

## Electronic supplementary materials for the paper

### **What kind of interactions we may get moving from zwitter to “dritter” ions: C–O···Re(O<sub>4</sub>) and Re–O···Re(O<sub>4</sub>) anion···anion interactions make structural difference between L-histidinium perrhenate and pertechnetate**

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## 1. XRD part

**Table S1. Bond Lengths for 1.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Re1	O11	1.733(4)	N21	C22	1.502(7)
Re1	O12	1.722(4)	N22	C24	1.380(7)
Re1	O13	1.724(4)	N22	C25	1.325(7)
Re1	O14	1.729(4)	N23	C25	1.336(8)
Re2	O21	1.733(4)	N23	C26	1.378(8)
Re2	O22	1.729(5)	N31	C32	1.496(7)
Re2	O23	1.722(4)	N32	C34	1.389(8)
Re2	O24	1.725(4)	N32	C35	1.330(7)
Re3	O31	1.733(4)	N33	C35	1.318(8)
Re3	O32	1.736(4)	N33	C36	1.366(8)
Re3	O33	1.725(4)	C11	C12	1.541(8)
Re3	O34	1.729(4)	C12	C13	1.524(8)
O15	C11	1.260(7)	C13	C14	1.487(8)
O16	C11	1.250(7)	C14	C16	1.369(8)
O25	C21	1.269(7)	C21	C22	1.535(8)
O26	C21	1.248(7)	C22	C23	1.529(8)
O35	C31	1.264(7)	C23	C24	1.483(8)
O36	C31	1.246(7)	C24	C26	1.376(8)
N11	C12	1.499(7)	C31	C32	1.541(7)
N12	C14	1.380(7)	C32	C33	1.530(8)
N12	C15	1.326(7)	C33	C34	1.494(7)
N13	C15	1.325(8)	C34	C36	1.356(8)
N13	C16	1.382(8)			

**Table S2. Bond Angles for 1.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O12	Re1	O11	110.5(2)	C14	C13	C12	114.5(5)
O12	Re1	O13	110.2(2)	N12	C14	C13	123.4(5)
O12	Re1	O14	109.5(2)	C16	C14	N12	106.6(5)
O13	Re1	O11	108.1(2)	C16	C14	C13	130.0(6)
O13	Re1	O14	108.2(2)	N13	C15	N12	108.8(5)
O14	Re1	O11	110.2(2)	C14	C16	N13	106.5(5)
O22	Re2	O21	107.8(2)	O25	C21	C22	115.9(5)
O23	Re2	O21	109.1(2)	O26	C21	O25	127.2(6)
O23	Re2	O22	110.2(2)	O26	C21	C22	116.8(5)
O23	Re2	O24	110.3(2)	N21	C22	C21	109.0(5)
O24	Re2	O21	108.5(2)	N21	C22	C23	111.7(5)
O24	Re2	O22	110.9(2)	C23	C22	C21	112.1(5)
O31	Re3	O32	109.7(2)	C24	C23	C22	112.9(5)
O33	Re3	O31	111.2(2)	N22	C24	C23	123.4(5)
O33	Re3	O32	112.1(2)	C26	C24	N22	106.0(5)
O33	Re3	O34	108.5(2)	C26	C24	C23	130.6(6)
O34	Re3	O31	108.75(19)	N22	C25	N23	108.8(5)
O34	Re3	O32	106.4(2)	C24	C26	N23	107.2(5)
C15	N12	C14	109.1(5)	O35	C31	C32	115.7(5)
C15	N13	C16	109.0(5)	O36	C31	O35	127.6(5)
C25	N22	C24	109.5(5)	O36	C31	C32	116.6(5)
C25	N23	C26	108.4(5)	N31	C32	C31	108.7(5)

C35	N32	C34	108.5(5)	N31	C32	C33	111.7(5)
C35	N33	C36	108.3(5)	C33	C32	C31	112.9(5)
O15	C11	C12	115.8(5)	C34	C33	C32	112.7(5)
O16	C11	O15	127.5(6)	N32	C34	C33	121.9(5)
O16	C11	C12	116.7(5)	C36	C34	N32	105.6(5)
N11	C12	C11	109.1(5)	C36	C34	C33	132.5(6)
N11	C12	C13	111.4(5)	N33	C35	N32	109.3(5)
C13	C12	C11	109.9(5)	C34	C36	N33	108.3(5)

