

An endohedral redox sytem in a fullerene cage: The Ce based mixed cluster fullerene

Lu₂CeN@C₈₀

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Supporting Information

Fig. S1 ¹³C NMR spectra of Lu₂CeN@C₈₀ in a temperature range of 268 to 308 K

Table S1. Redox potentials of Ce-based endohedral metallofullerenes and their lanthanide analogues (V, vs Fc⁺⁰).

Table S2 DFT-optimized Cartesian coordinates

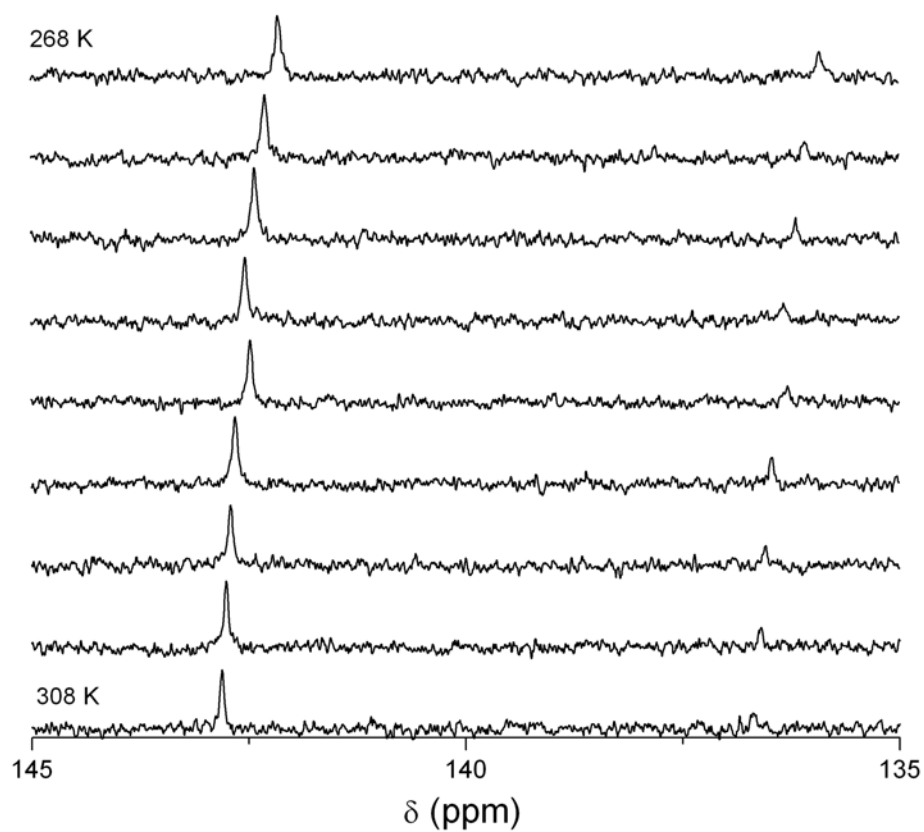


Fig. S1 ^{13}C NMR spectra of $\text{Lu}_2\text{CeN}@C_{80}$ in a temperature range of 268 to 308 K

Table S1. Redox potentials of Ce-based endohedral metallofullerenes and their lanthanide analogues (V, vs Fc⁺⁰).

compound	I _{red}	II _{red}	III _{red}	I _{ox}	II _{ox}
Ce@C ₈₂ ¹	-0.41	-1.41	-1.53	0.08	1.08
La@C ₈₂ ¹	-0.42	-1.37	-1.53	0.07	1.07
Ce ₂ @C ₈₀ (I _h) ²	-0.35	-1.69		0.57	0.95
La ₂ @C ₈₀ (I _h) ³	-0.39	-1.71		0.57	0.95
Ce ₂ @C ₈₀ (D _{5h}) ⁴	-0.40	-1.76		0.20	0.66
La ₂ @C ₈₀ (D _{5h}) ⁴	-0.36	-1.72		0.22	0.78
Ce ₂ @C ₇₈ ⁵	-0.52	-1.86	-2.23	0.25	0.79
La ₂ @C ₇₈	-0.40	-1.84	-2.28	0.26	0.62
Ce ₂ @C ₇₂ ⁶	-0.71	-1.86		0.18	0.82
La ₂ @C ₇₂ ⁷	-0.68	-1.92		0.24	0.75
Ce ₃ N@C ₈₈ ⁸	-1.30	-1.57		0.08	0.63
La ₃ N@C ₈₈ ⁸	-1.36	-1.67		0.21	0.66
Pr ₃ N@C ₈₈ ⁸	-1.34	-1.72		0.09	0.54
Ce ₃ N@C ₉₂ ⁹	-1.48			0.32	
La ₃ N@C ₉₂ ⁹	-1.44	-1.64		0.36	
Pr ₃ N@C ₉₂ ⁹	-1.46			0.35	
Ce ₃ N@C ₉₆ ⁹	-1.50	-1.84		0.18	0.67
La ₃ N@C ₉₆ ⁹	-1.54	-1.77		0.14	0.53
Pr ₃ N@C ₉₆ ⁹	-1.51	-1.86		0.14	0.53

