	1.45981600	3.80967700
C	1.10446400	0.71058300	3.91505900
C	2.29362200	1.14014900	3.23012500
C	3.03011800	-0.03355000	2.80593000
C	3.89375600	-0.04517000	1.65246300
C	3.94376200	-1.28805800	0.89481700
C	4.01394600	-1.29321800	-0.57878200
C	3.19664600	-2.40839800	-1.03408000
C	2.45032400	-2.39465700	-2.26383300
C	1.25090500	-3.17326200	-2.33340300
C	0.12379600	-2.70589000	-3.09557300
C	-1.07480300	-3.14879000	-2.43351700
C	-2.26976300	-2.35435100	-2.46610400
C	-3.13188300	-2.41753900	-1.29980500
C	-2.82268300	-3.23572000	-0.11058800
C	-3.23875100	-2.41976000	1.05074700
C	-2.47180100	-2.34996800	2.28295000
C	-2.50640500	-1.14080000	3.05580800
C	-1.36090900	-0.70034900	3.81224600
C	-0.14343800	-1.44929400	3.81330500
C	1.08742300	-0.72888800	3.91617500
C	2.26611900	-1.18834100	3.23222400
C	2.25749000	-2.38135700	2.45409700
C	3.09837100	-2.40171000	1.28848000
C	2.67943700	-3.11075300	0.10976200
C	1.44172900	-3.83899400	0.06106600
C	0.74872500	-3.89019000	-1.18899700
C	-0.70279500	-3.91209300	-1.24960300
C	-1.54257900	-3.96962200	-0.05948900
C	-0.80518400	-3.91394600	1.19788700
C	-1.27353800	-3.14235000	2.34342200

C	-0.13030700	-2.68950600	3.09250600
C	1.05444100	-3.15798300	2.42624300
C	0.64815300	-3.88313200	1.25047800
C	-2.21663300	1.19388700	-3.24775000
C	-1.02517800	0.72661400	-3.91049800
C	0.20298900	1.44973100	-3.81898900
C	1.42053800	0.69699900	-3.82113500
C	2.54849900	1.12941300	-3.04268100
C	2.50568200	2.32655800	-2.26984800
C	3.25338900	2.32531500	-1.04004100
C	2.75025500	3.04107100	0.10179000
C	1.53071100	3.80007000	0.05118800
C	0.73918800	3.86684700	1.24047100
C	-0.71272500	3.93206400	1.18788100
C	-1.44836200	4.00118600	-0.06964500
C	-2.74776900	3.30110400	-0.11891300
C	-3.07537400	2.48681200	-1.30615600
C	-2.21381600	2.39910700	-2.47202100
C	-1.00024500	3.16440800	-2.44159500
C	0.18747500	2.69193000	-3.10297100
C	1.32521400	3.13353500	-2.34123200
C	0.84006600	3.86549200	-1.19897500
C	-0.61034600	3.92082300	-1.25934800
Lu	-1.13854300	-1.64973300	-0.00360500
Lu	-1.11165400	1.66880700	-0.00401000
Lu	2.03780200	-0.00826700	0.01797600

La₃@C₈₀⁺ PBE/6-31G*~MWB46

C	1.56155000	-3.51454000	1.36654400
C	1.79983800	-2.71301400	2.51685200
C	0.70554400	-2.27800900	3.34250500
C	1.02300000	-0.96718400	3.84103700
C	0.00265400	0.01187100	4.05832000
C	0.33971000	1.38417100	3.83522000
C	-0.63194900	2.31235300	3.32020300
C	0.04989100	3.29775200	2.49262800
C	-0.59549100	3.99725600	1.39745800
C	0.26724200	4.28661800	0.23465500
C	-0.24617000	4.12941900	-1.15371900
C	0.84455600	3.54916900	-1.93781100
C	0.64724000	2.63620300	-3.03800200
C	1.68387300	1.68922400	-3.34316500
C	1.35531400	0.38104800	-3.84097900
C	2.32356900	-0.55057200	-3.32546300
C	1.96372500	-1.89385800	-3.02546300
C	2.65468000	-2.51590800	-1.92163500
C	1.92844200	-3.43452800	-1.08068400
C	2.45527700	-3.31399600	0.25199400
C	0.20441300	-3.92702400	1.10033600
C	-0.30332100	-4.11476800	-0.23201600
C	0.56106200	-3.81245800	-1.34684200
C	-0.06751400	-3.26784900	-2.50051500
C	0.62592500	-2.31940900	-3.33005400
C	-0.34222800	-1.38358500	-3.83433000
C	-0.00313400	-0.01192700	-4.05764500
C	-1.02199700	0.96880600	-3.84059300
C	-0.69700000	2.27472100	-3.33124600
C	-1.80097000	2.74696400	-2.50757300
C	-1.63106700	3.68805800	-1.41691500
C	-2.51725700	3.47871100	-0.25463000
C	-2.00205300	3.62874600	1.13406200
C	-2.61418500	2.55835600	1.92191700
C	-1.96078600	1.89762300	3.02630600
C	-2.33056700	0.54496400	3.33669100
C	-1.35508500	-0.38284900	3.84134400
C	-1.67448400	-1.69036100	3.33179500
C	-0.65200400	-2.63488000	3.03821400
C	-0.90141700	-3.53472000	1.93760900
C	-2.13683700	-3.54207500	1.15401200
C	-1.75539000	-3.92043100	-0.23438700
C	-2.38522000	-3.26328800	-1.39725900

