

Eu benchmark complexes

[Eu^{III}Cp*₂(THF)]

Eu	-0.162771	-0.019672	0.039573
O	1.806027	0.504265	-1.561649
C	0.573648	1.670600	2.096371
C	-0.742327	1.208470	2.439752
C	-1.671378	1.777642	1.500899
C	-0.926694	2.592976	0.581697
C	0.458503	2.533468	0.954694
C	1.844009	1.401635	2.867258
C	-1.109853	0.409786	3.665902
C	-3.175453	1.690358	1.593399
C	-1.508413	3.462965	-0.507018
C	1.575467	3.350772	0.354827
C	0.233977	-2.730181	-0.314581
C	-0.399584	-2.296787	-1.526557
C	-1.749611	-1.919763	-1.208535
C	-1.954146	-2.133835	0.197461
C	-0.723253	-2.626689	0.752513
C	1.617849	-3.320780	-0.185346
C	0.185766	-2.368918	-2.915758
C	-2.808804	-1.514561	-2.206004
C	-3.277747	-2.053358	0.917787
C	-0.513281	-3.118420	2.163974
C	3.197150	0.210368	-1.264012
C	1.694821	1.195489	-2.832741
C	4.012750	1.009848	-2.285812
C	3.065756	1.044627	-3.499477
H	0.871508	0.732854	-3.407136
H	3.355431	-0.881865	-1.365488
H	3.394850	0.502920	-0.215947
H	1.446416	2.258528	-2.638869
H	3.115723	0.094933	-4.064044
H	4.987191	0.541803	-2.507102
H	4.202863	2.032577	-1.910439
H	3.283437	1.867569	-4.201943

H	1.764838	4.282015	0.929361
H	2.538557	2.804154	0.330921
H	1.350464	3.666830	-0.681331
H	1.825229	0.423638	3.384582
H	2.738970	1.407023	2.213812
H	2.027017	2.167396	3.650039
H	-0.245338	-0.143659	4.073835
H	-1.485293	1.058506	4.484566
H	-1.904228	-0.333386	3.467448
H	-3.511857	0.729686	2.022086
H	-3.592295	2.490644	2.240641
H	-3.669357	1.799119	0.609584
H	-2.439915	3.042476	-0.932347
H	-1.764726	4.477979	-0.138094
H	-0.801253	3.605155	-1.347189
H	-3.966243	-1.327411	0.448493
H	-3.802223	-3.032073	0.915127
H	-3.169111	-1.760610	1.978698
H	-2.395562	-0.932073	-3.053110
H	-3.314547	-2.395015	-2.654353
H	-3.601491	-0.897631	-1.743539
H	1.275336	-2.172796	-2.932931
H	0.038023	-3.368261	-3.375627
H	-0.286757	-1.641024	-3.602580
H	2.274666	-3.032507	-1.026834
H	2.124592	-3.013527	0.750670
H	1.597511	-4.430710	-0.174598
H	-1.154013	-2.588715	2.891710
H	-0.742198	-4.200382	2.263957
H	0.532573	-2.986896	2.502575

[Eu^{II}Cp*₂]

Eu	-0.149543	0.352284	0.095317
C	-2.477978	-0.837167	0.849267
C	-1.583308	-1.925071	0.565851
C	-1.336408	-1.936442	-0.850572

C	-2.077917	-0.855766	-1.440376
C	-2.785290	-0.176015	-0.388963
C	-3.059346	-0.507013	2.203868
C	-1.118510	-2.970911	1.550902
C	-0.566957	-2.998973	-1.594445
C	-2.199816	-0.571436	-2.919302
C	-3.767204	0.958390	-0.560246
C	2.146105	1.763362	0.477187
C	2.151351	1.424544	-0.918412
C	2.330281	0.002327	-1.032047
C	2.439907	-0.536965	0.297869
C	2.321236	0.550814	1.228101
C	2.063232	3.155572	1.058004
C	2.081597	2.401085	-2.069440
C	2.549104	-0.757460	-2.318335
C	2.776752	-1.963603	0.656669
C	2.472177	0.460719	2.728611
H	3.049587	3.512593	1.418711
H	1.716647	3.889500	0.307801
H	1.375725	3.224818	1.925293
H	3.500643	0.719585	3.056266
H	1.796354	1.152181	3.269408
H	2.268775	-0.558176	3.107417
H	3.862100	-2.094122	0.847770
H	2.252454	-2.305206	1.568686
H	2.513448	-2.665111	-0.154759
H	3.614123	-0.734245	-2.630394
H	2.269965	-1.821914	-2.222396
H	1.967297	-0.339310	-3.161443
H	3.090421	2.704254	-2.418152
H	1.562288	1.979965	-2.951736
H	1.555058	3.334914	-1.793232
H	-4.805091	0.590037	-0.696683
H	-3.791440	1.631521	0.318323
H	-3.545305	1.585514	-1.444452
H	-3.080645	-1.079939	-3.362994

H	-2.320188	0.506740	-3.139389
H	-1.316142	-0.923912	-3.483390
H	-1.193464	-3.890317	-1.805944
H	-0.190808	-2.634731	-2.567244
H	0.305767	-3.355763	-1.017855
H	-1.851389	-3.799500	1.643929
H	-0.159929	-3.429830	1.247331
H	-0.978175	-2.563284	2.570245
H	-3.946988	-1.129200	2.441625
H	-2.337090	-0.675483	3.026430
H	-3.392877	0.545604	2.272723

[Eu^{III}Cp₃(THF)]

Eu	-0.024196	-0.492420	-0.027445
O	0.450640	2.076422	-0.302965
C	-0.010162	-0.028402	2.735172
C	-0.423107	-1.394833	2.579198
C	-1.716869	-1.398430	2.002876
C	-0.605342	-0.942241	-2.743784
C	-1.063510	0.803587	2.267414
C	-2.117803	-0.036241	1.807876
C	1.834882	-2.552402	0.281563
C	-1.258019	0.288726	-2.455749
C	-2.327133	0.021801	-1.556689
C	-2.343269	-1.390311	-1.297447
C	-1.279742	-1.982403	-2.022833
C	2.814717	-0.468586	0.063376
C	1.381746	4.263927	-0.118517
C	-0.129662	4.333822	0.161435
C	2.422479	-1.466390	1.003228
C	1.877269	-2.229004	-1.099374
C	2.470352	-0.930093	-1.236927
C	-0.624166	3.037036	-0.483543
C	1.671808	2.771304	0.071575
H	0.929635	0.313740	3.179238
H	-2.321402	-2.283422	1.784942

H	0.141026	-2.279429	2.887237
H	-1.075952	1.897146	2.295112
H	-3.085773	0.294093	1.421571
H	1.454795	-3.482846	0.714973
H	-1.000617	1.261350	-2.886211
H	-3.048254	0.749999	-1.174133
H	2.585029	-1.424910	2.083971
H	1.541645	-2.869433	-1.918871
H	0.236734	-1.067437	-3.430155
H	-1.039379	-3.049371	-2.058230
H	-3.073882	-1.918976	-0.678895
H	-0.615912	5.228080	-0.264952
H	-0.321848	4.327452	1.250900
H	-1.538579	2.624696	-0.022789
H	-0.806704	3.170129	-1.568498
H	1.983792	4.895196	0.557412
H	1.901260	2.529647	1.128940
H	2.494797	2.397726	-0.561845
H	1.597973	4.576083	-1.157404
H	3.343181	0.457802	0.304635
H	2.673582	-0.417782	-2.182519

[Eu^{III}CpCl₂(THF)₃]