1. T. Suzuki, K. Kikuchi, F. Oguri, Y. Nakao, S. Suzuki, Y. Achiba, K. Yamamoto, H. Funasaka and T. Takahashi, *Tetrahedron*, 1996, **52**, 4973-4982.
2. M. Yamada, T. Nakahodo, T. Wakahara, T. Tsuchiya, Y. Maeda, T. Akasaka, M. Kako, K. Yoza, E. Horn, N. Mizorogi, K. Kobayashi and S. Nagase, *J. Am. Chem. Soc.*, 2005, **127**, 14570-14571.
3. T. Suzuki, Y. Maruyama, T. Kato, K. Kikuchi, Y. Nakao, Y. Achiba, K. Kobayashi and S. Nagase, *Angew. Chem.-Int. Edit. Engl.*, 1995, **34**, 1094-1096.
4. M. Yamada, N. Mizorogi, T. Tsuchiya, T. Akasaka and S. Nagase, *Chem.-Eur. J.*, 2009, **15**, 9486-9493.
5. M. Yamada, T. Wakahara, T. Tsuchiya, Y. Maeda, M. Kako, T. Akasaka, K. Yoza, E. Horn, N. Mizorogi and S. Nagase, *Chem. Commun.*, 2008, 558-560.
6. M. Yamada, T. Wakahara, T. Tsuchiya, Y. Maeda, T. Akasaka, N. Mizorogi and S. Nagase, *J. Phys. Chem. A*, 2008, **112**, 7627-7631.
7. X. Lu, H. Nikawa, T. Tsuchiya, Y. Maeda, M. O. Ishitsuka, T. Akasaka, M. Toki, H. Sawa, Z. Slanina, N. Mizorogi and S. Nagase, *Angewandte Chemie International Edition*, 2008, **47**, 8642-8645.
8. M. N. Chaur, F. Melin, B. Elliott, A. Kumbhar, A. J. Athans and L. Echegoyen, *Chem.-Eur. J.*, 2008, **14**, 4594-4599.
9. M. N. Chaur, R. Valencia, A. Rodriguez-Forteza, J. M. Poblet and L. Echegoyen, *Angew. Chem.-Int. Edit.*, 2009, **48**, 1425-1428.

Table S2. DFT (PBE0)-optimized Cartesian coordinates.

Lu₂CeN@C₈₀ (PBE0, doublet)

C	-1.635485260	2.814349293	-2.484352773
C	-1.409633998	3.721095038	-1.390393642
C	-0.029644509	4.151022448	-1.138843416
C	-2.264962236	3.511965248	-0.240720085
C	-2.675559859	1.807935659	-2.484139515
C	-3.904306256	0.232193981	-1.072390395
C	-3.469631068	1.584318583	-1.338894641
C	-3.264412956	2.458472830	-0.234278410
C	-1.757734201	3.632734080	1.123415782
C	-0.374502973	3.978012180	1.398520217
C	0.219316982	3.250545337	2.490324009
C	-2.456021681	2.642309007	1.919973066
C	-2.285338735	0.649140673	3.330015589
C	-1.850856696	1.972468507	3.023294930
C	-0.507366150	2.318719236	3.318614465
C	-4.140672271	-0.272238940	0.250896163
C	-3.786270096	0.592225014	1.355486465
C	-3.400851255	1.950975973	1.093557485
C	-3.235734724	-0.027991360	2.500772614
C	1.599394843	2.808589199	2.504419703
C	2.401485733	2.959098321	1.355005972
C	1.816352223	3.678830710	0.250272792
C	3.381394995	1.942617619	1.091616992
C	1.714894127	1.647272154	3.331623758
C	2.284290435	-0.731859544	3.323324671
C	2.646632385	0.606630806	3.024296662
C	3.535869243	0.787812629	1.923492095
C	-1.365450343	-0.327887749	3.824633330
C	0.006200370	-0.006108293	4.044616016
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C	0.975715004	-1.030428756	3.826672250
C	3.757745325	1.572105172	-0.233231168
C	3.099028661	2.191370614	-1.335682536
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C	3.268566468	0.002509359	-2.486382697
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C	-0.222523267	-3.218882016	-2.482712324
C	1.661834054	-2.797360057	2.504641958
C	0.020520965	-3.914039943	1.095608047
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C	-1.052937311	-3.447849603	1.921643149
C	-0.774867896	-2.593736356	3.023717213
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C	0.487997734	4.281786380	0.249646247
N	-0.169064193	0.084580516	-0.036523285
Lu	-1.794149533	-1.096968033	-0.003051236
Lu	-0.229839671	2.097650148	-0.063217102
Ce	1.758012548	-0.766538117	0.049768062

