Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information available for

Interaction-determined extraction capacity between rare earth ions and extractants: taking lanthanum and lutetium as models through theoretical calculations

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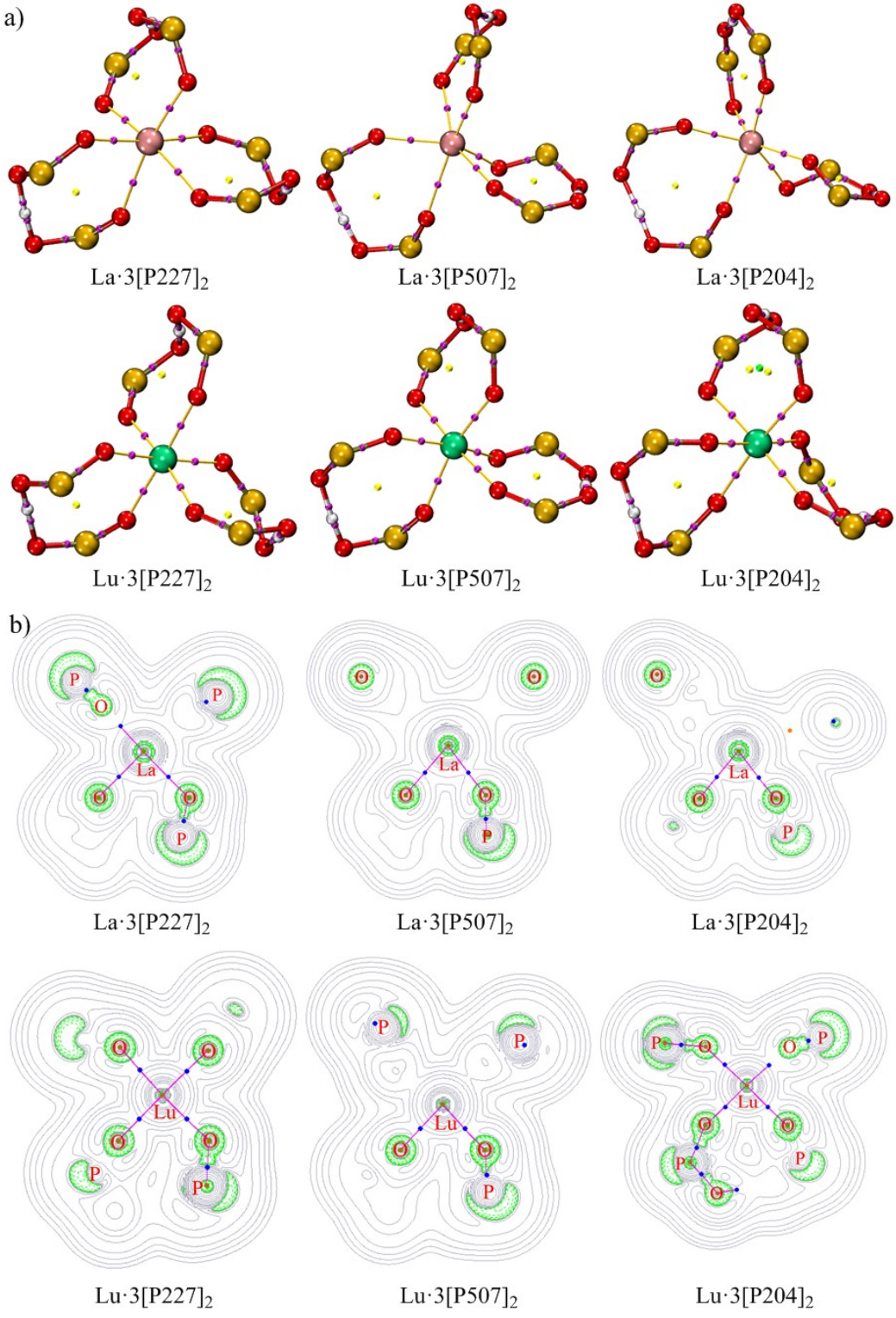
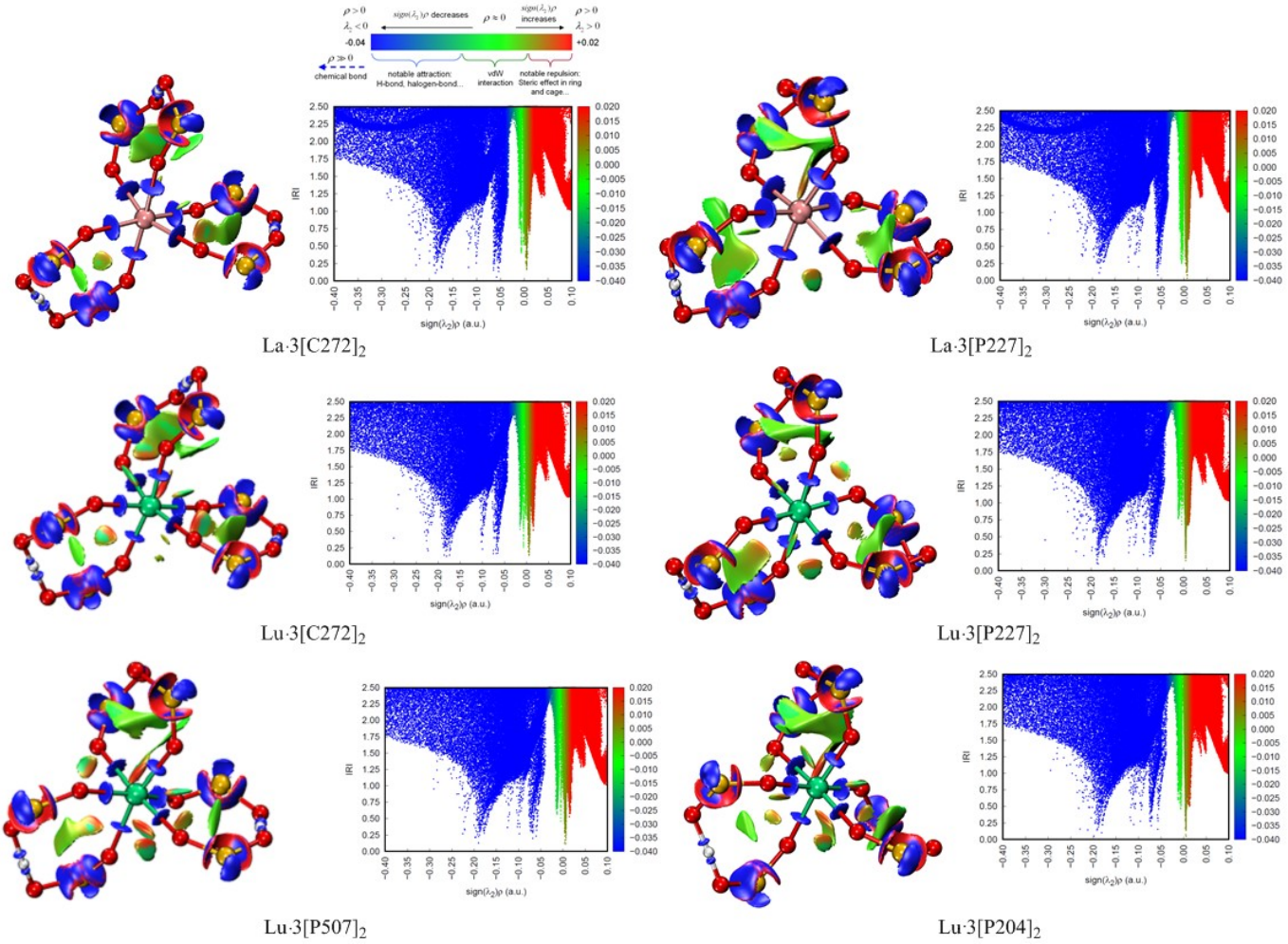
1. Fig. S1. a) The atoms in molecules graphs of the simplified structures of La·3[C272]$_2$ and Lu·3[C272]$_2$. Purple, yellow and green dots denote bond critical point (BCP), ring critical point (RCP) and cage ring critical point (CCP), respectively. b) The Laplacian distribution sectional diagram of one of the octatomic rings. Green dashed lines represent areas of charge concentration ($\nabla^2\rho(\mathbf{r}) < 0$) while solid gray lines show areas of charge depletion ($\nabla^2\rho(\mathbf{r}) > 0$). The solid magenta lines connecting the atomic nuclei are the bond paths.