Eu	0.192479	-0.274716	0.177052
Cl	-2.009862	0.106881	1.667051
Cl	1.911169	0.106796	-1.837386
O	-1.304737	-1.350694	-1.574578
O	1.348852	1.552835	1.483337
O	-0.810109	1.837812	-0.896417
C	-0.821870	-1.972254	-2.805447
C	-1.930101	-2.941121	-3.244849
C	-3.188964	-2.337952	-2.593287
C	-2.636577	-1.843037	-1.257405
C	2.640086	2.111147	1.099273
C	2.871077	3.270191	2.069807
C	2.208544	2.739102	3.355077

C	0.966146	2.030886	2.806148
C	-1.083913	1.962748	-2.313756
C	-2.270070	2.926183	-2.404730
C	-1.995162	3.883015	-1.230459
C	-1.404163	2.947026	-0.166592
C	0.067352	-2.618975	1.719264
C	1.085748	-1.805433	2.332447
C	2.194407	-1.747404	1.452664
C	1.867973	-2.511895	0.286708
C	0.552177	-3.047436	0.459950
H	3.140060	-1.225181	1.625111
H	2.520249	-2.657466	-0.578257
H	1.012272	-1.349996	3.324371
H	-0.907764	-2.852910	2.154688
H	0.023292	-3.694574	-0.246120
H	-0.179957	2.349845	-2.825369
H	-1.300983	0.953613	-2.701579
H	-2.328198	3.438385	-3.381047
H	-3.219645	2.381194	-2.245570
H	-1.258096	4.652201	-1.528925
H	-2.899609	4.403536	-0.870349
H	-2.159723	2.518271	0.518163
H	-0.614591	3.428138	0.439291
H	0.109912	2.723984	2.691571
H	0.625535	1.169346	3.405680
H	2.877009	2.019591	3.864270
H	1.954478	3.533713	4.077806
H	3.941813	3.507777	2.193234
H	2.356282	4.184691	1.719624
H	3.413866	1.326331	1.212987
H	2.585919	2.384915	0.032734
H	-0.644637	-1.166877	-3.543588
H	0.147241	-2.458937	-2.600407
H	-2.000164	-3.019740	-4.343551
H	-1.743233	-3.956795	-2.848795
H	-3.569834	-1.488822	-3.191285

H	-4.008015	-3.067261	-2.469609
H	-2.550953	-2.666010	-0.518610
H	-3.192182	-1.017966	-0.782915

[Eu^{III}Cp(NCS)₂(THF)₃]

Eu	0.186201	-0.342014	0.239120
N	-1.729739	-0.005089	1.616599
N	1.655507	0.095257	-1.589875
O	-1.300371	-1.406962	-1.516403
O	1.337321	1.547933	1.451446
O	-0.890956	1.725947	-0.819172
C	-0.816270	-2.017027	-2.752459
C	-1.882660	-3.045836	-3.149454
C	-3.161621	-2.460542	-2.521225
C	-2.629629	-1.910313	-1.198220
C	2.608821	2.112295	1.008511
C	2.992160	3.134476	2.082457
C	2.369869	2.520653	3.350498
C	1.048208	1.964571	2.816194
C	-1.046654	1.907531	-2.252150
C	-2.172656	2.932906	-2.407164
C	-1.969352	3.821473	-1.166889
C	-1.552637	2.801910	-0.098759
C	0.104922	-2.751240	1.612409
C	0.946636	-1.904976	2.407505
C	2.147496	-1.685015	1.688528
C	2.059903	-2.397983	0.445236
C	0.798749	-3.057246	0.406708
H	3.013033	-1.111771	2.035253
H	2.834720	-2.436620	-0.325700
H	0.699450	-1.521697	3.402122
H	-0.886229	-3.111933	1.904085
H	0.435561	-3.707193	-0.395057
C	-2.653259	0.085607	2.387187
S	-3.902601	0.225086	3.405223
C	2.393504	0.258923	-2.529234

S	3.369555	0.499761	-3.797259
H	4.084373	3.275145	2.153365
H	2.537523	4.119431	1.866065
H	3.348927	1.291620	0.935444
H	2.465361	2.534451	-0.000435
H	3.003917	1.700907	3.735936
H	2.222840	3.250571	4.164889
H	0.254765	2.738663	2.789821
H	0.659630	1.092233	3.369663
H	-0.704514	-1.217165	-3.509961
H	0.181443	-2.449468	-2.562614
H	-1.949458	-3.175350	-4.243273
H	-1.657020	-4.034003	-2.707342
H	-3.565034	-1.641927	-3.146226
H	-3.960622	-3.208053	-2.378158
H	-2.537941	-2.705717	-0.431527
H	-3.211495	-1.078902	-0.767072
H	-0.087324	2.264843	-2.674353
H	-1.277881	0.922256	-2.690598
H	-2.109944	3.488558	-3.358955
H	-3.160319	2.435080	-2.368759
H	-1.159628	4.553228	-1.346890
H	-2.874665	4.381265	-0.875609
H	-2.418514	2.376176	0.442095
H	-0.845413	3.211884	0.643788

[Eu^{III}(pta)₃(H₂O)₂]

Eu	-1.719583	-2.933655	-0.354813
F	-3.682390	1.451516	-1.266089
O	-2.943578	-4.257741	1.169165
O	-1.609215	-1.899202	1.890978
O	-3.211698	-1.124225	-0.344184
O	-1.097886	-1.611204	-2.302201
O	-0.867706	-4.397728	-2.028443
O	0.223488	-1.400495	0.125313
O	-0.356085	-4.928301	0.488984

C	-3.628791	-3.939288	2.198606
C	-3.471044	-2.823383	3.027331
C	-2.427504	-1.859577	2.860148
C	-1.040660	-1.846507	-3.545940
C	-1.004955	-3.171220	-4.089196
C	-0.893134	-4.321992	-3.302851
C	-2.295815	-0.714613	3.895840
C	-2.094699	-1.311399	5.311723
C	-1.094619	0.187072	3.551615
C	-1.009812	-0.637156	-4.517987
C	-2.290991	-0.690531	-5.392096
C	-0.982093	0.680522	-3.719375
O	-3.631111	-3.545596	-1.602194
C	-4.680779	0.648453	-0.831657
C	-4.266571	-0.826371	-0.991281
C	-4.763767	-4.935476	2.507252
C	-0.801869	-5.691201	-4.000853
C	-3.598580	0.126868	3.842404
C	0.242874	-0.721559	-5.426894
C	-4.711939	-3.038388	-2.022732
F	-4.898854	0.936058	0.469578
F	-5.796435	0.962588	-1.518636
C	-5.050474	-1.665479	-1.794826
F	-5.655606	-4.927153	1.491881
F	-5.425610	-4.637977	3.643330
F	-4.273322	-6.184285	2.617170
F	0.264699	-6.375269	-3.545155
F	-1.908315	-6.416374	-3.716768
F	-0.701014	-5.592396	-5.340799
C	-5.659832	-3.949543	-2.843746
C	-5.310647	-5.428364	-2.571551
C	-7.139040	-3.689256	-2.478196
C	-5.415035	-3.618745	-4.341038
H	-2.009318	-0.497957	6.056143
H	-2.934342	-1.960017	5.615334
H	-1.169321	-1.914068	5.359408