Lu₂CeN@C₈₀⁺ (PBE0, singlet)

C	-1.631702651	2.809664264	-2.483640669
C	-1.406895171	3.717639169	-1.391829705
C	-0.031085548	4.151899556	-1.141580856
C	-2.254736953	3.499283990	-0.242345019
C	-2.671779782	1.805296411	-2.486246661
C	-3.895610460	0.230292504	-1.072564796
C	-3.461478198	1.580249551	-1.339705448
C	-3.254296527	2.450326818	-0.235335177
C	-1.747541029	3.615446183	1.118892173
C	-0.371796755	3.963225141	1.393523166
C	0.219684556	3.247200971	2.492807751
C	-2.449238006	2.635064444	1.920024232
C	-2.284901756	0.650012416	3.336695112
C	-1.849485359	1.971769930	3.028033057
C	-0.506989296	2.319652310	3.323127457
C	-4.127576894	-0.272549872	0.250154545
C	-3.777622543	0.589671215	1.356570112
C	-3.389054278	1.944023705	1.092053146
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C	3.891548081	-0.631763753	-1.376513892
C	3.251656523	0.010312031	-2.486243114
C	2.741822526	-1.828796350	2.499359797
C	3.689731122	-1.688221033	1.417354576
C	4.045655634	-0.311405231	1.129388982
C	3.475261468	-2.560768070	0.258224231
C	1.755088336	1.605070086	-3.326148868
C	0.778170433	2.598944503	-3.027809456
C	1.009817935	3.492616261	-1.917824202
C	-0.574650632	2.301040559	-3.323524250
C	1.370456630	0.323429193	-3.836173731
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C	0.002167831	0.000398126	-4.055865504

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C	1.860744057	-1.967661379	-3.016042671
C	2.282292375	-0.651404383	-3.319000091
C	0.514582812	-2.315223715	-3.319596089
C	-1.703533729	-1.648326636	-3.325236574
C	-2.636248103	-0.626937117	-3.022299147
C	-2.263041517	0.716142846	-3.319622218
C	-3.530091112	-0.868338819	-1.912728959
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C	-1.885566469	-3.674066889	-0.240074095
C	-2.494681242	-3.046540346	-1.381242220
C	-3.574646480	-2.094739037	-1.134329184
C	1.754466110	-3.494070175	-1.069450461
C	-0.487228107	-4.030560241	-0.235549872
C	0.367601814	-3.786267517	-1.340584813
C	-0.224147968	-3.214055311	-2.485418375
C	1.657708517	-2.795859124	2.504443246
C	0.017897455	-3.906772941	1.093736645
C	1.387827769	-3.576869811	1.357151089
C	2.304315856	-3.440860650	0.252271690
C	-1.751291316	-1.605231848	3.318232097
C	-1.053157855	-3.441983025	1.920690329
C	-0.777127710	-2.592003433	3.024283170
C	0.590658770	-2.307620970	3.323783083
C	-3.969129331	-1.725556915	0.249468337
C	-2.250394293	-3.309406553	1.117322570
C	-3.258431925	-2.311553744	1.395278342
C	-2.922910159	-1.440083512	2.490726856
C	0.484729354	4.273874589	0.246477044
N	-0.025280632	0.016652329	0.006617620
Lu	-1.790017726	-1.102967523	-0.032102081
Lu	-0.196355587	2.096708396	-0.100170977
Ce	1.754130711	-0.871102434	0.153049170

Lu₂CeN@C₈₀⁺ (PBE0, triplet)