2. Fig. S2. Isosurface map of IRI = 1.2 and the scatter map between IRI and sign(λ_2)ρ of simplified structures.

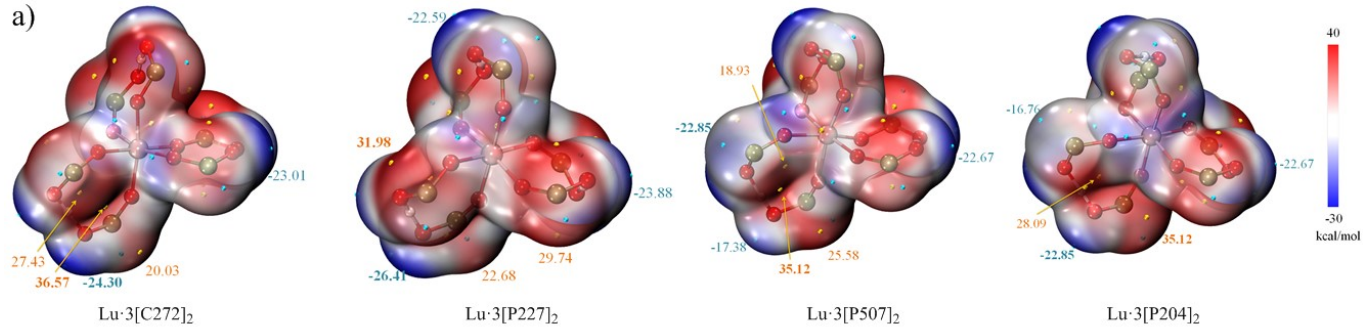


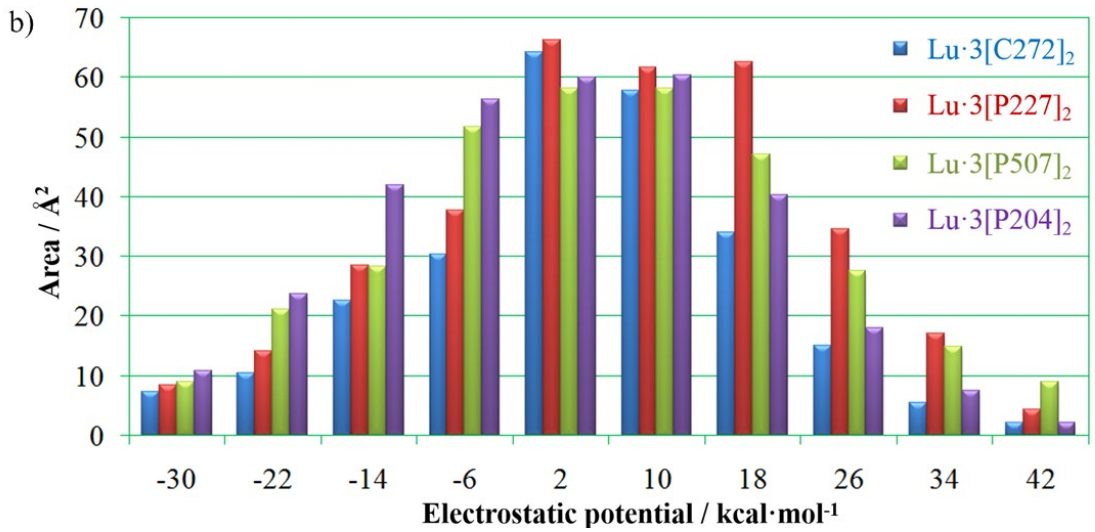
La·3[C272]$_2$ La·3[P227]$_2$

Lu·3[C272]$_2$ Lu·3[P227]$_2$

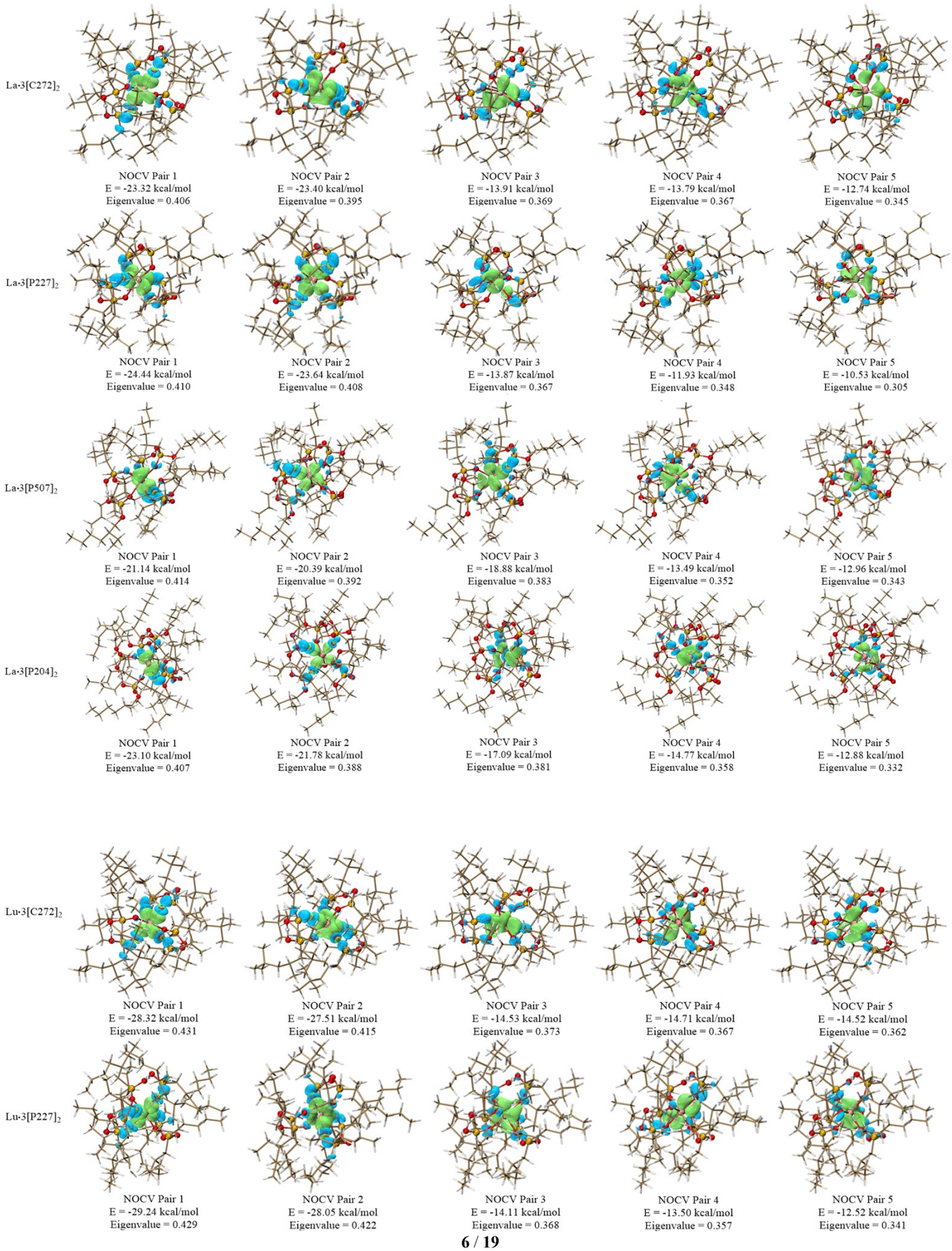
Lu·3[P507]$_2$ Lu·3[P204]$_2$

3. Fig. S3. a) ESP mapped van der Waals surface (isovalue = ±0.001) of simplified structures. The orange and cyan spheres are represented positive and negative, respectively. The unit is in kcal/mol. b) Area percent in each ESP range on the vdW surface of Lu-complexed.