H	-3.498717	1.014807	4.494928
H	-3.810744	0.471969	2.815043
H	-4.473875	-0.446218	4.194324
H	-1.009236	0.994980	4.300813
H	-0.146735	-0.380126	3.553328
H	-1.212839	0.658622	2.560045
H	0.276247	0.156987	-6.097904
H	1.173051	-0.730291	-4.829848
H	0.237398	-1.626496	-6.058720
H	-1.008615	1.541287	-4.412136
H	-1.839133	0.761157	-3.030080
H	-0.059765	0.760586	-3.116835
H	-2.314665	0.182399	-6.071034
H	-2.326586	-1.602483	-6.013755
H	-3.202866	-0.665694	-4.768566
H	-0.985372	-3.300962	-5.172834
H	-4.154436	-2.727581	3.873316
H	-5.963685	-1.249927	-2.225495
H	-5.979306	-6.085881	-3.156146
H	-4.268915	-5.654148	-2.849017
H	-5.434585	-5.674291	-1.501642
H	-7.791925	-4.385188	-3.036447
H	-7.316555	-3.850819	-1.399647
H	-7.464787	-2.663540	-2.727379
H	-6.047212	-4.262569	-4.980448
H	-5.659071	-2.566010	-4.570896
H	-4.358892	-3.793845	-4.617102
H	-0.303719	-5.338093	-0.402305
H	-1.073071	-5.397388	0.957415
H	0.109593	-0.699742	-0.542923
H	-0.183748	-1.081505	0.964472

[Eu^{III}(acac)₃(H₂O)₂]

Eu	-0.460092	0.066776	-0.405146
O	1.702929	-0.853990	-0.404727
O	0.252227	-0.054446	1.834263

O	-1.321057	2.117189	0.649486
O	0.857273	1.940424	-1.101306
O	-0.551696	-1.372653	-2.343806
O	-1.238697	-2.109785	0.288821
O	-1.295033	1.083611	-2.639154
O	-2.870423	0.082020	0.414889
C	2.314467	3.812384	-1.271932
C	-0.348246	-3.094274	-3.977925
C	-0.589927	-2.637158	-2.549497
C	-0.860641	-3.596800	-1.547614
C	-1.212967	-3.283931	-0.205917
C	-1.612291	-4.416272	0.729295
C	2.558802	-1.232428	0.459689
C	2.388870	-1.113078	1.865140
C	-1.661105	4.154521	1.834015
C	-0.853062	3.279760	0.890445
C	0.339456	3.793295	0.316975
C	1.108009	3.116284	-0.661841
C	3.838897	-1.848320	-0.084581
C	1.246091	-0.536297	2.474596
C	1.163037	-0.475152	3.992010
H	-2.675342	0.926398	0.890185
H	-2.788457	-0.649370	1.054834
H	-0.530763	1.681990	-2.746572
H	-1.027204	0.229181	-3.056564
H	-1.118445	-2.654741	-4.639082
H	0.630157	-2.713267	-4.323894
H	-0.369598	-4.190596	-4.086578
H	-0.870190	-4.651237	-1.842877
H	-2.614241	-4.209095	1.147324
H	-1.624068	-5.400526	0.233645
H	-0.907627	-4.448036	1.580549
H	0.277154	-1.043066	4.331166
H	2.061421	-0.878767	4.487167
H	1.012780	0.573147	4.308702
H	3.190614	-1.483106	2.513324

H	3.585807	-2.753416	-0.666316
H	4.314036	-1.138753	-0.785780
H	4.557235	-2.115854	0.707061
H	3.216426	3.204103	-1.076530
H	2.197200	3.863583	-2.369970
H	2.471310	4.828786	-0.876410
H	0.647815	4.806007	0.597006
H	-2.648668	4.360397	1.380622
H	-1.845598	3.605395	2.775055
H	-1.167856	5.112657	2.063020

[Eu^{III}(NO)₃(phen)₂]

Eu	10.632303	14.721739	3.228074
O	10.622590	16.939880	2.139977
O	8.906687	14.720841	1.414715
O	8.203334	15.360488	3.369198
O	6.798863	15.266724	1.684125
O	14.463838	15.275147	4.773639
O	10.630417	18.846188	3.228099
O	13.060480	15.363744	3.087389
O	12.357529	14.722765	5.041560
O	10.639808	16.939770	4.316028
N	10.630880	17.629513	3.228026
N	7.921169	15.129550	2.141016
N	9.094763	12.491802	3.346893
N	9.627078	14.018224	5.573517
N	11.637674	14.019034	0.882773
N	12.171700	12.493437	3.109485
N	13.342369	15.134197	4.315858
C	8.839969	11.760099	2.260046
C	7.948521	10.660185	2.258554
C	7.299141	10.325285	3.441855
C	7.542100	11.088328	4.615720
C	8.467570	12.178896	4.513326
C	6.894258	10.817027	5.872643
C	7.142668	11.595786	6.978361

C	8.062895	12.701797	6.915527
C	8.338263	13.541903	8.028843
C	8.739407	12.994119	5.687046
C	9.237098	14.592890	7.888172
C	9.866514	14.792842	6.634882
C	12.524499	12.994194	0.768637
C	11.397678	14.793492	-0.178551
C	12.797188	12.179383	1.942443
C	12.427629	11.762483	4.196551
C	13.199394	12.700878	-0.460485
C	12.025389	14.592420	-1.432554
C	13.721791	11.088113	1.839453
C	13.318384	10.662008	4.197548
C	12.923363	13.540680	-1.573870
C	14.118326	11.593878	-0.524043
C	14.367484	10.815503	0.581747
C	13.965937	10.325800	3.013550
H	9.351462	12.066569	1.338171
H	7.775928	10.099905	1.332704
H	6.592664	9.485879	3.479234
H	6.635857	11.388507	7.929745
H	6.186006	9.980484	5.927491
H	7.834573	13.354074	8.986015
H	9.468195	15.264159	8.722831
H	10.590547	15.604007	6.486726
H	10.674481	15.605334	-0.029846
H	11.917348	12.069998	5.118904
H	11.793883	15.263549	-2.267153
H	13.425644	13.351906	-2.531650
H	13.492191	10.102471	5.123631
H	14.671565	9.485826	2.975690
H	15.074504	9.978139	0.526274
H	14.623284	11.385526	-1.476128

[Eu^{III}Cl₃(phen)₂]

Eu	13.060175	2.731901	9.777208
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Cl	11.350733	1.959975	11.648705
Cl	12.989669	5.351012	10.152432
Cl	14.497785	2.428190	7.583092
N	10.665383	3.180959	8.712118
N	11.919666	0.743806	8.410207
N	15.590911	3.159713	10.513705
N	14.360068	0.755546	11.025653
C	10.633554	0.870295	7.986009
C	9.964127	2.147359	8.169378
C	8.599089	2.283184	7.755415
C	10.053464	4.358153	8.877974
C	8.702754	4.583821	8.516726
C	7.974346	3.544126	7.953270
C	9.931861	-0.206007	7.347434
C	12.567575	-0.397892	8.169722
C	7.917253	1.168105	7.151828
C	15.709826	0.839257	11.182213
C	13.736589	-0.374197	11.373917
C	8.561441	-0.028554	6.946004
C	10.642160	-1.416860	7.132556
C	14.421529	-1.514380	11.858593
C	16.495173	-0.266300	11.648438
C	16.361866	2.104679	10.892297
C	16.177433	4.334204	10.266466
C	11.971003	-1.510529	7.531075
C	18.380539	3.466342	10.758169
C	18.542803	1.062993	11.469983
C	17.922634	-0.126642	11.771310
C	15.806228	-1.463351	11.980570
C	17.575806	4.532263	10.374506
C	17.783405	2.207607	11.038487
H	8.258214	5.571316	8.685001
H	10.668385	5.153839	9.323908
H	6.927207	3.681848	7.653756
H	6.871074	1.299640	6.846325
H	13.620734	-0.432827	8.477056

H	8.041783	-0.869069	6.468328
H	15.498267	5.151305	9.982017
H	12.640686	-0.355638	11.286222
H	17.999123	5.518895	10.154757
H	16.372499	-2.330408	12.344643
H	19.467733	3.582559	10.856276
H	19.631498	1.163344	11.566646
H	18.505304	-0.990699	12.115718
H	13.857830	-2.413295	12.132676
H	10.136879	-2.259609	6.643405
H	12.557346	-2.420611	7.360677