C	-1.644045296	2.818449204	-2.483305750
C	-1.413296197	3.722458422	-1.391546803
C	-0.031903702	4.149598035	-1.139150007
C	-2.267553210	3.512511018	-0.239741641
C	-2.677912110	1.815053267	-2.480031625
C	-3.905771677	0.233543725	-1.073592368
C	-3.471063982	1.586025835	-1.338596064
C	-3.263992947	2.460221395	-0.232566565
C	-1.760462172	3.634952281	1.124297668
C	-0.377372499	3.977656432	1.398323017
C	0.219874929	3.251886543	2.486664798
C	-2.458182057	2.644025793	1.919468860
C	-2.276923086	0.646886841	3.319171288
C	-1.851109851	1.973008810	3.020019284
C	-0.505343376	2.312966345	3.312298766
C	-4.141626555	-0.271227541	0.248098313
C	-3.787999159	0.595071455	1.354422176
C	-3.403274661	1.953282382	1.095123322
C	-3.237253389	-0.029693293	2.494695572
C	1.596668460	2.808062605	2.498127554
C	2.398681328	2.952129997	1.353730617
C	1.811301892	3.674626467	0.246457749
C	3.382127836	1.936843772	1.093276930
C	1.707600534	1.637869557	3.322607364
C	2.284307577	-0.733994804	3.321944201
C	2.649300070	0.600658871	3.023049444
C	3.540251590	0.783377997	1.924780575
C	-1.362310200	-0.330615482	3.828882679
C	0.006805589	-0.008276458	4.050791275
C	0.408460424	1.338989234	3.830776993
C	0.976007235	-1.031557830	3.831925711
C	3.755397731	1.564684252	-0.229822462
C	3.093896108	2.184160770	-1.334682175
C	2.133810805	3.231390664	-1.071059557
C	2.912073207	1.396755542	-2.480438670
C	4.202633977	0.188631528	-0.232436375
C	3.599414411	-2.040869912	-1.121397901
C	3.930145480	-0.648453522	-1.378514710
C	3.274635879	0.002670275	-2.483922122
C	2.749804944	-1.839072666	2.503743598
C	3.683024611	-1.686394011	1.410069982
C	4.074582203	-0.314942102	1.135095456
C	3.477187883	-2.564507689	0.253707988
C	1.745157580	1.588863052	-3.308953185
C	0.770116388	2.594094716	-3.019694882
C	1.005675620	3.485766815	-1.912247983
C	-0.578484138	2.301001461	-3.323179471
C	1.370175188	0.319767816	-3.828601856
C	-0.402274424	-1.344171583	-3.835355853
C	0.001379449	0.000603544	-4.051888992

C	-0.963053890	1.024808111	-3.836464464
C	2.530813621	-2.632533474	-1.908121579
C	1.874703594	-1.975056767	-3.008126592
C	2.290875779	-0.656732637	-3.307495109
C	0.516251460	-2.307655640	-3.301771281
C	-1.698869407	-1.646221053	-3.319237289
C	-2.636375839	-0.626608060	-3.015327674
C	-2.256791808	0.714447748	-3.306879719
C	-3.534705426	-0.866222315	-1.910182384
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C	-2.493025530	-3.045849558	-1.377470963
C	-3.577407239	-2.092503762	-1.131975517
C	1.768364391	-3.505919208	-1.075640794
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C	1.668700827	-2.796590195	2.499331488
C	0.020990906	-3.912849442	1.098423595
C	1.393968088	-3.576103007	1.356522397
C	2.310091006	-3.438938459	0.248294957
C	-1.748870869	-1.603519116	3.315260453
C	-1.052687453	-3.447492261	1.923028469
C	-0.775207673	-2.592981327	3.023654799
C	0.590972672	-2.303273578	3.323166952
C	-3.978702235	-1.725422398	0.249045164
C	-2.252992031	-3.317422120	1.121955373
C	-3.266807593	-2.317805443	1.399450074
C	-2.932344256	-1.441923246	2.487530505
C	0.485797143	4.279434333	0.246800812
N	-0.165445254	0.083720365	-0.068773312
Lu	-1.791673059	-1.093790596	-0.008966334
Lu	-0.235234890	2.095773875	-0.063352578
Ce	1.762741455	-0.764720076	0.065389962

Lu₂CeN@C₈₀⁻ (PBE0, triplet)