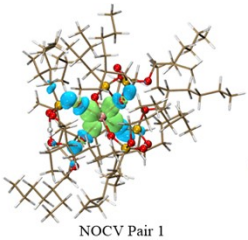




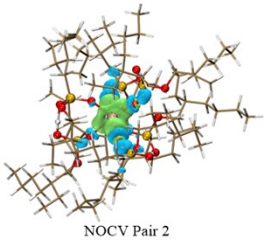
4. Fig. S4. The five major NOCV pairs of complexed structures.



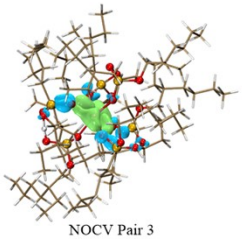
Lu-3[P507]$_2$



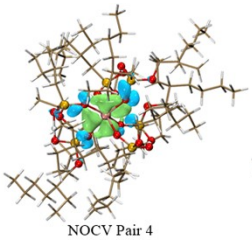
NOCV Pair 1
E = -29.33 kcal/mol
Eigenvalue = 0.434



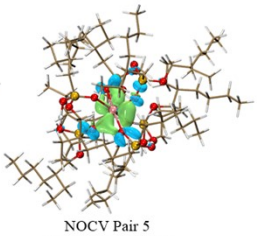
NOCV Pair 2
E = -28.28 kcal/mol
Eigenvalue = 0.422



NOCV Pair 3
E = -14.79 kcal/mol
Eigenvalue = 0.370

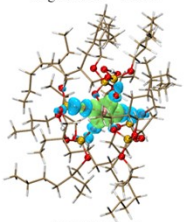


NOCV Pair 4
E = -13.88 kcal/mol
Eigenvalue = 0.349

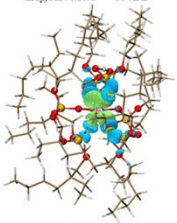


NOCV Pair 5
E = -12.81 kcal/mol
Eigenvalue = 0.330

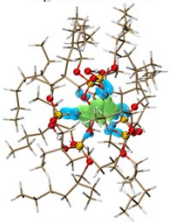
Lu-3[P204]$_2$



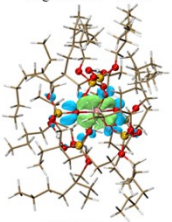
NOCV Pair 1
E = -30.44 kcal/mol
Eigenvalue = 0.431



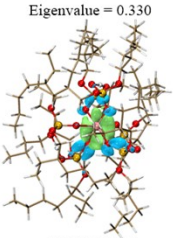
NOCV Pair 2
E = -28.16 kcal/mol
Eigenvalue = 0.420



NOCV Pair 3
E = -14.90 kcal/mol
Eigenvalue = 0.370



NOCV Pair 4
E = -14.17 kcal/mol
Eigenvalue = 0.357



NOCV Pair 5
E = -12.42 kcal/mol
Eigenvalue = 0.328

5. Table S1. The bond length and Mayer bond order (MBO) between Ln-O in four extractant complexes at the level of BP86/ECP28MWB.

			L_{Ln-O} / Å						
			La-O_1	La-O_2	La-O_3	La-O_4	La-O_5	La-O_6	La-O_{ave}
La·3(HA_2)	A = C272	Bond length	2.437	2.343	2.421	2.327	2.375	2.428	2.389
		MBO	0.412	0.529	0.433	0.478	0.425	0.486	0.461
	A = P227	Bond length	2.418	2.425	2.411	2.401	2.404	2.369	2.405
		MBO	0.509	0.423	0.462	0.455	0.487	0.430	0.461
	A = P507	Bond length	2.390	2.514	2.422	2.424	2.428	2.365	2.424
		MBO	0.535	0.387	0.428	0.533	0.500	0.452	0.473
	A = P204	Bond length	2.390	2.395	2.366	2.491	2.590	2.495	2.455
		MBO	0.522	0.422	0.524	0.423	0.430	0.521	0.474
			Lu-O_1	Lu-O_2	Lu-O_3	Lu-O_4	Lu-O_5	Lu-O_6	Lu-O_{ave}
Lu·3(HA_2)	A = C272	Bond length	2.213	2.154	2.187	2.232	2.191	2.193	2.195
		MBO	0.476	0.585	0.558	0.462	0.484	0.530	0.516
	A = P227	Bond length	2.235	2.174	2.208	2.189	2.176	2.200	2.197
		MBO	0.481	0.554	0.488	0.556	0.559	0.492	0.522
	A = P507	Bond length	2.164	2.222	2.175	2.236	2.152	2.249	2.200
		MBO	0.573	0.476	0.509	0.531	0.573	0.476	0.523
	A = P204	Bond length	2.161	2.176	2.169	2.261	2.163	2.161	2.182
		MBO	0.558	0.486	0.519	0.539	0.561	0.451	0.519

6. Table S2. Topological properties of the complex structures between La/Lu and six coordination oxygen atoms, including density of all electrons ρ(**r**), Laplacian of electron density ∇2ρ(**r**).