C	-1.48823200	-2.94313900	-2.49180100
C	-1.63390700	-1.75376400	-3.31939000
C	-2.61781400	-0.76907300	-3.02562800
C	-2.31721500	0.60079000	-3.33677000
C	-2.79275200	1.67969300	-2.51291500
C	-3.58031600	1.41361000	-1.35901800
C	-3.41146200	2.31858500	-0.24816300
C	-3.50537600	1.79215400	1.08685100
C	-3.82693700	0.41194700	1.35914700
C	-3.25352700	-0.18947500	2.51338500
C	-2.87131000	-1.59540100	2.50797500
C	-3.15802300	-2.50757200	1.41725900
C	-3.84564500	-1.91064700	0.25509100
C	-3.45924200	-2.28294600	-1.13360600
C	-3.50403300	-1.05068000	-1.92174400
C	-3.93735200	0.04195600	-1.08672800
C	-4.09854500	-0.46778400	0.24835800
C	2.82680800	-1.67945900	2.50449500
C	2.31323000	-0.59218300	3.32605900
C	2.61922200	0.76466200	3.02679500
C	1.63163900	1.76281700	3.33057300
C	1.45846600	2.92485300	2.50115400
C	2.26801700	3.11502700	1.34712600
C	1.64332900	3.78419900	0.23216600
C	2.00627200	3.38300900	-1.10047000
C	3.01592600	2.38648800	-1.36638300
C	2.85472300	1.56611900	-2.51690300
C	3.28384900	0.17363800	-2.50434300
C	4.01288100	-0.43876800	-1.40954600
C	3.70214000	-1.85784200	-1.13978100
C	3.57859900	-2.37380300	0.25134800
C	3.75714300	-1.47600900	1.41008400
C	4.14141800	-0.07491200	1.14026800
C	3.51931900	0.99431100	1.92195500
C	3.30271700	2.14495300	1.08093200
C	3.71408200	1.79379300	-0.25175600
C	4.27225400	0.43936600	-0.25084700
La	1.92215500	-0.47322700	-0.00023200
La	-1.37085800	-1.42715000	-0.00013400
La	-0.55042600	1.90002800	-0.00110800

Nd₃@C₈₀⁺ PBE/6-31G*~MWB49

C	-2.29444100	3.05726800	1.36760500
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C	-2.35557600	2.24054900	2.52558400
C	-1.19346900	2.06347500	3.35466700
C	-1.21177800	0.71473400	3.85218600
C	0.00092100	-0.01382500	4.07088100
C	-0.02314400	-1.42711500	3.84626100
C	1.12972300	-2.11381800	3.32626900
C	0.68592000	-3.22144700	2.49433900
C	1.46711800	-3.75896200	1.39790000
C	0.69662400	-4.22713100	0.23306200
C	1.16042400	-3.96086000	-1.15563800
C	-0.03067300	-3.63685700	-1.94009400
C	-0.04529600	-2.71027800	-3.04493600
C	-1.26572200	-2.02059800	-3.35278700
C	-1.23812700	-0.67306000	-3.85308100
C	-2.38811200	0.01956000	-3.33271200
C	-2.33619800	1.40866200	-3.03043300
C	-3.14301300	1.85425500	-1.92096600
C	-2.63380600	2.90101700	-1.07609300
C	-3.12361200	2.67114200	0.25464300
C	-1.06450200	3.76465500	1.10073500
C	-0.61383000	4.06456300	-0.22994800
C	-1.38411900	3.57207400	-1.34361900
C	-0.66192400	3.19740600	-2.50575500
C	-1.12946600	2.12208500	-3.33879300
C	0.02305400	1.42650300	-3.84526100
C	-0.00079000	0.01374300	-4.07100600
C	1.21099000	-0.71518800	-3.85195800
C	1.18460300	-2.05921400	-3.33954200
C	2.36224700	-2.27372100	-2.51333000
C	2.40755100	-3.22560400	-1.42138400
C	3.21846000	-2.82910100	-0.25717400
C	2.75205200	-3.09021200	1.13206000
C	3.10858700	-1.91151400	1.92164600
C	2.33263500	-1.41393600	3.03121900
C	2.39495700	-0.01511500	3.34699700
C	1.23747100	0.67232800	3.85281200
C	1.25712400	2.01680000	3.34001200
C	0.05012700	2.70992300	3.04538000
C	0.09581100	3.63632900	1.94108000
C	1.29660900	3.91934900	1.15574800
C	0.84160500	4.20179800	-0.23280900
C	1.59485100	3.70708900	-1.39853400
C	0.79459600	3.19559600	-2.49432500
C	1.19939700	2.07348100	-3.32672000

