Supporting Information
Is the chemistry of lawrencium peculiar?

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Table S 1 Excitation energies (in eV) of the Lr atom from the $7p_{1/2}$ ground state to the $6d_{3/2}$ excited state. Non-relativistic (NR) reference values in parentheses. 'DF': Single-jj-configuration Dirac-Fock. 'PW'= Present work.

Ref. [1]	DF(PW)	MCDF [2]
0.156	0.626	0.165
	(-2.297)	

Table S 2 Cartesian coordinates of optimized structures of the hydrides studied. Lengths in Å, angles in degree. ZORA2c, PBE, TZ2P. ADF outputs bonding energy instead of total energy by default.

LuH, Bond energy = -15.97329756 a.u.			
Lu	0.000000	0.000000	-0.001116
H	0.000000	0.000000	1.893789
LrH, Bond energy = -206.85080914 a.u.			
Lr	0.000000	0.000000	-0.001003
H	0.000000	0.000000	1.958639
LuH_2, Bond energy = -16.10361981 a.u.			
Lu	0.000000	-0.054547	0.023366
H	1.601334	-0.872929	0.681107
H	-1.601334	-0.872929	0.681107
LrH_2, Bond energy = -206.96678954 a.u.			
Lr	0.000000	-0.021740	-0.003001
H	1.606069	-0.889333	0.694291
H	-1.606069	-0.889333	0.694291
LuH_3, Bond energy = -16.25528212 a.u.			
Lu	0.101430	0.000000	-0.000485
H	0.641310	-1.596787	0.921607
H	0.641310	1.596787	0.921607
H	0.640251	0.000000	-1.844728
LrH_3, Bond energy = -207.11349376 a.u.			
Lr	-0.131551	0.000000	0.002248
H	0.592051	-1.559353	-0.897596
H	0.592051	1.559353	-0.897596
H	0.591449	0.000000	1.802944

Table S 3 Cartesian coordinates of optimized structures of the trichlorides and monocarbonyls studied. Lengths in Å, angles in degree. ZORA2c, PBE, TZ2P.

$LuCl_3$, Bond energy = -16.42018352 a.u.			
Lu	0.000000	0.000000	0.000000
Cl	1.194041	2.068139	0.000000
Cl	1.194041	-2.068139	0.000000
Cl	-2.388081	0.000000	0.000000
$LrCl_3$, Bond energy = -207.25782680 a.u.			
Lr	0.000000	0.000000	0.186717
Cl	1.167489	2.022151	-0.462759
Cl	1.167489	-2.022151	-0.462759
Cl	-2.334978	0.000000	-0.462759
LuCO, Bond energy = -16.40676579 a.u.			
Lu	-0.000223	-0.000402	0.032047
C	-0.003583	-0.006479	2.329114
O	-0.005290	-0.009566	3.495924
LrCO, Bond energy = -207.28264400 a.u.			
Lr	-0.000373	-0.000674	-0.026497
C	-0.003576	-0.006466	2.357064
O	-0.005147	-0.009307	3.526518

Table S 4 Cartesian coordinates of optimized structures of $[(Cp')_3M]^-$, Cp' = $C_5H_4SiMe_3$. Lengths in Å. TPSSh, def2-TZVP, COSMO.

Total energy = -2814.630460158 a.u.			
Lr	-0.4531807	-0.2877815	-0.3841826
Si	2.5802096	-2.9304156	-1.0528258
Si	2.0802987	3.0248059	0.0947735
Si	-3.9540284	0.3293947	1.5668960
C	0.2290485	-1.9104392	-2.4903269
C	-1.1747461	-1.9705142	-2.4221018
C	-1.5232380	-2.6562810	-1.2281307
C	-0.3294503	-3.0177081	-0.5754978
C	0.7895600	-2.5244246	-1.3226513
C	2.9363403	-4.6833893	-1.6860098
C	3.6896134	-1.7463548	-2.0158931
C	3.0627326	-2.8974186	0.7714167
C	-0.6684139	2.4337808	-0.7723118
C	-1.3360849	1.7976800	-1.8483001
C	-0.3410147	1.2058229	-2.6726486
C	0.9086478	1.4143503	-2.0635294
C	0.7301831	2.1882723	-0.8705046
C	2.7703558	4.4599559	-0.9331810
H	3.5738928	4.9836262	-0.4029943
H	1.9870162	5.1900257	-1.1623422
H	3.1752174	4.1005165	-1.8849338
C	1.4231671	3.7618492	1.7039779
H	1.0867530	2.9926185	2.4034095
H	0.5806644	4.4353520	1.5165840
H	2.2074854	4.3451149	2.1988398
C	3.5227294	1.8686100	0.4725898
H	3.1953822	1.0047218	1.0574469
H	4.3064472	2.3920013	1.0318659
H	3.9712404	1.4886526	-0.4507429
C	-1.5705242	-1.3616476	1.8794222
C	-0.2047481	-1.2371670	2.1798833
C	0.1063043	0.1476018	2.2414814
C	-1.0847416	0.8643913	2.0003536
C	-2.1457418	-0.0585471	1.7222078
C	-4.2289983	2.0812044	0.9210123
C	-4.7774192	0.2279481	3.2729597
C	-4.8401501	-0.9027370	0.4450075
H	0.7990789	-1.4297090	-3.2732384
H	-1.8702756	-1.5630911	-3.1436794
H	-2.5284945	-2.8658925	-0.8888632
H	-0.2675356	-3.5420465	0.3680112
H	2.7050711	-4.7703941	-2.7529133
H	2.3263386	-5.4221093	-1.1552677
H	3.9886704	-4.9561702	-1.5469713
H	3.5665960	-0.7211807	-1.6569098
H	3.4558105	-1.7599342	-3.0853127
H	4.7433890	-2.0236986	-1.9027734
H	2.9371220	-1.8939141	1.1874783
H	4.1085145	-3.1981587	0.9011940
H	2.4453572	-3.5844082	1.3593670
H	-1.1525863	2.9986630	0.0107774
H	-2.3963260	1.8330537	-2.0560805
H	-0.5231326	0.6419304	-3.5759214
H	1.8579474	1.0600243	-2.4435877
H	-2.0962896	-2.2958037	1.7349096
H	0.4978495	-2.0477861	2.3132317
H	1.0745366	0.5670870	2.4755401
H	-1.1751340	1.9401403	1.9922529
H	-3.7345847	2.8222985	1.5574550
H	-5.2978764	2.3209382	0.9039283
H	-3.8385745	2.1974039	-0.0931065
H	-4.3210606	0.9378153	3.9709097
H	-4.6675460	-0.7734411	3.7022842
H	-5.8484280	0.4534589	3.2172911
H	-4.4438247	-0.8518184	-0.5731842
H	-5.9159037	-0.6972162	0.4100481
H	-4.7095181	-1.9295118	0.8021117

References

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2 S. Fritzsche, C. Z. Dong, F. Koike and A. Uvarov, *Eur. Phys. J. D*, 2007, **45**, 107–113.