		$La-O_1$	$La-O_2$	$La-O_3$	$La-O_4$	$La-O_5$	$La-O_6$	Average
$La·3[C272]_2$	$\rho(r_n)$	0.0514	0.0633	0.0541	0.0651	0.0582	0.0554	0.0579
	$\nabla^2\rho(r_n)$	0.202	0.250	0.206	0.259	0.235	0.197	0.225
$La·3[P227]_2$	$\rho(r_n)$	0.0562	0.0526	0.0605	0.0573	0.0584	0.0577	0.0571
	$\nabla^2\rho(r_n)$	0.204	0.207	0.232	0.212	0.205	0.214	0.212
$La·3[P507]_2$	$\rho(r_n)$	0.0587	0.0430	0.0603	0.0537	0.0552	0.0533	0.0540
	$\nabla^2\rho(r_n)$	0.215	0.164	0.235	0.202	0.200	0.205	0.204
$La·3[P204]_2$	$\rho(r_n)$	0.0629	0.0542	0.0545	0.0591	0.0571	0.0600	0.0580
	$\nabla^2\rho(r_n)$	0.232	0.215	0.201	0.237	0.221	0.211	0.220
		$Lu-O_1$	$Lu-O_2$	$Lu-O_3$	$Lu-O_4$	$Lu-O_5$	$Lu-O_6$	Average
$Lu·3[C272]_2$	$\rho(r_n)$	0.0650	0.0752	0.0698	0.0674	0.0684	0.0652	0.0685
	$\nabla^2\rho(r_n)$	0.312	0.372	0.329	0.333	0.340	0.295	0.330
$Lu·3[P227]_2$	$\rho(r_n)$	0.0619	0.0721	0.0665	0.0709	0.0732	0.0680	0.0688
	$\nabla^2\rho(r_n)$	0.295	0.351	0.317	0.332	0.348	0.324	0.328
$Lu·3[P507]_2$	$\rho(r_n)$	0.0742	0.0693	0.0734	0.0686	0.0758	0.0605	0.0703
	$\nabla^2\rho(r_n)$	0.348	0.345	0.351	0.334	0.360	0.283	0.337
$Lu·3[P204]_2$	$\rho(r_n)$	0.0747	0.0717	0.0751	0.0747	0.0730	0.0576	0.0711
	$\nabla^2\rho(r_n)$	0.360	0.349	0.362	0.365	0.340	0.261	0.340

7. Table S3. The values of ESP nearby three types atoms of simplified structures.

		O_1	O_2	O_3	O_4	O_5	O_6	Average
La·3[C272]$_2$	Coordination oxygen	43.36	43.36	40.64	35.57	39.76	43.36	41.01
	phosphorus atom	38.85	34.88	35.53	33.87	41.50	27.72	35.39
	Hydrogen bonding oxygen	-18.26	-25.52	-17.63	-26.42	-16.58	-21.90	-21.05
La·3[P227]$_2$	Coordination oxygen	31.79	27.06	31.79	26.37	31.79	27.09	29.32
	phosphorus atom	21.59	23.60	32.23	27.65	31.59	32.80	28.24
	Hydrogen bonding oxygen	-23.73	-18.86	-17.89	-23.15	-19.99	-15.25	-19.81
La·3[P507]$_2$	Coordination oxygen	60.13	63.89	62.64	63.68	58.90	63.60	62.14
	phosphorus atom	27.22	41.69	39.99	56.43	34.75	32.42	38.75
	Hydrogen bonding oxygen	-24.47	-20.30	-14.52	-22.06	-23.39	-16.97	-20.29
La·3[P204]$_2$	Coordination oxygen	55.49	63.09	59.24	64.18	73.58	67.33	63.82
	phosphorus atom	27.01	45.78	38.27	57.72	40.89	42.22	41.98
	Hydrogen bonding oxygen	-25.70	-17.42	-14.77	-26.83	-16.86	-21.43	-20.50
Lu·3[C272]$_2$	Coordination oxygen	28.74	29.34	26.65	40.96	34.30	19.41	29.90
	phosphorus atom	36.71	28.28	26.79	42.20	43.92	25.07	33.83
	Hydrogen bonding oxygen	-17.79	-24.30	-23.01	-17.11	-16.22	-20.73	-19.86
Lu·3[P227]$_2$	Coordination oxygen	24.94	29.74	27.56	22.69	19.26	24.66	24.81
	phosphorus atom	31.98	22.68	33.99	27.18	26.46	31.77	29.01
	Hydrogen bonding oxygen	-16.52	-26.41	-16.21	-23.88	-22.59	-18.06	-20.61
Lu·3[P507]$_2$	Coordination oxygen	18.93	28.09	29.35	25.92	33.42	31.00	27.79
	phosphorus atom	25.58	35.12	34.46	32.28	34.39	34.75	32.76
	Hydrogen bonding oxygen	-22.85	-17.38	-17.86	-22.67	-23.22	-13.23	-19.54
Lu·3[P204]$_2$	Coordination oxygen	23.09	29.72	35.56	21.72	17.83	24.91	25.47
	phosphorus atom	27.11	35.53	40.11	25.06	22.79	31.88	30.41
	Hydrogen bonding oxygen	-23.80	-16.76	-16.50	-22.18	-25.27	-15.23	-19.96

8. Table S4. The Gibbs free energy of complexation structures between Ln (Ln = La/Lu) and four organophosphoric extractants in three forms (Ln^{3+}, $(Ln\cdot 8H_2O)^{3+}$ and $(Ln\cdot 9H_2O)^{3+}$)).