C	-1.638908673	2.820414425	-2.494837355
C	-1.418792096	3.744111176	-1.405669533
C	-0.023151331	4.172270200	-1.148746148
C	-2.264758168	3.510076108	-0.244600513
C	-2.678729359	1.815220606	-2.494420637
C	-3.908007505	0.236325942	-1.078715472
C	-3.472171816	1.586681748	-1.344656200
C	-3.266579863	2.459274645	-0.238267749
C	-1.757919190	3.621561769	1.113936129
C	-0.368587033	3.971278540	1.393242783
C	0.226648466	3.251307414	2.492043969
C	-2.454726555	2.638894853	1.913274574
C	-2.281802101	0.650233043	3.323344387
C	-1.848363790	1.972179596	3.019278297
C	-0.501156894	2.322852379	3.319187921
C	-4.144875017	-0.271840610	0.244864448
C	-3.788064595	0.591378942	1.351676676
C	-3.404862007	1.948273743	1.090176960
C	-3.237927641	-0.031230812	2.500403997
C	1.605635037	2.820699706	2.513973441
C	2.401807017	2.961649909	1.354718722
C	1.816313342	3.675182548	0.244127409
C	3.382744919	1.950153822	1.091513000
C	1.722588666	1.647031484	3.331463174
C	2.291055188	-0.737675184	3.323119254
C	2.653399661	0.609814794	3.027579195
C	3.540394531	0.789614526	1.920735080
C	-1.362656824	-0.329222116	3.816324082
C	0.009723919	-0.007000530	4.036775279
C	0.412516583	1.342052065	3.822777959
C	0.981031667	-1.032735787	3.818623304
C	3.753118635	1.578131204	-0.234974850
C	3.102159577	2.195706750	-1.342097308
C	2.143193083	3.239790112	-1.078521676
C	2.915997271	1.408383627	-2.496335478
C	4.183147599	0.195948694	-0.234713683
C	3.591025252	-2.041718978	-1.120929452
C	3.918216027	-0.638402289	-1.381844255
C	3.268647373	0.007428241	-2.491307035
C	2.754258838	-1.841440732	2.507878796
C	3.696926396	-1.696159187	1.413578559
C	4.067954690	-0.306384953	1.130123277
C	3.481354059	-2.569894515	0.250628203
C	1.755125256	1.604173140	-3.318381321
C	0.779518177	2.601617084	-3.027915266
C	1.014744843	3.501213581	-1.922096125
C	-0.582673380	2.311405096	-3.334332432
C	1.375203925	0.319979506	-3.827717687
C	-0.400844283	-1.347553794	-3.832601497
C	0.003399256	0.000198328	-4.047874893

C	-0.963106885	1.025867194	-3.831197395
C	2.525030092	-2.630459980	-1.909048999
C	1.871171965	-1.975417211	-3.015667466
C	2.296509905	-0.653148999	-3.323178928
C	0.519859420	-2.316360945	-3.314336003
C	-1.705992729	-1.657477546	-3.332415366
C	-2.637451570	-0.627312981	-3.021662873
C	-2.264383291	0.714884420	-3.316243292
C	-3.537564420	-0.867092389	-1.914561787
C	-1.611813455	-2.820052282	-2.490681362
C	-1.883712312	-3.679280680	-0.238183925
C	-2.500014577	-3.055456514	-1.385063482
C	-3.587512144	-2.093956060	-1.137726406
C	1.765595377	-3.513290379	-1.079595468
C	-0.482252546	-4.036468168	-0.236117449
C	0.375477019	-3.792425636	-1.342758937
C	-0.224515596	-3.221103422	-2.490208540
C	1.672864652	-2.805693674	2.507694736
C	0.026589560	-3.916126030	1.092859375
C	1.399242166	-3.584202844	1.353555297
C	2.315904522	-3.454836205	0.246177925
C	-1.755534412	-1.608785446	3.313487882
C	-1.051914644	-3.450272303	1.916528940
C	-0.772131001	-2.598614161	3.022766205
C	0.593310874	-2.315315173	3.321895979
C	-3.987497708	-1.729258743	0.244830375
C	-2.252059549	-3.326495493	1.116868261
C	-3.281101850	-2.326670972	1.398370292
C	-2.930461741	-1.444506010	2.488326300
C	0.489722574	4.277677933	0.239139158
N	-0.182820751	0.088575388	-0.041953950
Lu	-1.806884799	-1.103705534	-0.008787820
Lu	-0.230873157	2.104437075	-0.140224615
Ce	1.729087344	-0.816658160	0.111128589

Lu₃N@C₈₀ (PBE0, singlet)