[Eu^{III}(NCS)₃(bipy)₃]

Eu	2.608263	3.023173	3.696728
N	2.962401	0.598532	3.652713
N	1.883268	4.801848	5.194177
N	2.434421	2.418744	1.003651
N	2.247867	5.010566	1.858062
N	1.323905	1.959157	5.796680
N	4.040532	2.365992	5.864982
N	5.185253	2.695432	2.471395
N	4.745716	5.026603	3.779880
N	0.319374	2.931301	2.915644
S	-1.850848	3.318698	1.147193
S	0.791043	6.284648	7.338414
S	3.228193	-1.958572	4.828115
C	2.369542	1.124755	0.638765
C	2.206349	4.792822	0.519474
C	1.834062	7.367992	1.490204
C	2.045316	6.257801	2.321938
C	5.377444	2.516098	5.843917
C	6.228662	2.059953	6.860527
C	5.650653	1.400628	7.954951
C	4.261999	1.235742	7.982294
C	3.469238	1.735176	6.922761
C	1.984449	1.584109	6.919156

C	1.290556	1.076878	8.040824
C	5.429533	1.495054	1.915593
C	6.370067	1.296930	0.891308
C	7.068956	2.413565	0.409910
C	6.840683	3.661819	1.004705
C	5.906233	3.767171	2.060641
C	5.721302	5.030121	2.839237
C	6.573221	6.144776	2.666174
C	6.431672	7.257986	3.505519
C	5.449554	7.227313	4.505604
C	4.628206	6.090330	4.595330
C	3.068102	-0.491076	4.156947
C	1.406588	5.419840	6.111467
C	2.278351	3.374453	0.055083
C	2.189237	0.703683	-0.687984
C	2.030344	5.865533	-0.385474
C	1.848797	7.164708	0.103099
C	-0.102599	0.946848	7.993879
C	-0.014527	1.833062	5.756749
C	-0.606235	3.096898	2.166177
C	2.118527	3.031050	-1.307691
C	2.080427	1.683504	-1.684632
C	-0.773575	1.330279	6.825481
H	2.455694	0.402410	1.462376
H	1.659815	8.357689	1.927128
H	2.031481	6.356079	3.415336
H	5.784264	3.018241	4.959179
H	7.311149	2.212896	6.783767
H	6.269400	1.010411	8.772148
H	3.798974	0.707087	8.819912
H	1.825752	0.789267	8.950439
H	4.833081	0.667387	2.322976
H	7.391775	4.538480	0.648946
H	7.356891	6.139302	1.902476
H	7.090395	8.127203	3.387241
H	3.826360	6.020447	5.341317

H	5.309941	8.060329	5.203802
H	6.533598	0.293912	0.481470
H	7.791789	2.317790	-0.409655
H	2.130345	-0.365765	-0.919872
H	1.702299	8.000102	-0.592496
H	-0.487801	2.159016	4.821535
H	2.016520	5.695360	-1.466031
H	-0.649581	0.555543	8.860186
H	1.944385	1.407982	-2.737607
H	2.001554	3.805133	-2.071608
H	-1.862631	1.252634	6.733111

Np benchmark complexes

[Np^{III}(COT)]⁻

Np	8.259958	10.511427	5.852163
C	8.201939	11.223806	3.226259
C	8.202056	9.797797	3.228176
C	8.976160	12.232688	3.873013
C	8.974619	8.788463	3.872097
C	10.069948	12.232317	4.785358
C	10.070069	8.788387	4.786390
C	10.847182	11.222996	5.428218
C	10.844813	9.797528	5.428353
C	5.570149	10.509502	6.240484
C	5.997558	11.828260	6.579685
C	5.998704	9.193601	6.579000
C	7.028269	12.372829	7.399893
C	7.029005	8.646687	7.399896
C	8.059280	11.828853	8.221347
C	8.060137	9.193824	8.220845
C	8.484475	10.510125	8.563129
H	7.365404	11.642789	2.648526
H	7.363408	9.378930	2.653014
H	8.590695	13.244453	3.679767
H	8.589040	7.776938	3.678074
H	10.329385	13.243867	5.130200

H	10.329786	7.776817	5.130792
H	11.563450	11.641258	6.150132
H	11.558826	9.378829	6.152588
H	4.772619	10.509161	5.483106
H	5.451431	12.603134	6.022279
H	5.454578	8.418621	6.019416
H	7.091392	13.467996	7.320916
H	7.090509	7.551429	7.323483
H	8.725522	12.604275	8.626717
H	8.728108	8.418758	8.624543
H	9.402724	10.510152	9.168723

[Np^{IV}(COT)₂]

Np	-0.017700	-0.029799	0.035424
C	-0.128101	0.714778	-2.537810
C	-0.114809	-0.708304	-2.544141
C	0.634893	1.724297	-1.887866
C	0.680787	-1.710752	-1.919132
C	1.728175	1.729815	-0.976921
C	1.793966	-1.705265	-1.032534
C	2.521931	0.727037	-0.350767
C	2.555221	-0.695694	-0.381266
H	-0.979904	1.126804	-3.095576
H	-0.959339	-1.132003	-3.104051
H	0.237899	2.731574	-2.071745
H	0.308631	-2.724355	-2.119460
H	1.973106	2.739786	-0.621975
H	2.074622	-2.716232	-0.707988
H	3.234520	1.147950	0.371096
H	3.289911	-1.112887	0.320457
C	-1.822981	1.647410	1.112754
C	-2.587619	0.639194	0.463144
C	-2.556367	-0.783571	0.431718
C	-1.761835	-1.787689	1.055057
C	-0.664476	-1.783905	1.961032
C	0.103781	-0.775645	2.607106

C	0.092283	0.647356	2.614511
C	-0.705195	1.650699	1.993414
H	0.940606	1.069875	3.169507
H	0.957574	-1.189422	3.160534
H	-0.269065	-2.791988	2.143863
H	-2.010167	-2.797338	0.701546
H	-3.272377	-1.203492	-0.287354
H	-3.324252	1.057878	-0.235697
H	-2.104080	2.658702	0.791201
H	-0.331577	2.663840	2.193476

[Np^{IV}Cp₃Cl]

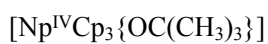
Np	6.129664	11.974729	5.240250
Cl	6.526716	14.535084	5.102124
C	6.129572	12.273619	7.961978
C	5.939921	10.871798	7.763959
C	4.034179	11.961864	7.055940
C	4.654769	10.679686	7.184701
C	4.921391	10.503782	3.251424
C	3.847876	11.014396	4.032723
C	5.531079	11.603878	2.569320
C	4.944368	12.942585	7.535652
C	8.625475	11.191000	6.152816
C	8.515647	11.717703	3.913570
C	8.881380	12.213618	5.199473
C	8.099890	10.056435	5.458595
C	8.052455	10.376460	4.072843
C	4.840066	12.789821	2.939265
C	3.809831	12.431850	3.856624
H	7.011709	12.755338	8.393039
H	6.643527	10.080758	8.034873
H	4.204603	9.715069	6.930239
H	3.025389	12.153149	6.682042
H	6.363694	11.542041	1.863928
H	4.774878	14.021496	7.562041
H	3.158329	10.421452	4.638812

H	5.199694	9.449562	3.158099
H	8.823386	11.252760	7.225889
H	9.273691	13.210251	5.413631
H	8.606492	12.265282	2.971411
H	7.742134	9.703064	3.270079
H	7.825668	9.095389	5.904590
H	5.069964	13.801981	2.599476
H	3.098810	13.124204	4.315953