	ΔG_{B3LYP} / kcal·mol^{-1}					
	La^{3+}	$(La\cdot 8H_2O)^{3+}$	$(La\cdot 9H_2O)^{3+}$	Lu^{3+}	$(Lu\cdot 8H_2O)^{3+}$	$(Lu\cdot 9H_2O)^{3+}$
A = C272	-1.27	-36.12	-8.83	-112.26	-49.53	-31.99
A = P227	-20.86	-55.72	-28.43	-143.28	-80.45	-62.92
A = P507	-29.79	-65.64	-37.35	-143.14	-80.31	-62.78
A = P204	-56.23	-91.09	-63.80	-178.51	-115.68	-98.15
	ΔG_{BP86} / kcal·mol^{-1}					
	La^{3+}	$(La\cdot 8H_2O)^{3+}$	$(La\cdot 9H_2O)^{3+}$	Lu^{3+}	$(Lu\cdot 8H_2O)^{3+}$	$(Lu\cdot 9H_2O)^{3+}$
A = C272	-22.31	-54.79	-30.18	-134.21	-68.96	-52.78
A = P227	-36.57	-69.05	-44.44	-160.57	-95.31	-79.14
A = P507	-56.25	-88.73	-64.13	-168.46	-103.20	-87.03
A = P204	-73.87	-106.35	-81.75	-192.74	-127.48	-111.30

9. Table S5. The contribution of various types of shells of complexes structures.

Contribution of various types of shells to NOCV pair/orbitals								
	$La·3(C272)_2$		$La·3(P227)_2$		$La·3(P507)_2$		$La·3(P204)_2$	
	type	Contribution (%)	type	Contribution (%)	type	Contribution (%)	type	Contribution (%)
pair 1	s	17.49	s	16.17	s	18.99	s	12.29
	p	34.49	p	38.01	p	35.48	p	32.75
	d	47.04	d	45.44	d	42.46	d	51.50
	f	0.87	f	0.30	f	2.95	f	3.20
pair 2	s	11.88	s	15.30	s	20.07	s	16.30
	p	32.83	p	35.03	p	33.48	p	28.96
	d	53.26	d	48.64	d	43.85	d	50.34
	f	1.87	f	0.92	f	2.51	f	4.20
pair 3	s	20.37	s	32.57	s	18.80	s	17.65
	p	40.36	p	33.26	p	32.56	p	35.48
	d	38.03	d	32.42	d	46.90	d	45.79
	f	1.18	f	1.69	f	1.44	f	1.01
pair 4	s	22.39	s	14.89	s	18.17	s	16.88
	p	37.41	p	39.17	p	35.06	p	32.99
	d	38.78	d	44.75	d	45.57	d	48.88
	f	1.39	f	1.15	f	1.11	f	0.98
pair 5	s	20.50	s	28.06	s	16.91	s	22.59
	p	36.57	p	38.53	p	38.18	p	33.17
	d	41.42	d	29.04	d	43.16	d	43.05
	f	1.40	f	4.26	f	1.59	f	0.94

Contribution of various types of shells to NOCV pair/orbitals								
	$Lu·3(C272)_2$		$Lu·3(P227)_2$		$Lu·3(P507)_2$		$Lu·3(P204)_2$	
	type	Contribution (%)	type	Contribution (%)	type	Contribution (%)	type	Contribution (%)
pair 1	s	13.30	s	12.51	s	10.97	s	9.19
	p	29.96	p	27.50	p	30.11	p	25.34
	d	56.30	d	59.59	d	58.51	d	65.03
	f	0.15	f	0.02	f	0.17	f	0.02
pair 2	s	10.11	s	11.89	s	11.38	s	11.20
	p	26.95	p	28.75	p	27.53	p	26.26
	d	62.38	d	58.94	d	60.50	d	61.98
	f	0.13	f	0.06	f	0.23	f	0.17
	s	22.79	s	18.92	s	17.97	s	20.53

pair 3	p	45.83	p	44.61	p	43.90	p	41.12
	d	31.29	d	36.44	d	37.99	d	38.28
	f	0.06	f	0.01	f	0.10	f	0.04
pair 4	s	20.02	s	19.25	s	17.38	s	25.31
	p	44.30	p	44.36	p	40.82	p	36.96
	d	35.56	d	36.33	d	41.71	d	37.69
	f	0.09	f	0.02	f	0.05	f	0.01
pair 5	s	25.62	s	23.55	s	18.25	s	20.13
	p	40.20	p	41.10	p	45.86	p	41.00
	d	34.08	d	35.32	d	35.71	d	38.80
	f	0.06	f	0.01	f	0.14	f	0.03

10. Table S6. The atoms contribution of complexes structures.

La·3(C272)$_2$										
	pair 1 / -22.32		pair 2 / -23.40		pair 3 / -13.91		pair 4 / -13.79		pair 5 / -12.74	
	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)
La		49.67		55.07		42.21		45.92		46.33
Phosphorus atoms	1	0.38	1	1.85	1	2.52	1	3.11	1	0.15
	2	5.24	2	0.34	2	8.31	2	1.34	2	4.97
	3	1.95	3	0.27	3	0.94	3	0.80	3	3.11
	4	2.14	4	2.10	4	0.51	4	1.99	4	2.05
	5	0.16	5	4.10	5	5.07	5	2.80	5	0.81
	6	0.93	6	1.13	6	1.16	6	4.25	6	2.32
Ln coordinate oxygen	1	0.79	1	4.03	1	2.24	1	3.40	1	0.16
	2	8.30	2	0.93	2	6.19	2	2.24	2	4.90
	3	3.37	3	0.38	3	1.82	3	0.26	3	4.65
	4	4.53	4	2.99	4	0.61	4	4.28	4	3.01
	5	0.31	5	7.21	5	5.86	5	4.17	5	0.98
	6	1.46	6	2.54	6	1.33	6	4.23	6	4.50
hydrogen bonding oxygen	1	0.01	1	0.03	1	0.25	1	0.14	1	0.01
	2	0.21	2	0.07	2	1.16	2	0.14	2	0.17
	3	0.10	3	0.02	3	0.14	3	0.02	3	0.34
	4	0.09	4	0.15	4	0.03	4	0.15	4	0.39
	5	0.06	5	0.45	5	0.14	5	0.56	5	0.09
	6	0.08	6	0.02	6	0.12	6	0.32	6	0.11