C	0.418851574	3.217659867	2.496206532
C	-2.996000973	-1.246093830	2.496206532
C	2.577149399	-1.971566037	2.496206532
C	-0.143214631	3.915809213	1.377733771
C	-3.319582939	-2.081932115	1.377733771
C	3.462797570	-1.833877098	1.377733771
C	-1.574228503	3.805692514	1.129289096
C	-2.508712145	-3.266168132	1.129289096
C	4.082940647	-0.539524382	1.129289096
C	0.719219061	4.056070282	0.239170360
C	-3.872269434	-1.405173164	0.239170360
C	3.153050374	-2.650897119	0.239170360
C	1.765606007	2.703088235	2.493315777
C	-3.223746083	0.177515538	2.493315777
C	1.458140076	-2.880603773	2.493315777
C	-3.249505129	2.169247216	1.077032479
C	-0.253870632	-3.898777599	1.077032479
C	3.503375761	1.729530383	1.077032479
C	-3.719118580	0.833623273	1.344464413
C	1.137620358	-3.637662806	1.344464413
C	2.581498222	2.804039533	1.344464413
C	2.058452248	3.518979152	0.234570587
C	-4.076751465	0.023182364	0.234570587
C	2.018299217	-3.542161516	0.234570587
C	0.207349679	3.985288004	-1.115808642
C	-3.555035493	-1.813073912	-1.115808642
C	3.347685813	-2.172214092	-1.115808642
C	-1.197221390	3.798944975	-1.392665504
C	-2.691372161	-2.936296626	-1.392665504
C	3.888593552	-0.862648350	-1.392665504
C	-1.462422213	2.912480585	-2.493613479
C	-1.791071068	-2.722735080	-2.493613479
C	3.253493281	-0.189745505	-2.493613479
C	1.244767007	3.383181321	-1.924993478
C	-3.552304473	-0.613590810	-1.924993478
C	2.307537466	-2.769590511	-1.924993478
C	-2.218849616	0.865083079	-3.340073259
C	0.360240885	-2.354121674	-3.340073259
C	1.858608731	1.489038595	-3.340073259
C	0.944767376	2.539571428	-3.030611023
C	-2.671717059	-0.451593166	-3.030611023
C	1.726949683	-2.087978262	-3.030611023
C	-0.429701261	2.340449656	-3.324216024
C	-1.812038228	-1.542357036	-3.324216024
C	2.241739489	-0.798092620	-3.324216024
C	-3.130717372	2.708617170	-0.248353761
C	-0.780372593	-4.065589362	-0.248353761
C	3.911089965	1.356972191	-0.248353761
C	-3.377148724	1.815262277	-1.358168316
C	0.116511116	-3.832327726	-1.358168316

C	3.260637608	2.017065449	-1.358168316
C	2.384608886	3.119583191	-1.097946447
C	-3.893942735	0.505340278	-1.097946447
C	1.509333849	-3.624923469	-1.097946447
C	-2.563929913	1.975446888	-2.505439227
C	-0.428822232	-3.208151882	-2.505439227
C	2.992752145	1.232704994	-2.505439227
C	-0.895787182	1.087317885	-3.835522161
C	-0.493751320	-1.319433399	-3.835522161
C	1.389538502	0.232115513	-3.835522161
C	0.000000000	0.000000000	-4.055523263
C	-2.115095887	3.757270312	-0.248399925
C	-2.196343595	-3.710361925	-0.248399925
C	4.311439482	-0.046908386	-0.248399925
C	-2.236627463	0.798921964	3.325954058
C	0.426427015	-2.336437183	3.325954058
C	1.810200447	1.537515220	3.325954058
C	-1.721805662	2.092544234	3.027798880
C	-0.951293634	-2.537399561	3.027798880
C	2.673099296	0.444855327	3.027798880
C	-2.287894400	2.816999900	1.914575796
C	-1.295646276	-3.389874622	1.914575796
C	3.583540676	0.572874722	1.914575796
C	-0.361444229	2.347859407	3.335722992
C	-1.852583776	-1.486949588	3.335722992
C	2.214028005	-0.860909819	3.335722992
C	0.492917672	1.318287246	3.845440324
C	-1.388129081	-0.232264397	3.845440324
C	0.895211409	-1.086022849	3.845440324
C	0.000000000	0.000000000	4.061310242
N	0.000000000	0.000000000	0.007485178
Lu	-0.765761306	1.894086193	0.005822898
Lu	-1.257446107	-1.610211841	0.005822898
Lu	2.023207413	-0.283874352	0.005822898

Lu₃N@C₈₀⁺ (PBE0, doublet)