[Np^{IV}Cp₃{OCH(CH₃)₂}]

Np	-0.417080	0.063383	0.178800
C	-0.143441	2.534308	1.421471
C	-0.892967	1.723113	2.320996
C	-2.182757	1.503937	1.744824
C	-2.216838	2.156885	0.482383
C	-0.952128	2.794527	0.281797
H	0.879066	2.886756	1.579613
H	-0.548555	1.365987	3.295570
H	-3.009123	0.956567	2.205315
H	-3.074928	2.197620	-0.194671
H	-0.669787	3.404077	-0.580248
C	0.800743	-0.186057	-2.305513
C	0.170352	1.092431	-2.307528
C	-1.242711	0.884285	-2.339677
C	-1.482106	-0.517592	-2.327677
C	-0.214288	-1.179634	-2.309029
H	1.877446	-0.370718	-2.292321
H	0.683266	2.057907	-2.322761
H	-2.005719	1.664683	-2.395178
H	-2.462835	-1.001607	-2.361072
H	-0.051607	-2.260173	-2.326714
C	0.001912	-2.014311	1.967130
C	-0.137553	-2.620171	0.682706
C	-1.502929	-2.490803	0.284330
C	-2.194713	-1.780985	1.304364
C	-1.263541	-1.494821	2.349755

H	0.921708	-1.958086	2.554269
H	0.655119	-3.125889	0.124048
H	-1.946875	-2.890672	-0.630394
H	-3.260626	-1.533238	1.304528
H	-1.491340	-0.988601	3.290926
O	1.616349	0.248760	0.601553
C	2.953334	0.489189	0.987758
C	3.651212	1.395175	-0.039552
H	2.933529	1.029843	1.962133
C	3.703871	-0.835750	1.185920
H	3.203301	-1.465592	1.940763
H	3.742963	-1.400590	0.236583
H	4.739900	-0.652698	1.524489
H	3.716684	0.891853	-1.021399
H	3.089237	2.336076	-0.173103
H	4.676103	1.647564	0.288234



Np	-0.309696	-0.009147	-0.043680
C	-0.191190	2.549418	1.036128
C	-0.916975	1.757808	1.972982
C	-2.182236	1.439418	1.389783
C	-2.222111	2.007737	0.087194
C	-0.988049	2.697381	-0.130322
H	0.807422	2.966807	1.185630
H	-0.576633	1.480486	2.974492
H	-2.989665	0.881365	1.870251
H	-3.064176	1.956222	-0.609355
H	-0.716433	3.265217	-1.023782
C	1.009513	-0.383739	-2.458830
C	0.393495	0.899711	-2.541551
C	-1.018166	0.701886	-2.630885
C	-1.273054	-0.695940	-2.570593
C	-0.014723	-1.367377	-2.469885
H	2.082825	-0.578756	-2.396963
H	0.915295	1.860255	-2.571751

H	-1.769983	1.485292	-2.752926
H	-2.256196	-1.172895	-2.628603
H	0.137030	-2.449080	-2.438450
C	0.121438	-2.032850	1.808307
C	-0.012769	-2.677641	0.543729
C	-1.377983	-2.564111	0.137256
C	-2.074381	-1.826304	1.133568
C	-1.145245	-1.500867	2.170335
H	1.039828	-1.955959	2.395345
H	0.782526	-3.199476	0.004071
H	-1.818497	-2.992256	-0.766467
H	-3.141211	-1.583502	1.123691
H	-1.374708	-0.962590	3.093333
O	1.700590	0.220774	0.460186
C	3.085397	0.373952	0.751263
C	3.663648	1.474161	-0.163125
C	3.234112	0.775517	2.233171
C	3.796932	-0.969874	0.487676
H	3.379080	-1.762574	1.132715
H	3.663400	-1.278098	-0.564194
H	4.880554	-0.894325	0.690817
H	3.547603	1.196479	-1.225342
H	3.135313	2.429864	0.001598
H	4.738693	1.634604	0.036370
H	2.719718	1.732600	2.429157
H	2.787352	0.005835	2.886955
H	4.297830	0.892105	2.509084

[Np^{IV}Cp₃{OCH(CF₃)₂}]

Np	-0.959683	-0.024979	-0.089367
C	-0.705054	2.430073	1.166328
C	-1.374132	1.579696	2.094450
C	-2.686467	1.325854	1.589122
C	-2.814202	1.993950	0.340256
C	-1.587648	2.682074	0.081334
H	0.310479	2.821738	1.267774

H	-0.961920	1.215039	3.039648
H	-3.466702	0.745497	2.087364
H	-3.709518	2.011224	-0.288174
H	-1.375376	3.316604	-0.782375
C	0.254022	-0.125926	-2.568455
C	-0.436073	1.120320	-2.522771
C	-1.838969	0.848711	-2.558426
C	-2.012644	-0.561925	-2.598272
C	-0.715299	-1.164394	-2.606516
H	1.337485	-0.257812	-2.554963
H	0.033617	2.106868	-2.502225
H	-2.638457	1.593640	-2.582360
H	-2.970377	-1.087968	-2.651758
H	-0.503365	-2.234784	-2.665573
C	-0.468523	-2.195345	1.553658
C	-0.688422	-2.729448	0.250365
C	-2.071215	-2.558439	-0.066982
C	-2.694068	-1.890876	1.023064
C	-1.700460	-1.671559	2.028488
H	0.483515	-2.176274	2.086429
H	0.066407	-3.214612	-0.374627
H	-2.570341	-2.905266	-0.974833
H	-3.754270	-1.629856	1.094312
H	-1.864925	-1.211279	3.005979
O	1.104218	0.164734	0.386418
C	2.403581	0.441058	0.722679
C	3.184123	1.000951	-0.484725
H	2.475548	1.230446	1.507516
C	3.067412	-0.812779	1.329207
F	2.489299	-1.085485	2.523251
F	2.910477	-1.889686	0.542965
F	4.381848	-0.629707	1.541658
F	3.373292	0.070433	-1.443234
F	2.495299	2.025341	-1.029340
F	4.388027	1.465528	-0.112001

[Np^{IV}Cp₄]

Np	-0.000419	-0.001092	-0.000379
C	-1.487737	0.044023	2.462447
C	-1.344806	-1.336930	2.120294
C	-2.152787	-1.582111	0.977351
C	-2.735091	-0.351664	0.566531
C	-2.332621	0.651962	1.505628
H	-1.058711	0.540382	3.334946
H	-0.783469	-2.089422	2.680855
H	-2.323725	-2.558600	0.523157
H	-3.422024	-0.214820	-0.273186
H	-2.658948	1.693644	1.527324
C	1.488166	-0.046115	2.460245
C	1.341685	1.335493	2.121914
C	2.148898	1.586097	0.979805
C	2.733951	0.358290	0.564929
C	2.334078	-0.648957	1.501332
H	1.059770	-0.546200	3.330799
H	0.779679	2.085090	2.685630
H	2.315881	2.563892	0.526875
H	3.420414	0.224831	-0.275785
H	2.662837	-1.689891	1.520323
C	0.045898	1.486954	-2.461403
C	0.649998	2.332855	-1.503073
C	-0.356703	2.733860	-0.566474
C	-1.585014	2.149496	-0.980561
C	-1.335593	1.341528	-2.122421
H	0.546383	1.057352	-3.331207
H	1.691425	2.660108	-1.522740
H	-0.222093	3.420393	0.274005
H	-2.562538	2.317295	-0.527516
H	-2.085335	0.779495	-2.685994
C	-0.045227	-1.489223	-2.459798
C	-0.648361	-2.335741	-1.501328
C	0.358820	-2.735514	-0.564919
C	1.586695	-2.150177	-0.979361