La·3(P227)$_2$										
	pair 1 / -24.44		pair 2 / -23.64		pair 3 / -13.87		pair 4 / -11.93		pair 5 / -10.53	
	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)

La		47.42		50.69		53.37		46.99		41.65
Phosphorus atoms	1	6.61	1	1.34	1	4.67	1	3.36	1	5.95
	2	0.28	2	2.42	2	0.24	2	2.33	2	1.08
	3	1.75	3	4.21	3	0.54	3	2.59	3	2.48
	4	2.60	4	3.08	4	2.94	4	0.46	4	6.39
	5	1.31	5	2.44	5	2.87	5	1.04	5	2.18
	6	2.81	6	0.30	6	1.91	6	6.44	6	0.23
Ln coordinate oxygen	1	5.35	1	1.42	1	4.19	1	1.85	1	2.22
	2	0.26	2	3.70	2	0.55	2	3.55	2	1.86
	3	0.31	3	7.05	3	0.65	3	4.37	3	2.62
	4	2.85	4	2.31	4	4.00	4	0.18	4	3.92
	5	3.02	5	3.01	5	4.73	5	1.15	5	3.24
	6	4.80	6	0.31	6	1.28	6	7.27	6	0.82
hydrogen bonding oxygen	1	0.11	1	0.08	1	0.38	1	0.05	1	0.32
	2	0.05	2	0.10	2	0.01	2	0.23	2	0.17
	3	0.09	3	0.32	3	0.03	3	0.07	3	0.15
	4	0.16	4	0.12	4	0.07	4	0.04	4	0.45
	5	0.04	5	0.08	5	0.30	5	0.24	5	0.27
	6	0.09	6	0.01	6	0.15	6	0.37	6	0.07

$La{\cdot}3(P507)_2$										
	pair 1 / -21.14		pair 2 / -20.39		pair 3 / -18.88		pair 4 / -13.49		pair 5 / -12.96	
	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)
La		52.20		50.63		53.46		49.76		48.11
Phosphorus	1	1.21	1	5.60	1	1.41	1	3.33	1	0.45
	2	0.50	2	1.31	2	1.80	2	0.62	2	0.72
	3	0.57	3	2.04	3	4.15	3	0.82	3	1.76

	4	0.67	4	0.93	4	2.20	4	1.95	4	3.82
	5	1.63	5	1.62	5	1.26	5	2.73	5	2.97
	6	6.93	6	1.64	6	0.30	6	1.77	6	2.55
Ln coordinate oxygen	1	1.22	1	9.95	1	1.25	1	5.11	1	1.06
	2	0.27	2	2.54	2	1.57	2	1.59	2	1.39
	3	1.38	3	2.36	3	5.58	3	1.16	3	2.53
	4	0.77	4	0.77	4	5.01	4	3.12	4	4.85
	5	3.01	5	1.31	5	2.13	5	4.99	5	4.72
	6	12.32	6	0.31	6	1.07	6	1.96	6	2.95
hydrogen bonding oxygen	1	0.30	1	0.14	1	0.15	1	0.03	1	0.23
	2	0.01	2	0.14	2	0.02	2	0.00	2	0.30
	3	0.02	3	0.09	3	0.12	3	0.07	3	0.57
	4	0.03	4	0.03	4	0.12	4	0.05	4	0.44
	5	0.19	5	0.18	5	0.24	5	0.19	5	0.11
	6	0.42	6	0.03	6	0.07	6	0.13	6	0.67
methyl oxygen	1	0.10	1	0.27	1	0.07	1	0.61	1	0.02
	2	0.05	2	0.43	2	0.21	2	0.08	2	0.03
	3	0.19	3	0.41	3	0.26	3	0.16	3	0.08
	4	0.03	4	0.01	4	0.04	4	0.17	4	0.21
	5	0.32	5	0.10	5	0.07	5	0.54	5	0.23
	6	1.46	6	0.19	6	0.56	6	1.03	6	0.24

$La{\cdot}3(204)_2$										
	pair 1 / -23.10		pair 2 / -21.78		pair 3 / -17.09		pair 4 / -14.77		pair 5 / -12.88	
	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)
La		58.10		59.59		51.40		52.44		48.78