C	2.37837000	1.33282400	-3.03355500
C	2.39195700	-0.06799000	-3.34835200
C	3.09223400	-1.01367000	-2.52157900
C	3.78132700	-0.58118400	-1.35950800
C	3.82637900	-1.49982900	-0.25027700
C	3.79604000	-0.96615200	1.08328400
C	3.80056200	0.45094600	1.35786800
C	3.12734300	0.90648800	2.52065000
C	2.44039000	2.19067900	2.51246300
C	2.51742700	3.14045200	1.42037500
C	3.31284400	2.71603100	0.25544500
C	2.85536200	2.99333900	-1.13362700
C	3.17112900	1.80330000	-1.92374200
C	3.82587600	0.83497700	-1.08536800
C	3.87555600	1.36727200	0.24825200
C	-3.12529200	1.00424200	2.50972700
C	-2.38476100	0.06221400	3.33413600
C	-2.38080000	-1.32816200	3.03274900
C	-1.19869700	-2.08292600	3.34050600
C	-0.76979000	-3.17303500	2.50659400
C	-1.50585100	-3.52284700	1.34547700
C	-0.75304300	-4.04030600	0.23136100
C	-1.19377800	-3.72484100	-1.09885000
C	-2.39930200	-2.97725200	-1.36572500
C	-2.43294500	-2.15870700	-2.52381500
C	-3.15958600	-0.89639800	-2.50705500
C	-4.00518800	-0.46520200	-1.41108500
C	-4.01776600	0.98169200	-1.13799600
C	-4.01073300	1.50936600	0.25366400
C	-3.98482100	0.60200400	1.41398400
C	-4.04843600	-0.84350800	1.14142300
C	-3.20357000	-1.74546900	1.92389900
C	-2.73203000	-2.80943800	1.07871700
C	-3.21414200	-2.56240800	-0.25195900
C	-4.06156400	-1.37118800	-0.25043600
Nd	1.03387400	1.72067200	-0.00081900
Nd	-2.00973700	0.03238300	-0.00071000
Nd	0.97820600	-1.75226900	-0.00065400

Gd₃@C₈₀⁺ PBE/6-31G*~MWB53

C	-0.14491400	-2.88286600	2.88993100
C	1.07294900	-2.24727300	3.26156900
C	1.08117800	-0.93681600	3.85382800

C	2.27402500	-0.26096200	3.42164600
C	2.26530300	1.15262400	3.18698000
C	3.08266600	1.67908600	2.12307900
C	2.78831100	2.90374900	1.39059500
C	3.31562800	2.73786400	0.01175100
C	2.56748900	3.23422900	-1.16000700
C	2.51623900	2.33989000	-2.30422900
C	1.35971100	2.21206400	-3.17953500
C	1.35728400	0.89927200	-3.76719200
C	0.12855000	0.22599200	-4.06938300
C	0.09862700	-1.19783400	-3.92552300
C	-1.09269500	-1.88343400	-3.50236100
C	-0.68969700	-3.01800400	-2.71458000
C	-1.45435100	-3.43358900	-1.59616200
C	-0.74030400	-4.01347100	-0.48669900
C	-1.22210300	-3.77551700	0.84584400
C	-0.09061300	-3.74171800	1.73037300
C	-1.37462800	-2.21343700	3.19850600
C	-2.51083100	-2.30008300	2.32129700
C	-2.43663000	-3.04442200	1.11784800
C	-3.20447100	-2.56668300	0.00296800
C	-2.68688400	-2.73716400	-1.32487900
C	-3.12195100	-1.62304600	-2.11988200
C	-2.27959500	-1.14647800	-3.18362900
C	-2.27645000	0.26007300	-3.40418500
C	-1.09117300	0.94166200	-3.85057100
C	-1.09135600	2.26129500	-3.27711700
C	0.13869500	2.88538800	-2.88622500
C	0.14582300	3.73884700	-1.72717000
C	1.32074500	3.96012600	-0.88453600
C	0.81221500	4.12873300	0.49816100
C	1.51270800	3.56912700	1.64838000
C	0.69331100	3.03096900	2.70575200
C	1.07647000	1.87268300	3.48827300
C	-0.11375500	1.19964600	3.93564400
C	-0.14027600	-0.22317300	4.07679000
C	-1.36719700	-0.89749000	3.78078800
C	-2.49748600	-0.17458800	3.26242200
C	-3.23323400	-1.03743100	2.35489800
C	-4.03255100	-0.54023000	1.25565800
C	-4.02728900	-1.36394900	0.04641600
C	-3.96936200	-0.76070200	-1.30524400
C	-3.91878600	0.68738700	-1.49737100
C	-3.03686000	1.15063100	-2.54657100

C	-2.27719900	2.38850800	-2.47185600
C	-2.25700700	3.12956600	-1.26475600
C	-1.03896800	3.81654100	-0.91727900
C	-0.63552700	4.02242500	0.44452200
C	-1.43441800	3.48241200	1.50883200
C	-0.75714900	3.04430900	2.67311400
C	-1.25021900	1.92450900	3.43148200
C	-2.44119800	1.23138700	3.04326600
C	-3.20850000	1.73933500	1.92967100
C	-4.05803900	0.91729700	1.06830400
C	-4.00320200	1.52267600	-0.29061800
C	-3.11666300	2.67961800	-0.19761500
C	-2.67227600	2.82859800	1.16097300
C	2.27220400	-2.41065900	2.45712500
C	3.00165100	-1.15496600	2.56191900
C	3.72420700	-0.65853000	1.44843100
C	3.77605100	0.77119400	1.25476800
C	3.88194000	1.38630200	-0.04052500
C	3.83261700	0.53414200	-1.20314700
C	3.20191400	1.05326800	-2.36242300
C	2.49853100	0.18309600	-3.26634300
C	2.42492600	-1.23054800	-3.03229600
C	1.23385100	-1.91256200	-3.40670500
C	0.76264500	-3.06069500	-2.65292800
C	1.49957600	-3.65054000	-1.55814300
C	0.70668300	-4.20225900	-0.45061200
C	1.12519700	-4.02599300	0.96728300
C	2.35339300	-3.29582400	1.31460700
C	3.17889800	-2.81750600	0.20143900
C	3.80463800	-1.50382200	0.29042900
C	3.81817000	-0.89570500	-1.00966200
C	3.15291400	-1.78280600	-1.92273700
C	2.75683600	-2.99071100	-1.20887800
Gd	-2.01751000	0.11996500	-0.01125300
Gd	0.91747000	-1.79876600	-0.00940600
Gd	1.13576200	1.66820400	0.00228600