C	0.422470773	3.221751215	2.492489402
C	-3.001353654	-1.245005368	2.492489402
C	2.578882880	-1.976745847	2.492489402
C	-0.143277386	3.917872773	1.377958506
C	-3.321338669	-2.083018397	1.377958506
C	3.464616055	-1.834854376	1.377958506
C	-1.574685969	3.806204732	1.129534659
C	-2.508927235	-3.266820183	1.129534659
C	4.083612675	-0.539384549	1.129534659
C	0.718528511	4.056580714	0.237002615
C	-3.872366176	-1.406026596	0.237002615
C	3.153837665	-2.650554118	0.237002615
C	1.762898971	2.707370820	2.488290910
C	-3.226101052	0.173029848	2.488290910
C	1.463202611	-2.880400668	2.488290910
C	-3.245612346	2.169126119	1.077095310
C	-0.255712205	-3.895346227	1.077095310
C	3.501324552	1.726219579	1.077095310
C	-3.714320511	0.832096298	1.343008995
C	1.136543612	-3.632743605	1.343008995
C	2.577776370	2.800647836	1.343008995
C	2.054090394	3.516332019	0.231344122
C	-4.072278228	0.020728931	0.231344122
C	2.018187305	-3.537060421	0.231344122
C	0.207306775	3.989046584	-1.117811266
C	-3.558269316	-1.814990650	-1.117811266
C	3.350962541	-2.174055934	-1.117811266
C	-1.197204258	3.800650488	-1.393423711
C	-2.692857605	-2.937134819	-1.393423711
C	3.890061863	-0.863515668	-1.393423711
C	-1.465760654	2.914797189	-2.490072121
C	-1.791407866	-2.726784746	-2.490072121
C	3.257168519	-0.188012443	-2.490072121
C	1.244180910	3.385859134	-1.925602983
C	-3.554330649	-0.615437374	-1.925602983
C	2.310149739	-2.770421760	-1.925602983
C	-2.210087613	0.861392609	-3.331215233
C	0.359056289	-2.344688609	-3.331215233
C	1.851031854	1.483296000	-3.331215233
C	0.942965811	2.540836094	-3.028885687
C	-2.671911711	-0.453785896	-3.028885687
C	1.728945900	-2.087050199	-3.028885687
C	-0.429826866	2.335860345	-3.320401496
C	-1.808000748	-1.540171442	-3.320401496
C	2.237828143	-0.795688904	-3.320401496
C	-3.128425516	2.708909668	-0.245766319
C	-0.781772071	-4.063750537	-0.245766319
C	3.910197587	1.354840869	-0.245766319
C	-3.377336206	1.813866677	-1.357744993
C	0.117813377	-3.831792040	-1.357744993

C	3.259522300	2.017925362	-1.357744993
C	2.383622296	3.121245639	-1.099974289
C	-3.894889547	0.503654501	-1.099974289
C	1.511266722	-3.624900669	-1.099974289
C	-2.562751441	1.978182034	-2.498776028
C	-0.431780060	-3.208499029	-2.498776028
C	2.994531500	1.230316995	-2.498776028
C	-0.894435495	1.086446401	-3.839399492
C	-0.493672101	-1.317827037	-3.839399492
C	1.388107596	0.231380635	-3.839399492
C	0.000000000	0.000000000	-4.061293567
C	-2.114964299	3.756289559	-0.246101817
C	-2.195560110	-3.709757416	-0.246101817
C	4.310524409	-0.046532143	-0.246101817
C	-2.226984772	0.795005736	3.319459561
C	0.424997066	-2.326128246	3.319459561
C	1.801987706	1.531122511	3.319459561
C	-1.719277832	2.093229401	3.025708507
C	-0.953150886	-2.535553318	3.025708507
C	2.672428717	0.442323916	3.025708507
C	-2.285927709	2.817696868	1.913842018
C	-1.297233046	-3.388519838	1.913842018
C	3.583160755	0.570822969	1.913842018
C	-0.359555303	2.341687116	3.331920627
C	-1.848182764	-1.482227591	3.331920627
C	2.207738066	-0.859459525	3.331920627
C	0.492123729	1.316787204	3.853096716
C	-1.386433280	-0.232201919	3.853096716
C	0.894309551	-1.084585285	3.853096716
C	0.000000000	0.000000000	4.071551138
N	0.000000000	0.000000000	0.007935542
Lu	-0.759414862	1.896754885	0.004070961
Lu	-1.262930189	-1.606050305	0.004070961
Lu	2.022345580	-0.290704580	0.004070961

Lu₃N@C₈₀⁻ (PBE0, doublet)