C	1.336212	-1.342692	-2.121296
H	-0.545795	-1.060495	-3.330003
H	-1.689203	-2.664496	-1.521295
H	0.225497	-3.421768	0.275956
H	2.564543	-2.316895	-0.526400
H	2.085372	-0.780237	-2.685207



Np	0.567455	-0.021572	-0.571829
C	-0.797154	-0.213235	-3.006030
C	-0.112856	1.036176	-3.037251
C	0.173941	-1.251089	-3.048573
C	1.287789	0.768722	-3.126512
C	1.466432	-0.642557	-3.121097
C	-1.840066	0.101246	-0.013001
C	0.244669	-2.670233	0.014950
C	0.270460	-2.027218	1.290391
C	1.592272	-1.555045	1.512041
C	2.385531	-1.891293	0.372733
C	1.556854	-2.601586	-0.540805
C	0.315625	2.420984	0.700122
C	1.136395	1.624922	1.548814
C	2.392741	1.436190	0.894706
C	2.335625	2.096304	-0.364003
C	1.049783	2.708925	-0.484843
C	-2.602776	0.109181	1.249768
C	-3.023647	-1.100308	1.874891
C	-2.972312	1.310995	1.913083
C	-3.723212	-1.104339	3.088018
C	-3.671003	1.301812	3.129169
C	-4.055686	0.097146	3.754933
C	-4.797092	0.083536	5.073275
H	-5.060504	1.104298	5.401150
H	-5.733251	-0.503339	5.009234
H	-4.189043	-0.375765	5.876925
H	-3.932833	2.259386	3.600675

H	-2.730196	2.277633	1.451412
H	-4.027477	-2.066028	3.525100
H	-2.817736	-2.057349	1.375848
H	-2.039194	1.001396	-0.634495
H	-2.076525	-0.800212	-0.620836
H	-1.881503	-0.347318	-2.966629
H	-0.583056	2.023636	-3.044519
H	2.082327	1.514580	-3.212851
H	2.423120	-1.169441	-3.192907
H	-0.033247	-2.324035	-3.059041
H	-0.623042	-3.155184	-0.443304
H	1.875911	-3.028730	-1.494226
H	3.451369	-1.678189	0.242798
H	-0.566839	-1.924760	1.985076
H	1.947200	-1.056616	2.416593
H	3.261057	0.909627	1.298491
H	3.153124	2.158099	-1.088722
H	0.707033	3.323237	-1.321630
H	-0.694428	2.760017	0.936611
H	0.852793	1.257677	2.538654

[Np^{IV}Cp₃(*n*-C₄H₉)]

Np	-0.475822	0.022237	-0.126956
C	0.218600	2.319591	1.249067
C	-0.834328	1.739237	2.009439
C	-2.038305	1.832668	1.244165
C	-1.727180	2.477190	0.014363
C	-0.328980	2.766492	0.011039
H	1.258498	2.425382	1.566321
H	-0.744153	1.324576	3.016538
H	-3.032526	1.505304	1.562563
H	-2.437995	2.727938	-0.777211
H	0.223424	3.277996	-0.782152
C	0.430840	0.092359	-2.750114
C	-0.630914	1.039061	-2.716242
C	-1.852852	0.326503	-2.516953

C	-1.544608	-1.060496	-2.437251
C	-0.129870	-1.205632	-2.568654
H	1.490322	0.318131	-2.898830
H	-0.532388	2.118702	-2.852493
H	-2.854026	0.765238	-2.466088
H	-2.266706	-1.872816	-2.319957
H	0.426678	-2.147202	-2.566747
C	0.180346	-2.337815	1.168400
C	-0.845961	-2.699136	0.251858
C	-2.062490	-2.086684	0.684425
C	-1.785866	-1.359575	1.876363
C	-0.395696	-1.502028	2.168009
H	1.223784	-2.659749	1.123954
H	-0.730488	-3.358177	-0.612224
H	-3.042891	-2.192246	0.209437
H	-2.516150	-0.812254	2.477462
H	0.134515	-1.071430	3.022102
C	1.948337	-0.008566	0.099916
H	2.214887	0.889205	-0.508865
C	2.823080	-0.057559	1.358807
H	2.187815	-0.884366	-0.550326
H	2.585694	0.797933	2.026013
H	2.578387	-0.960854	1.956210
C	4.346714	-0.054385	1.099870
H	4.601414	-0.916049	0.449452
H	4.609133	0.849986	0.513836
C	5.192790	-0.105213	2.380535
H	4.983776	0.761615	3.036053
H	4.979876	-1.018930	2.967644
H	6.275616	-0.099213	2.158329

[Np^{IV}(MeCp)Cl₃(THF)₂]

Np	-0.158210	-0.395265	0.113450
Cl	0.837596	-1.090722	-2.212176
Cl	-0.417661	1.107228	2.261858
Cl	0.975574	-2.390879	1.297197

O	2.140597	0.680281	0.259927
O	-0.369718	1.842266	-1.150591
C	2.978446	0.525233	1.446712
C	4.404344	0.562177	0.903240
C	4.289874	1.603130	-0.226318
C	2.897824	1.320626	-0.810751
C	-0.478826	1.980307	-2.604350
C	-0.771028	3.090623	-0.499241
C	-2.118804	-2.274302	0.086281
C	-2.512783	-1.382380	1.134275
C	-2.233582	-1.595830	-1.162288
C	-2.691329	-0.271315	-0.895154
C	-2.860201	-0.139440	0.513960
C	-1.211058	3.304499	-2.831443
C	-0.770245	4.136793	-1.614252
C	-2.617471	-1.708790	2.599532
H	-3.665900	-1.941976	2.869713
H	-1.999221	-2.583730	2.863031
H	-2.286083	-0.858860	3.221234
H	-1.779945	-3.303963	0.231420
H	-2.000781	-2.014518	-2.143983
H	-3.204157	0.752385	1.044958
H	-2.897942	0.499651	-1.643797
H	2.765547	1.359284	2.143962
H	2.692588	-0.427755	1.921330
H	5.142463	0.835658	1.676795
H	4.680200	-0.428356	0.497216
H	4.338924	2.626934	0.188971
H	5.082946	1.508558	-0.987585
H	2.911659	0.616202	-1.662286
H	2.357429	2.234170	-1.116406
H	0.545420	1.988445	-3.021841
H	-0.995566	1.090781	-2.999221
H	-0.945917	3.762705	-3.799805
H	-2.306774	3.153377	-2.817170
H	-1.779009	2.949245	-0.064200

H	-0.066679	3.280344	0.325990
H	-1.446133	4.980749	-1.393248
H	0.245954	4.546521	-1.768627

Table S1 Calculated ρ_0 values (a_0^{-3}) of various functionals

(a) Eu system

Eu complex	[Eu ^{II} Cp* ₂]	[Eu ^{III} Cp ₃ (THF)]	[Eu ^{III} CpCl ₂ (THF) ₃]	[Eu ^{III} (acac) ₃ (H ₂ O) ₂]	[Eu ^{III} Cl ₃ (phen) ₂]
$\delta_{\text{Eu}} / \text{mms}^{-1}$	-12.7	-1.77	0.06	0.36	0.57
BP86	462665.761	462674.919	462679.088	462683.225	462684.269
PBE	462597.555	462606.715	462610.797	462614.791	462615.908
TPSS	462421.840	462431.771	462435.898	462440.273	462441.070
TPSSh	462382.054	462394.200	462399.141	462404.269	462404.881
B3LYP	462413.186	462426.701	462432.949	462438.041	462438.652
PBE0	462454.055	462469.584	462476.315	462479.985	462480.807
BHandHLYP	462330.965	462356.088	462359.230	462360.216	462361.241
B2PLYP	462313.149	462338.763	462341.734	462342.645	462343.695
M06-2X	462467.630	462491.549	462494.790	462495.790	462496.698