Tb₃@C₈₀⁺ PBE/6-31G*~MWB54

C	2.17037200	-3.15387200	-1.33525400
C	2.27325100	-2.35540700	-2.50107700
C	3.08827100	-1.15046800	-2.48401400
C	2.40159000	-0.18619200	-3.32582000
C	2.45521600	1.20570900	-3.03240500

C	1.31355500	2.00802300	-3.35676200
C	0.92501600	3.11775200	-2.52781700
C	-0.52569500	3.21998800	-2.52281200
C	-1.28466900	3.78611400	-1.42969700
C	-2.58943000	3.17602300	-1.16735500
C	-3.07530200	2.94700400	0.21635300
C	-3.74922200	1.65406100	0.21302700
C	-3.75440200	0.74974200	1.33097400
C	-3.85488100	-0.66347100	1.06197500
C	-3.24544700	-1.64800100	1.91137500
C	-2.96965600	-2.84890700	1.12820000
C	-1.74753000	-3.60694900	1.40823100
C	-1.01510400	-4.13251800	0.25268900
C	0.44130000	-4.07110600	0.26037900
C	0.91084500	-3.80256100	-1.06950400
C	2.99872600	-2.79604800	-0.21513800
C	2.49394300	-2.99561600	1.11418300
C	1.21788800	-3.61218200	1.37978700
C	0.51079000	-3.20322500	2.53719200
C	-0.94172500	-3.13303400	2.51168000
C	-1.30644500	-1.99675400	3.33881300
C	-2.45117900	-1.20941000	3.03069600
C	-2.41139000	0.18884300	3.34066400
C	-3.06253900	1.15622400	2.49839900
C	-2.27489800	2.37940400	2.48508200
C	-2.26866600	3.31741800	1.38394200
C	-0.99604600	3.99464500	1.12121600
C	-0.51315200	4.22746300	-0.26355600
C	0.92526900	3.98986600	-0.25065500
C	1.65829600	3.44038200	-1.35958900
C	2.84749900	2.67647400	-1.07618300
C	3.27534200	1.59017600	-1.91205300
C	4.06570900	0.65697600	-1.11433600
C	3.94747700	-0.77881300	-1.38084400
C	3.92404700	-1.66872900	-0.21464700
C	3.94060700	-1.13463000	1.17077100
C	3.03417600	-1.96607500	1.95660700
C	2.24984100	-1.48579400	3.06553200
C	1.01618800	-2.14688700	3.37263200
C	-0.10927200	-1.39936100	3.86638000
C	-0.02840000	0.01313900	4.08355700
C	-1.20836900	0.78955800	3.85203500
C	-1.11971100	2.12574000	3.32773400
C	0.13909400	2.72371400	3.03749700

C	0.17164900	3.63213500	1.91951500
C	1.34021900	3.66842700	1.08572900
C	2.50988400	2.87459200	1.36896300
C	3.30418000	2.41897200	0.26016000
C	4.08641300	1.18924000	0.27147400
C	3.98451300	0.30474000	1.43556000
C	3.16479300	0.77766800	2.52878700
C	2.35734800	-0.09734800	3.35954000
C	1.23741900	0.64677600	3.87019400
C	1.32611200	1.98987100	3.36262300
C	2.50025700	2.07097100	2.53532000
C	1.12899000	-2.13526100	-3.34434400
C	1.20817400	-0.79187400	-3.85236500
C	0.02969300	-0.01280300	-4.08348400
C	0.11410900	1.39962800	-3.86784100
C	-1.01119900	2.13543100	-3.35704600
C	-2.24564500	1.48948500	-3.06598400
C	-2.99665000	2.01796600	-1.95632600
C	-3.73192600	1.11432900	-1.11721600
C	-3.79668600	-0.30031000	-1.38634300
C	-3.91634100	-1.19866400	-0.26913500
C	-3.40359400	-2.56390500	-0.26331900
C	-2.62584000	-3.02408000	-1.41906000
C	-1.44554000	-3.84373700	-1.13792200
C	-0.23256700	-3.62671600	-1.91987300
C	-0.14124800	-2.72355500	-3.03825600
C	-1.31587000	-1.98077700	-3.34636800
C	-1.23735600	-0.64365500	-3.87089500
C	-2.36749800	0.09605900	-3.37613300
C	-3.14100200	-0.78630800	-2.54409900
C	-2.50476100	-2.09402600	-2.52020500
Tb	2.02169800	-0.12931200	0.00167200
Tb	-1.12629400	-1.68196100	0.00058200
Tb	-0.90197700	1.81203900	-0.00038300

Dy₃@C₈₀⁺ PBE/6-31G*~MWB55

C	-3.25538500	0.52074800	2.36253300
C	-2.30384600	0.46129300	3.40770500
C	-1.36332700	1.53985800	3.59561200
C	-0.11427000	0.95841700	4.01913200
C	1.13312900	1.53199800	3.63962400
C	2.23565200	0.63948800	3.41698100
C	3.23384700	0.91572600	2.42063700