Phosphorus atoms	1	0.46	1	3.51	1	2.86	1	2.68	1	1.03
	2	0.54	2	2.15	2	2.32	2	1.25	2	1.58
	3	2.08	3	1.07	3	2.81	3	0.68	3	3.39
	4	0.91	4	1.00	4	2.15	4	1.04	4	1.56
	5	6.28	5	2.55	5	0.68	5	0.77	5	2.37
	6	0.73	6	1.94	6	0.89	6	0.93	6	1.76
Ln coordinate oxygen	1	1.03	1	6.64	1	3.04	1	5.90	1	1.65
	2	0.72	2	4.80	2	3.58	2	1.85	2	2.68
	3	3.92	3	0.58	3	5.48	3	4.28	3	3.30
	4	2.00	4	2.38	4	1.90	4	2.88	4	2.61
	5	8.11	5	0.42	5	2.45	5	0.72	5	3.32
	6	2.69	6	2.84	6	1.66	6	2.15	6	2.24
hydrogen bonding oxygen	1	0.11	1	0.30	1	0.50	1	0.08	1	0.25
	2	0.05	2	0.18	2	0.03	2	0.10	2	0.59
	3	0.19	3	0.05	3	0.14	3	0.03	3	0.68
	4	0.02	4	0.02	4	0.10	4	0.08	4	0.54
	5	0.72	5	0.04	5	0.21	5	0.03	5	0.32
	6	0.13	6	0.04	6	0.28	6	0.04	6	0.15
methyl oxygen	1	0.01	1	1.00	1	0.36	1	0.18	1	0.09
	2	0.05	2	0.21	2	0.09	2	0.82	2	0.02
	3	0.06	3	0.79	3	0.36	3	0.01	3	0.03
	4	0.02	4	0.02	4	0.09	4	0.35	4	0.05
	5	0.28	5	0.10	5	0.35	5	0.47	5	0.20
	6	0.27	6	0.02	6	0.47	6	0.14	6	0.13
	7	0.01	7	0.31	7	0.31	7	0.31	7	0.06
	8	0.47	8	0.24	8	0.07	8	0.26	8	0.08

	9	0.45	9	0.18	9	1.29	9	1.47	9	0.03
	10	0.34	10	0.02	10	0.04	10	0.07	10	0.25
	11	0.17	11	0.38	11	0.02	11	0.22	11	0.08
	12	0.02	12	0.04	12	0.16	12	0.08	12	0.27

$Lu{\cdot}3(C272)_2$										
	pair 1 / -28.32		pair 2 / -27.51		pair 3 / -14.53		pair 4 / -14.71		pair 5 / -14.52	
	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)
Lu		56.81		62.64		33.91		36.09		39.14
Phosphorus atoms	1	0.31	1	1.55	1	4.40	1	4.08	1	3.23
	2	2.85	2	0.38	2	5.98	2	5.97	2	6.99
	3	1.83	3	0.55	3	1.27	3	1.89	3	3.42
	4	1.93	4	1.03	4	1.17	4	3.45	4	1.61
	5	1.60	5	1.10	5	4.18	5	4.99	5	3.67
	6	0.21	6	1.38	6	6.51	6	1.97	6	3.16
Ln coordinate oxygen	1	0.54	1	5.62	1	3.26	1	1.53	1	1.61
	2	5.87	2	1.40	2	3.63	2	5.05	2	4.09
	3	4.04	3	0.61	3	1.51	3	1.62	3	2.44
	4	4.33	4	2.21	4	1.74	4	2.62	4	2.06
	5	3.07	5	3.44	5	2.49	5	4.37	5	2.68
	6	0.19	6	5.28	6	3.94	6	1.66	6	2.25
hydrogen bonding oxygen	1	0.01	1	0.06	1	0.50	1	0.06	1	0.04
	2	0.15	2	0.02	2	0.78	2	0.33	2	0.54
	3	0.20	3	0.03	3	0.17	3	0.18	3	0.09
	4	0.11	4	0.08	4	0.04	4	0.48	4	0.13
	5	0.09	5	0.04	5	0.58	5	0.70	5	0.15

	6	0.03	6	0.13	6	0.18	6	0.24	6	0.31

$Lu{\cdot}3(P227)_2$										
	pair 1 / -29.24		pair 2 / -28.05		pair 3 / -14.11		pair 4 / -13.50		pair 5 / -12.52	
	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)	No.	Percent (%)
Lu		59.50		59.36		36.78		36.63		35.49
Phosphorus atoms	1	1.33	1	1.07	1	2.71	1	3.51	1	5.89
	2	1.03	2	0.78	2	4.53	2	7.77	2	2.40
	3	0.27	3	1.26	3	3.07	3	0.93	3	4.76
	4	2.20	4	0.85	4	2.66	4	3.05	4	2.79
	5	1.62	5	0.75	5	3.15	5	5.67	5	2.14
	6	0.09	6	2.66	6	5.70	6	2.39	6	4.89
Ln coordinate oxygen	1	4.28	1	1.32	1	1.98	1	1.20	1	3.06
	2	4.48	2	1.14	2	3.47	2	5.38	2	2.25
	3	0.12	3	5.42	3	3.24	3	0.72	3	3.24
	4	4.19	4	2.77	4	2.00	4	2.44	4	3.69
	5	4.65	5	1.68	5	2.76	5	5.83	5	1.61
	6	0.31	6	5.98	6	4.18	6	0.99	6	2.93
hydrogen bonding oxygen	1	0.02	1	0.02	1	0.39	1	0.16	1	0.22
	2	0.06	2	0.05	2	0.28	2	1.18	2	0.18
	3	0.01	3	0.04	3	0.11	3	0.06	3	0.67
	4	0.07	4	0.04	4	0.11	4	0.04	4	0.65
	5	0.04	5	0.03	5	0.40	5	0.49	5	0.17
	6	0.03	6	0.10	6	0.19	6	0.25	6	0.43