(b) Np system

Np complex	[Np ^{III} (COT) ₂] ⁺	[Np ^{IV} (COT) ₂]	[Np ^{IV} Cp ₄]	[Np ^{IV} Cp ₃ (<i>n</i> -C ₄ H ₉)]	[Np ^{IV} (MeCp)Cl ₃ (THF) ₂]
$\delta_{\text{Np}} / \text{mms}^{-1}$	39.2	19.4	7.1	2.7	-3.1
BP86	13197253.055	13197306.306	13197296.747	13197358.411	13197374.832
PBE	13196016.275	13196069.773	13196060.710	13196121.644	13196137.200
TPSS	13184514.850	13184571.421	13184565.190	13184626.665	13184642.727
TPSSh	13182645.248	13182710.809	13182708.062	13182770.869	13182787.835
B3LYP	13187769.138	13187842.138	13187839.345	13187903.265	13187924.087
PBE0	13188458.596	13188536.560	13188536.879	13188600.054	13188617.403
BHandHLYP	13181423.004	13181528.758	13181536.313	13181594.780	13181613.754
B2PLYP	13180491.943	13180572.760	13180606.834	13180664.857	13180686.967
M06-2X	13190069.581	13190163.902	13190171.480	13190233.729	13190250.559

Table S2 R^2 and RMSD values obtained by linear regression to five Eu and five Np benchmark complexes

Functional	Hartree-Fock exchange admixture (%)	R^2 value		RMSD / mms ⁻¹	
		Eu	Np	Eu	Np
BP86	0	0.872	0.816	1.813	7.206
PBE	0	0.876	0.821	1.786	7.102
TPSS	0	0.884	0.842	1.726	6.678
TPSSh	10	0.894	0.873	1.649	5.971
B3LYP	20	0.900	0.883	1.600	5.745
PBE0	25	0.937	0.903	1.274	5.242
BHandHLYP	50	0.999	0.944	0.159	3.990
B2PLYP	53	0.999	0.962	0.185	3.274
M062X	54	0.999	0.935	0.132	4.269

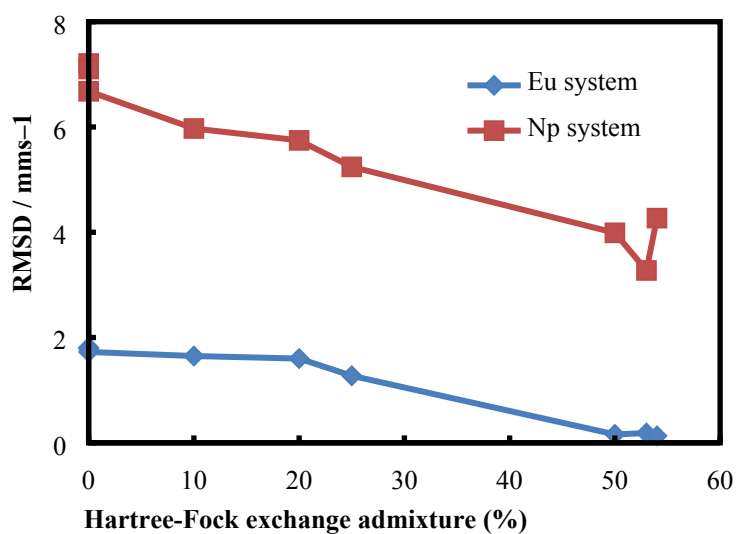


Figure S1 RMSD vs Hartree-Fock exchange admixture plot for Eu and Np system.

Table S3 Mulliken's population analyses for ten Eu and ten Np complexes
by BP86, B3LYP and B2PLYP methods

(a) Eu complexes

Eu complexes	Eu atomic charge / electrons			Eu spin population / electrons		
	BP86	B3LYP	B2PLYP	BP86	B3LYP	B2PLYP
[Eu ^{II} Cp* ₂ (THF)]	1.106	1.188	1.182	7.080	7.060	7.083
[Eu ^{II} Cp* ₂]	1.027	1.074	1.076	7.086	7.066	7.087
[Eu ^{III} Cp ₃ (THF)]	1.087	1.271	1.367	6.648	6.534	6.173
[Eu ^{III} CpCl ₂ (THF) ₃]	1.053	1.283	1.444	6.470	6.302	6.103
[Eu ^{III} Cp(NCS) ₂ (THF) ₃]	1.588	1.875	2.031	6.478	6.259	6.099
[Eu ^{III} (acac) ₃ (H ₂ O) ₂]	1.447	1.720	1.915	6.278	6.090	6.048
[Eu ^{III} (pta) ₃ (H ₂ O) ₂]	1.462	1.748	1.940	6.273	6.090	6.046
[Eu ^{III} (NO ₃) ₃ (phen) ₂]	1.134	1.433	1.591	6.337	6.118	6.069
[Eu ^{III} Cl ₃ (phen) ₂]	0.990	1.181	1.333	6.322	6.136	6.078
[Eu ^{III} (NCS) ₃ (bipy) ₃]	1.795	2.074	2.144	6.428	6.160	6.065

(b) Np complexes

Np complexes	Np atomic charge / electrons			Np spin population / electrons		
	BP86	B3LYP	B2PLYP	BP86	B3LYP	B2PLYP
[Np ^{III} (COT) ₂] ⁻	1.472	1.592	1.641	4.117	4.053	4.079
[Np ^{IV} (COT) ₂]	1.316	1.464	1.519	3.457	3.465	3.592
[Np ^{IV} Cp ₃ Cl]	0.939	1.183	1.302	3.408	3.326	3.276
[Np ^{IV} Cp ₃ {OCH(CH ₃) ₂ }]	1.305	1.591	1.724	3.385	3.282	3.229
[Np ^{IV} Cp ₃ {OC(CH ₃) ₃ }]	1.337	1.631	1.757	3.387	3.281	3.228
[Np ^{IV} Cp ₃ {OCH(CF ₃) ₂ }]	1.269	1.547	1.679	3.389	3.297	3.244
[Np ^{IV} Cp ₄]	1.032	1.296	1.392	3.545	3.445	3.354
[Np ^{IV} Cp ₃ (<i>p</i> -CH ₃ C ₆ H ₄ CH ₂)]	1.047	1.288	1.390	3.440	3.328	3.277
[Np ^{IV} Cp ₃ (<i>n</i> -C ₄ H ₉)]	1.173	1.418	1.530	3.389	3.306	3.271
[Np ^{IV} (MeCp)Cl ₃ (THF) ₂]	1.165	1.435	1.618	3.264	3.166	3.129

Table S4 Löwdin's population analyses for ten Eu and ten Np complexes
by BP86, B3LYP and B2PLYP methods

(a) Eu complexes

Eu complexes	Eu atomic charge / electrons			Eu spin population / electrons		
	BP86	B3LYP	B2PLYP	BP86	B3LYP	B2PLYP
[Eu ^{II} Cp* ₂ (THF)]	-0.268	-0.233	-0.191	7.020	7.036	7.059
[Eu ^{II} Cp* ₂]	-0.561	-0.521	-0.475	7.008	7.028	7.054
[Eu ^{III} Cp ₃ (THF)]	-0.896	-0.798	-0.612	6.556	6.474	6.134
[Eu ^{III} CpCl ₂ (THF) ₃]	-1.624	-1.488	-1.315	6.413	6.269	6.080
[Eu ^{III} Cp(NCS) ₂ (THF) ₃]	-1.034	-0.884	-0.716	6.419	6.230	6.070
[Eu ^{III} (acac) ₃ (H ₂ O) ₂]	-0.875	-0.700	-0.529	6.250	6.078	6.039
[Eu ^{III} (pta) ₃ (H ₂ O) ₂]	-0.992	-0.815	-0.641	6.241	6.077	6.038
[Eu ^{III} (NO ₃) ₃ (phen) ₂]	-1.216	-1.027	-0.857	6.297	6.101	6.050
[Eu ^{III} Cl ₃ (phen) ₂]	-1.778	-1.648	-1.521	6.271	6.112	6.060
[Eu ^{III} (NCS) ₃ (bipy) ₃]	-1.177	-1.008	-0.862	6.370	6.138	6.045