C	3.71906000	-0.34850500	1.86750500
C	4.26969300	-0.48636100	0.52547300
C	3.89001000	-1.73177700	-0.15848700
C	3.46852800	-1.74831200	-1.57507300
C	2.45234400	-2.76425600	-1.73376100
C	1.39179700	-2.67019100	-2.69439800
C	0.13245400	-3.27995400	-2.35542200
C	-1.11345100	-2.72972500	-2.80221500
C	-2.15178000	-3.10122100	-1.85971500
C	-3.20309800	-2.13678200	-1.58345100
C	-3.66756600	-2.05105300	-0.21085300
C	-3.99630800	-0.74389300	0.32600700
C	-3.61453800	-0.70677900	1.70771200
C	-3.32104800	1.72778500	1.57912800
C	-3.70039200	1.70759600	0.19521400
C	-4.00705500	0.45930300	-0.46240300
C	-3.65851300	0.34105000	-1.82859500
C	-3.22781000	-0.92954500	-2.37155000
C	-2.23371100	-0.63782300	-3.37867100
C	-1.13166900	-1.51896200	-3.58455300
C	0.12153100	-0.95732600	-3.97728800
C	1.36907500	-1.53066900	-3.53728900
C	2.32575600	-0.46292200	-3.34533300
C	3.36733400	-0.53479200	-2.35739600
C	3.78270500	0.69762300	-1.71076900
C	4.22367100	0.73957500	-0.29588200
C	3.64119600	1.96902700	0.25799800
C	3.14424300	2.08381400	1.60682900
C	2.09065500	3.02296700	1.87860500
C	1.09985300	2.74950500	2.88661500
C	-0.14301300	3.33376700	2.46165400
C	-1.39016000	2.70889600	2.77306200
C	-2.45215200	2.85570400	1.79736400
C	-2.31582800	3.61074600	0.54072200
C	-3.09494400	2.84738900	-0.46973900
C	-2.61959300	2.64455400	-1.83268100
C	-2.94588000	1.40763400	-2.49588500
C	-2.06187000	0.78849700	-3.45509800
C	-0.78325500	1.35378300	-3.73962400
C	0.29348600	0.46944800	-4.05398700
C	1.64515200	0.77415000	-3.65937700
C	1.95066800	1.96134900	-2.94624400
C	3.01587300	1.89610100	-1.98261000
C	2.94886000	2.68066000	-0.78458500

C	1.84611300	3.57342900	-0.52236800
C	1.45755500	3.77435300	0.82937600
C	0.05811600	3.99549600	1.17625300
C	-0.99834900	4.18647700	0.19118000
C	-0.56181000	4.00612800	-1.19652200
C	-1.36646400	3.26817500	-2.18447000
C	-0.46366400	2.59769100	-3.09473300
C	0.88285800	2.89079200	-2.69886600
C	0.83315200	3.71679400	-1.52392900
C	-1.64376100	-0.78127300	3.72512200
C	-0.28709400	-0.47145600	4.09504700
C	0.78255900	-1.36234800	3.79072300
C	2.06179200	-0.78470600	3.48893800
C	2.95291700	-1.39385400	2.54132300
C	2.57643900	-2.58953100	1.85857600
C	3.05633700	-2.73220000	0.51183700
C	2.21536900	-3.37932000	-0.45902800
C	0.93914600	-3.95270300	-0.11456600
C	-0.10010200	-3.96149900	-1.11015100
C	-1.52964700	-3.91550600	-0.78828500
C	-1.95733900	-3.79283400	0.61784900
C	-3.06109400	-2.85271900	0.87829300
C	-3.01085300	-1.96722600	2.04340900
C	-1.94937100	-1.98547400	3.01951900
C	-0.89647600	-2.92349900	2.79407300
C	0.45303900	-2.61307200	3.17458600
C	1.34022100	-3.22419500	2.22024200
C	0.53494300	-3.90907200	1.24604900
C	-0.87466800	-3.74705900	1.59035300
Dy	-0.87311200	1.82205600	-0.04220300
Dy	-1.17241100	-1.65073800	-0.04368500
Dy	2.01225300	-0.17108100	-0.10711200

Ho₃@C₈₀⁺ PBE/6-31G*~MWB56

C	2.46595500	2.91359500	1.36669200
C	1.66619800	2.78911800	2.52944200
C	1.75572400	1.62061200	3.36416400
C	0.43856900	1.33737600	3.87023200
C	-0.00281200	-0.00647700	4.08818700
C	-1.38683500	-0.29572400	3.86626300
C	-1.79599900	-1.57041600	3.34188700
C	-2.96630200	-1.38024700	2.50514800
C	-3.30218300	-2.24867000	1.40089000