C	2.582294486	-1.973105108	2.498996695
C	0.417612397	3.222885242	2.498996695
C	-2.999906354	-1.249779605	2.498996695
C	3.484762891	-1.847214369	1.387186299
C	-0.142647136	3.941500538	1.387186299
C	-3.342116285	-2.094286168	1.387186299
C	4.094539656	-0.536960917	1.132987540
C	-1.582247912	3.814456193	1.132987540
C	-2.512291744	-3.277494747	1.132987540
C	3.166894056	-2.658449442	0.236252770
C	0.718838079	4.071835836	0.236252770
C	-3.885732135	-1.413385864	0.236252770
C	1.464616572	-2.883250817	2.500535013
C	1.764660072	2.710020411	2.500535013
C	-3.229276645	0.173230406	2.500535013
C	3.490359470	1.727286400	1.076765633
C	-3.241053484	2.159096623	1.076765633
C	-0.249305456	-3.886383023	1.076765633
C	2.575020415	2.803803320	1.344692307
C	-3.715675205	0.828131702	1.344692307
C	1.140654260	-3.631935022	1.344692307
C	2.020944318	-3.537731947	0.232975576
C	2.053293982	3.519055165	0.232975576
C	-4.074237771	0.018677311	0.232975576
C	3.359917807	-2.185059117	-1.119237399
C	0.212357772	4.002303533	-1.119237399
C	-3.572275579	-1.817244416	-1.119237399
C	3.893276086	-0.859807194	-1.398733476
C	-1.202023475	3.801579723	-1.398733476
C	-2.691252611	-2.941772529	-1.398733476
C	3.255265598	-0.185223679	-2.501093295
C	-1.467224358	2.911754420	-2.501093295
C	-1.788041240	-2.726531270	-2.501093295
C	2.312946441	-2.767349886	-1.925118785
C	1.240122120	3.386745506	-1.925118785
C	-3.553068562	-0.619395091	-1.925118785
C	1.855947911	1.493906004	-3.343827644
C	-2.221734275	0.860345367	-3.343827644
C	0.365786365	-2.354251371	-3.343827644
C	1.729901065	-2.087596310	-3.036273531
C	0.942960520	2.541936254	-3.036273531
C	-2.672862114	-0.454340473	-3.036273531
C	2.248503236	-0.793569020	-3.334621547
C	-0.437000922	2.344045659	-3.334621547
C	-1.811502843	-1.550476639	-3.334621547
C	3.888668539	1.350719107	-0.248255040
C	-3.114091162	2.692325782	-0.248255040
C	-0.774576848	-4.043045418	-0.248255040
C	3.252539277	2.013846464	-1.362120231
C	-3.370311907	1.809858160	-1.362120231

C	0.117772630	-3.823704624	-1.362120231
C	1.508576914	-3.619115703	-1.099212273
C	2.379957744	3.116023718	-1.099212273
C	-3.888534658	0.503091986	-1.099212273
C	2.999147514	1.235334125	-2.518108990
C	-2.569404786	1.979670610	-2.518108990
C	-0.429742727	-3.215005264	-2.518108990
C	1.390757187	0.233799505	-3.839633388
C	-0.897855038	1.087531215	-3.839633388
C	-0.492902149	-1.321330719	-3.839633388
C	0.000000000	0.000000000	-4.057789355
C	4.297563271	-0.046318355	-0.246246283
C	-2.108668677	3.744958286	-0.246246283
C	-2.188894594	-3.698639931	-0.246246283
C	1.811241429	1.538246295	3.327092943
C	-2.237781046	0.799457704	3.327092943
C	0.426539617	-2.337703999	3.327092943
C	2.672992291	0.446107004	3.029213248
C	-1.722836019	2.091826023	3.029213248
C	-0.950156272	-2.537933028	3.029213248
C	3.583248069	0.572086115	1.915003033
C	-2.287065440	2.817140703	1.915003033
C	-1.296183158	-3.389226818	1.915003033
C	2.219202691	-0.866544679	3.345189217
C	-0.359152070	2.355158381	3.345189217
C	-1.860050622	-1.488613702	3.345189217
C	0.897854509	-1.086371258	3.846119514
C	0.491897770	1.320750212	3.846119514
C	-1.389752279	-0.234379483	3.846119514
C	0.000000000	0.000000000	4.063858489
N	0.000000000	0.000000000	-0.025984720
Lu	2.014919106	-0.372755629	0.041821936
Lu	-0.684643704	1.931348789	0.041821936
Lu	-1.330275402	-1.558593689	0.041821936