(b) Np complexes

Np complexes	Np atomic charge / electrons			Np spin population / electrons		
	BP86	B3LYP	B2PLYP	BP86	B3LYP	B2PLYP
[Np ^{III} (COT) ₂] ⁻	-0.516	-0.416	-0.346	4.040	4.018	4.043
[Np ^{IV} (COT) ₂]	-0.416	-0.326	-0.272	3.364	3.394	3.607
[Np ^{IV} Cp ₃ Cl]	-0.816	-0.690	-0.560	3.296	3.252	3.200
[Np ^{IV} Cp ₃ {OCH(CH ₃) ₂ }]	-0.520	-0.378	-0.230	3.262	3.211	3.163
[Np ^{IV} Cp ₃ {OC(CH ₃) ₃ }]	-0.528	-0.385	-0.237	3.263	3.211	3.162
[Np ^{IV} Cp ₃ {OCH(CF ₃) ₂ }]	-0.504	-0.365	-0.218	3.270	3.226	3.176
[Np ^{IV} Cp ₄]	-0.532	-0.400	-0.262	3.414	3.366	3.276
[Np ^{IV} Cp ₃ (<i>p</i> -CH ₃ C ₆ H ₄ CH ₂)]	-0.462	-0.338	-0.217	3.329	3.253	3.197
[Np ^{IV} Cp ₃ (<i>n</i> -C ₄ H ₉)]	-0.472	-0.352	-0.234	3.271	3.228	3.188
[Np ^{IV} (MeCp)Cl ₃ (THF) ₂]	-1.470	-1.312	-1.148	3.188	3.121	3.087

Table S5 Natural population analyses for ten Eu and ten Np complexes
by BP86 and B2PLYP methods

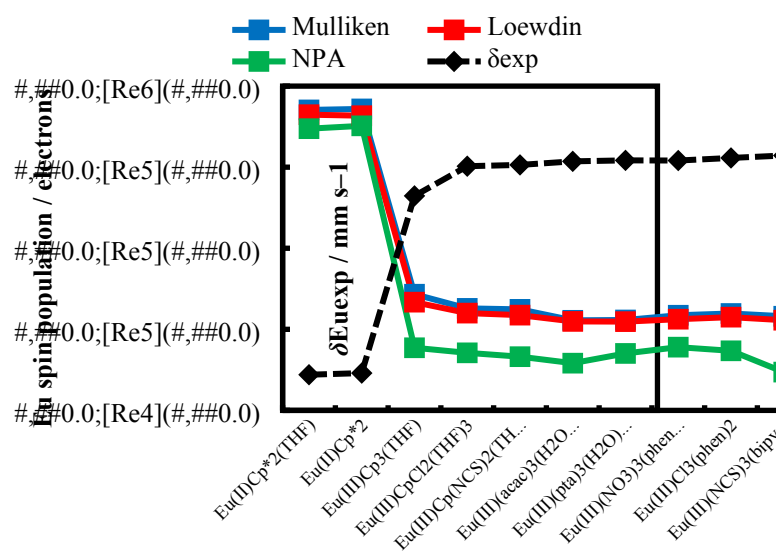
(a) Eu complexes

Eu complexes	Eu atomic charge		Eu spin population	
	BP86	B2PLYP	BP86	B2PLYP
[Eu ^{II} Cp* ₂ (THF)]	1.388	1.438	6.930	6.990
[Eu ^{II} Cp* ₂]	1.514	1.564	6.960	7.004
[Eu ^{III} Cp ₃ (THF)]	0.991	1.355	6.431	5.909
[Eu ^{III} CpCl ₂ (THF) ₃]	1.124	1.507	6.278	5.884
[Eu ^{III} Cp(NCS) ₂ (THF) ₃]	1.492	1.927	6.277	5.865
[Eu ^{III} (acac) ₃ (H ₂ O) ₂]	1.501	1.829	6.041	5.833
[Eu ^{III} (pta) ₃ (H ₂ O) ₂]	1.701	2.088	6.088	5.881
[Eu ^{III} (NO ₃) ₃ (phen) ₂]	1.060	1.312	6.031	5.912
[Eu ^{III} Cl ₃ (phen) ₂]	1.109	1.545	6.145	5.894
[Eu ^{III} (NCS) ₃ (bipy) ₃]	1.452	1.857	6.167	5.789

(b) Np complexes

Np complexes	Np atomic charge		Np spin population	
	BP86	B2PLYP	BP86	B2PLYP
[Np ^{III} (COT) ₂] ⁻	0.202	0.640	4.087	4.000
[Np ^{IV} (COT) ₂]	0.218	0.566	3.383	3.616
[Np ^{IV} Cp ₃ Cl]	0.035	0.523	3.298	3.154
[Np ^{IV} Cp ₃ {OCH(CH ₃) ₂ }]	0.464	0.962	3.256	3.138
[Np ^{IV} Cp ₃ {OC(CH ₃) ₃ }]	0.491	0.991	3.254	3.131
[Np ^{IV} Cp ₃ {OCH(CF ₃) ₂ }]	0.445	0.926	3.265	3.151
[Np ^{IV} Cp ₄]	-0.065	0.443	3.404	3.193
[Np ^{IV} Cp ₃ (<i>p</i> -CH ₃ C ₆ H ₄ CH ₂)]	0.337	0.779	3.337	3.180
[Np ^{IV} Cp ₃ (<i>n</i> -C ₄ H ₉)]	0.351	0.798	3.279	3.171
[Np ^{IV} (MeCp)Cl ₃ (THF) ₂]	0.376	0.928	3.149	3.053

(a) Eu system



(b) Np system

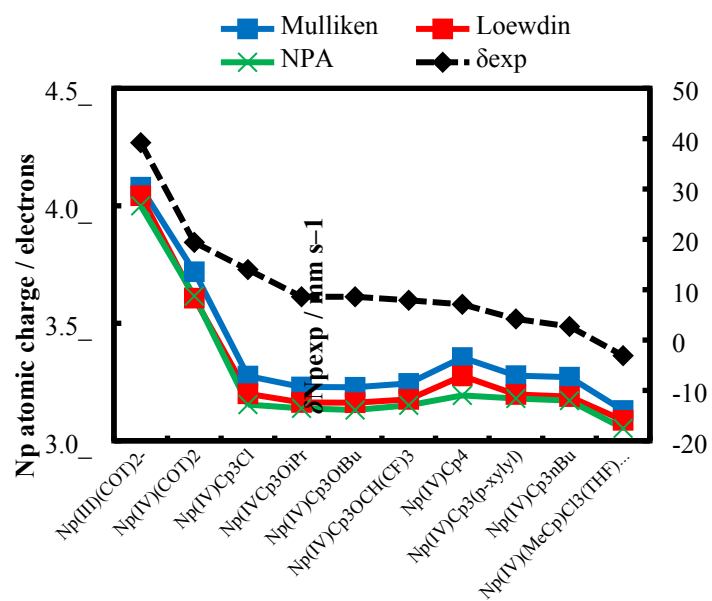


Figure S2 Spin population obtained by Mulliken, Löwdin and natural population at ZORA-B2PLYP/SARC level.