C	-3.91596800	-1.60643500	0.24087100
C	-3.56378200	-1.99711000	-1.14264100
C	-3.53691600	-0.77364000	-1.93392500
C	-2.65668000	-0.55844500	-3.05079100
C	-2.26342000	0.78252700	-3.36427300
C	-0.94327900	1.05764600	-3.86619200
C	-0.52295400	2.32871600	-3.34187900
C	0.84457900	2.58885000	-3.04346400
C	1.09865400	3.45597400	-1.92463300
C	2.23524300	3.20524500	-1.08359700
C	1.90436500	3.61926500	0.25027800
C	3.42373800	1.87174600	1.09188600
C	3.81291000	1.50328300	-0.24099600
C	3.16698300	2.14207000	-1.35818000
C	2.95933700	1.36365100	-2.52343200
C	1.80949700	1.57865900	-3.36055700
C	1.38674700	0.29951700	-3.86501900
C	0.00310100	0.00648800	-4.08721600
C	-0.43452200	-1.33936500	-3.86994100
C	-1.74710300	-1.61209200	-3.34942300
C	-1.68494400	-2.79883600	-2.51577600
C	-2.58922800	-3.04983100	-1.41622900
C	-2.03036800	-3.75012700	-0.25469200
C	-2.38051000	-3.35346600	1.13320800
C	-1.15644500	-3.44208100	1.92267400
C	-0.84712900	-2.58853500	3.04316500
C	0.52725500	-2.34066200	3.35744700
C	0.94037300	-1.06000500	3.86733000
C	2.25018200	-0.77651000	3.34611500
C	2.65804300	0.55470200	3.04997900
C	3.55453600	0.71515000	1.93198800
C	4.09205000	-0.38788200	1.14198600
C	4.26478100	0.11607700	-0.24410400
C	3.94029700	-0.71617700	-1.40826300
C	3.27303900	-0.05621900	-2.50809700
C	2.27772000	-0.70178300	-3.34439600
C	1.81943100	-2.01760100	-3.05065200
C	0.46214900	-2.34635800	-3.36819000
C	-0.29854800	-3.23693200	-2.53310600
C	0.27217000	-3.80929600	-1.36945700
C	-0.60348700	-4.05234800	-0.25280700
C	-0.09001300	-3.90441200	1.08070600
C	1.29049000	-3.59636000	1.35582300
C	1.58320500	-2.84517500	2.52079800

C	2.67210300	-1.88371000	2.50802000
C	3.59410800	-1.73860700	1.40592100
C	3.34760500	-2.58914100	0.24400600
C	3.51417100	-2.08684900	-1.13827200
C	2.44347100	-2.67454000	-1.93357600
C	1.65862900	-3.53571200	-1.09461500
C	2.18231100	-3.46002700	0.23954200
C	0.28895800	3.25137700	2.51438500
C	-0.46067900	2.33072400	3.34863200
C	-1.81701800	2.01931100	3.04942500
C	-2.28944000	0.70403200	3.35982400
C	-3.25483000	0.04372000	2.52216800
C	-3.75941000	0.67612100	1.35905100
C	-4.08706200	-0.16158500	0.24057900
C	-3.89054800	0.33398900	-1.09192900
C	-3.43558000	1.67284700	-1.36329500
C	-2.65459600	1.88436300	-2.52655100
C	-1.58178800	2.86599200	-2.50687800
C	-1.34703000	3.77236500	-1.40542700
C	0.05217300	4.08845700	-1.13115600
C	0.56718900	4.19277700	0.25253600
C	-0.29534300	3.97833400	1.41174300
C	-1.71319700	3.73436400	1.14382300
C	-2.40189000	2.71688500	1.93087000
C	-3.33591800	2.02683800	1.08752700
C	-3.20877700	2.55016600	-0.24447800
C	-2.23294300	3.63438000	-0.24400200
Ho	1.95134400	-0.55966700	0.00271400
Ho	-0.48959800	1.96869600	0.00180300
Ho	-1.46287100	-1.40705100	0.00147300

Er₃@C₈₀⁺ PBE/6-31G*~MWB57

C	2.80963400	-2.61352300	1.31423300
C	2.73593000	-1.81259000	2.48117100
C	1.57585800	-1.85067500	3.33170600
C	1.36312700	-0.52545500	3.85206300
C	0.04519700	-0.02040700	4.08972400
C	-0.17824800	1.37686500	3.87815300
C	-1.43775900	1.84913200	3.37078900
C	-1.19975700	3.01088300	2.53685500
C	-2.05746700	3.37838900	1.43802900
C	-1.39892900	3.95668200	0.27858700
C	-1.82665200	3.64003600	-1.09639200

C	-0.62054800	3.58071400	-1.90917800
C	-0.46582600	2.70014900	-3.03200200
C	0.84958300	2.24444200	-3.36618300
C	1.05384300	0.91430000	-3.87520900
C	2.30996900	0.43058900	-3.37013200
C	2.50647600	-0.95054400	-3.08291000
C	3.36831500	-1.25460400	-1.97676200
C	3.08275800	-2.38637600	-1.14028900
C	3.52186900	-2.08178300	0.19159100
C	1.71926800	-3.51912400	1.04798300
C	1.31798300	-3.88929500	-0.28292300
C	1.97338000	-3.26228800	-1.40554100
C	1.18903700	-3.00466300	-2.55810700
C	1.44769500	-1.86311500	-3.39379300
C	0.18330000	-1.37621800	-3.87737900
C	-0.04489100	0.02157200	-4.08877000
C	-1.36496500	0.52321700	-3.85026700
C	-1.56765600	1.84422800	-3.32017700
C	-2.74567800	1.83336300	-2.47215300
C	-2.94366800	2.74354100	-1.36595100
C	-3.66978500	2.21950500	-0.19865500
C	-3.22626900	2.53433000	1.18561800
C	-3.35836800	1.31089300	1.96955100
C	-2.50596400	0.95457000	3.08004900
C	-2.32067200	-0.43153100	3.38254100
C	-1.05598200	-0.90910300	3.87753100
C	-0.84113400	-2.22683200	3.34381300
C	0.46409300	-2.69859600	3.02783700
C	0.56807000	-3.59807100	1.90228200
C	-0.56773400	-4.08387300	1.12457900
C	-0.08930900	-4.28099200	-0.27012500
C	-0.91909400	-3.89088300	-1.41997500
C	-0.24416400	-3.24887000	-2.52486800
C	-0.85313600	-2.22092400	-3.34832500
C	-2.14125400	-1.69994600	-3.03525500
C	-2.40872900	-0.32730900	-3.34338900
C	-3.25099200	0.46920500	-2.49210400
C	-3.84063800	-0.07892200	-1.32493900
C	-4.03456300	0.80441200	-0.20032900
C	-3.88509300	0.27381600	1.12863900
C	-3.64039700	-1.12280600	1.39323100
C	-2.88515900	-1.45659000	2.54517100
C	-1.97633900	-2.58767900	2.51667400
C	-1.88156800	-3.49923000	1.40336900

C	-2.72468100	-3.19492700	0.25769100
C	-2.25145200	-3.37980500	-1.12627500
C	-2.81271200	-2.29288500	-1.91401600
C	-3.63282700	-1.47755200	-1.06194300
C	-3.55940500	-2.00750800	0.27013300
C	3.26086800	-0.45948300	2.46917800
C	2.39067600	0.32839000	3.32107300
C	2.14387600	1.70019200	3.03242500
C	0.85717900	2.23242200	3.36013100
C	0.23386200	3.23273500	2.53452200
C	0.87638400	3.71701300	1.36811000
C	0.04642900	4.08642700	0.26095400
C	0.51341800	3.88409900	-1.08103300
C	1.82314200	3.36486100	-1.37042100
C	1.97803300	2.57735300	-2.53894300
C	2.90529500	1.45762400	-2.53592700
C	3.80993300	1.17417000	-1.44553900
C	4.03804100	-0.23945000	-1.17930300
C	4.13347900	-0.76520500	0.19452100
C	3.99284200	0.09729900	1.35776300
C	3.83874700	1.53249900	1.10562400
C	2.85854000	2.25981000	1.90794600
C	2.20222800	3.22990900	1.07741900
C	2.70681500	3.09018100	-0.26252100
C	3.74998700	2.06767000	-0.27965500
Er	-0.54361800	-1.95643300	0.00513400
Er	1.96881700	0.50625000	0.00537000
Er	-1.42658400	1.44507900	0.00788400

Tm₃@C₈₀⁺ PBE/6-31G*~MWB58

C	3.67620500	1.04523600	1.36219600
C	2.93168600	1.41654700	2.51047000
C	2.34294000	0.42071700	3.36605600
C	1.09511200	0.94003400	3.86206500
C	-0.02877000	0.08459700	4.09321800
C	-1.33290200	0.62166500	3.85314400
C	-2.38440500	-0.21262900	3.33843000
C	-3.23375200	0.58534900	2.47692300
C	-3.97078900	0.02941800	1.37113600
C	-4.09100800	0.87529000	0.19895000
C	-4.02155900	0.32711000	-1.16340500
C	-3.34164600	1.31635600	-1.98355000
C	-2.49535600	0.97042100	-3.08794000

C	-1.41416900	1.84886900	-3.41840300
C	-0.16436600	1.31940500	-3.89568400
C	0.89656200	2.14401500	-3.38403400
C	2.17184600	1.59373100	-3.06818000
C	2.86401000	2.18175500	-1.95980800
C	3.67211900	1.36218000	-1.09934000
C	3.61408900	1.91171100	0.22597700
C	3.88441000	-0.36119000	1.11843700
C	4.02184500	-0.91845600	-0.20249900
C	3.84096200	-0.04518800	-1.34029700
C	3.22574400	-0.59472300	-2.49490600
C	2.40039200	0.20966800	-3.35513000
C	1.33191600	-0.62024900	-3.84278700
C	0.02479500	-0.08702400	-4.08522200
C	-1.09722400	-0.94644900	-3.85471200
C	-2.33746300	-0.42084500	-3.35286500
C	-2.95510400	-1.41869400	-2.49976000
C	-3.84777800	-1.09575900	-1.41033400
C	-3.81319800	-1.97624100	-0.23121600
C	-3.87084500	-1.41329100	1.14364400
C	-2.90873600	-2.15340000	1.95403400
C	-2.17593000	-1.59505000	3.06840000
C	-0.90349800	-2.15587700	3.39801500
C	0.15603700	-1.32085300	3.90070400
C	1.39968400	-1.83399100	3.39503700
C	2.49018600	-0.97392000	3.08536900
C	3.32879800	-1.36903200	1.97627400
C	3.16128600	-2.59920000	1.21152700
C	3.61737200	-2.32520100	-0.17662500
C	2.86453500	-2.84266800	-1.33272700
C	2.68442400	-1.94449800	-2.45185500
C	1.50236100	-1.93804700	-3.29421200
C	0.37814400	-2.75882600	-2.98921800
C	-0.92603300	-2.27452000	-3.32818800
C	-2.05828100	-2.56302500	-2.48928700
C	-1.92196300	-3.33948300	-1.31034100
C	-2.79649900	-3.02761600	-0.20273300
C	-2.28625600	-3.15701800	1.13733800
C	-0.97220400	-3.67388700	1.43023200
C	-0.31133200	-3.18531800	2.58509700
C	1.12573100	-3.00009900	2.58012700
C	1.96268400	-3.39479500	1.47797700
C	1.28403100	-3.96942600	0.33399500
C	1.71635300	-3.68974100	-1.04323200

C	0.51149300	-3.62605800	-1.85615300
C	-0.62698900	-3.89162400	-1.01993200
C	-0.16030700	-4.07941800	0.32466300
C	2.05224600	2.56925900	2.46906100
C	0.91257400	2.25389300	3.30828700
C	-0.38089800	2.75825800	2.99179500
C	-1.51209500	1.94398700	3.31088000
C	-2.67623000	1.92386400	2.46485700
C	-2.73480800	2.70902900	1.28584900
C	-3.46171800	2.18071200	0.17308400
C	-3.02627400	2.45582400	-1.16697600
C	-1.89442700	3.29484400	-1.44872600
C	-1.12205900	2.99527400	-2.60012400
C	0.31704700	3.19869300	-2.57480800
C	1.01118200	3.83329100	-1.47915100
C	2.32332900	3.28304400	-1.18181600
C	2.79719800	3.10929000	0.19888500
C	1.97339800	3.46161600	1.34066800
C	0.67930300	4.08984800	1.06113200
C	-0.46590100	3.64429200	1.85135400
C	-1.62229700	3.58169900	1.00196900
C	-1.21775700	3.92318800	-0.33689100
C	0.20029700	4.27798900	-0.33477900
Tm	1.44603400	-1.42837800	0.00636700
Tm	0.52949500	1.96053000	-0.00032800
Tm	-1.96522500	-0.52333700	0.00357700

Lu₃@C₈₀⁺ PBE/6-31G*~MWB60

C	-3.70248800	0.19383100	-1.62220700
C	-2.98431300	0.15256000	-2.83924500
C	-2.31539500	-1.05814900	-3.25211400
C	-1.09570800	-0.67274000	-3.91701900
C	0.08123500	-1.47128600	-3.81963800
C	1.34720400	-0.80211000	-3.82547300
C	2.44691100	-1.30434600	-3.04804000
C	3.22758600	-0.17995300	-2.56251500
C	4.02055200	-0.21962900	-1.35660600
C	4.09214100	1.02465500	-0.59225500
C	4.02321900	1.02937100	0.88700400
C	3.23024100	2.18476000	1.27443300
C	2.38537000	2.22496900	2.43665600
C	1.23036200	3.07607900	2.40040400
C	0.02139800	2.69712200	3.07513800

C	-1.09264000	3.23076800	2.33363900
C	-2.33223200	2.51280300	2.27235300
C	-3.08794500	2.62527400	1.03846900
C	-3.74809100	1.43317700	0.55806700
C	-3.68643400	1.42453300	-0.87593000
C	-3.81867800	-1.02817900	-0.87083800
C	-3.87988700	-1.02332600	0.56317700
C	-3.82240200	0.20680600	1.30930700
C	-3.19959200	0.17596500	2.57845800
C	-2.44105800	1.31158400	3.04773700
C	-1.32736400	0.79971200	3.80758600
C	-0.06654100	1.46537700	3.80608600
C	1.11664400	0.66816200	3.91342700
C	2.32247500	1.04675700	3.22732200
C	3.01205300	-0.15614100	2.80131400
C	3.87760300	-0.20501600	1.64984900
C	3.88485100	-1.44994400	0.89197200
C	3.95314700	-1.45912000	-0.58622900
C	3.07386300	-2.52784100	-1.03882600
C	2.32126800	-2.48258600	-2.26269600
C	1.08651600	-3.21085800	-2.32791400
C	-0.01877800	-2.70492000	-3.09453300
C	-1.23538800	-3.10118400	-2.43796800
C	-2.38897300	-2.25468000	-2.47002400
C	-3.24195200	-2.27901800	-1.29831800
C	-2.97094600	-3.11231800	-0.11092000
C	-3.34893100	-2.27607800	1.04853300
C	-2.58597400	-2.24033900	2.28224100
C	-2.56709200	-1.03190800	3.05368600
C	-1.40476500	-0.63885500	3.81158600
C	-0.22186700	-1.43559200	3.81336800
C	1.03931200	-0.76828800	3.91516600
C	2.19775300	-1.27645400	3.23117600
C	2.13443800	-2.45909300	2.44683000
C	2.97778100	-2.51520700	1.28514900
C	2.51667000	-3.19057300	0.10606200
C	1.24536500	-3.86443400	0.05784600
C	0.55774600	-3.90861100	-1.18921700
C	-0.89961900	-3.87936800	-1.24609200
C	-1.74400000	-3.92938100	-0.05937100
C	-1.00034400	-3.88269400	1.19564500
C	-1.43080700	-3.08691900	2.34746200
C	-0.26614700	-2.67297600	3.08752800
C	0.89516800	-3.18284900	2.41533000

C	0.45775200	-3.89633100	1.24731500
C	-2.18979600	1.28293300	-3.25696500
C	-1.01828200	0.76638200	-3.91924700
C	0.23705900	1.43527300	-3.82690900
C	1.42403300	0.63419700	-3.82887800
C	2.57124900	1.01927900	-3.05360200
C	2.57265900	2.20731300	-2.27347900
C	3.32698100	2.17679300	-1.04946500
C	2.84152100	2.89887900	0.09221500
C	1.65073500	3.70677900	0.04072300
C	0.87162900	3.82787300	1.22990600
C	-0.57930100	3.97061200	1.17851000
C	-1.31345300	4.08982900	-0.07709300
C	-2.62202100	3.41055200	-0.12510200
C	-2.97961200	2.60482500	-1.30856600
C	-2.13424800	2.48368400	-2.47986400
C	-0.89699900	3.20165900	-2.45164400
C	0.26994300	2.67567000	-3.10719600
C	1.42300000	3.06311300	-2.34190400
C	0.97229000	3.81891200	-1.20664700
C	-0.47977400	3.94389500	-1.26299500
Lu	-1.15215000	-1.67872300	0.01083400
Lu	-0.97311000	1.78669100	0.01095500
Lu	2.05783300	-0.09642600	0.02172100