**Table S3.** Hydrogen Bonds for **1**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N11	H11A	O21	0.91	2.08	2.946(7)	158.7
N11	H11B	O31 <sup>1</sup>	0.91	1.92	2.801(6)	163.4
N11	H11C	O32 <sup>2</sup>	0.91	2.11	2.950(7)	153.1
N12	H12	O26 <sup>3</sup>	0.88	1.78	2.651(7)	172.8
N13	H13	O15 <sup>4</sup>	0.88	1.77	2.616(7)	160.1
N21	H21A	O34 <sup>5</sup>	0.91	2.42	3.264(7)	154.0
N21	H21B	O24	0.91	1.89	2.799(6)	173.7
N21	H21C	O11 <sup>6</sup>	0.91	1.94	2.830(6)	165.8
N22	H22	O36 <sup>7</sup>	0.88	1.78	2.645(6)	165.4
N23	H23	O25 <sup>4</sup>	0.88	1.78	2.653(7)	170.8
N31	H31A	O13 <sup>8</sup>	0.91	2.30	2.839(6)	118.0
N31	H31B	O14	0.91	1.92	2.787(6)	158.2
N31	H31C	O22 <sup>9</sup>	0.91	2.45	3.087(7)	127.7
N31	H31C	O34	0.91	2.08	2.844(6)	140.5
N32	H32	O16	0.88	1.81	2.684(7)	169.4
N33	H33	O35 <sup>10</sup>	0.88	1.80	2.680(6)	176.6
C13	H13A	O36	0.99	2.38	3.189(7)	138.0
C13	H13B	O12 <sup>8</sup>	0.99	2.39	3.219(7)	140.4
C15	H15	O23 <sup>4</sup>	0.95	2.41	3.235(8)	144.8
C23	H23A	O16 <sup>6</sup>	0.99	2.44	3.252(7)	138.4
C25	H25	O33 <sup>1</sup>	0.95	2.41	3.053(7)	125.1
C26	H26	O13 <sup>6</sup>	0.95	2.42	3.143(8)	132.4
C33	H33A	O26 <sup>11</sup>	0.99	2.54	3.377(7)	142.4
C35	H35	O12 <sup>12</sup>	0.95	2.37	3.071(7)	130.1
C36	H36	O34	0.95	2.43	3.016(8)	119.6

<sup>1</sup>3/2-X,1-Y,-1/2+Z; <sup>2</sup>1-X,1/2+Y,3/2-Z; <sup>3</sup>1-X,-1/2+Y,1/2-Z; <sup>4</sup>1+X,+Y,+Z; <sup>5</sup>1/2-X,1-Y,-1/2+Z; <sup>6</sup>1-X,1/2+Y,1/2-Z; <sup>7</sup>-1/2+X,3/2-Y,1-Z; <sup>8</sup>1/2+X,1/2-Y,1-Z; <sup>9</sup>3/2-X,1-Y,1/2+Z; <sup>10</sup>-1+X,+Y,+Z; <sup>11</sup>1/2+X,3/2-Y,1-Z; <sup>12</sup>-1/2+X,1/2-Y,1-Z

**Table S4.** Torsion Angles for **1**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O15	C11	C12	N11	5.9(7)	C15	N12	C14	C13	179.3(5)
O15	C11	C12	C13	128.4(6)	C15	N12	C14	C16	-0.9(7)
O16	C11	C12	N11	-174.0(5)	C15	N13	C16	C14	0.5(7)
O16	C11	C12	C13	-51.5(7)	C16	N13	C15	N12	-1.1(7)
O25	C21	C22	N21	22.4(7)	C21	C22	C23	C24	177.4(5)
O25	C21	C22	C23	146.5(5)	C22	C23	C24	N22	-65.4(8)
O26	C21	C22	N21	-159.4(5)	C22	C23	C24	C26	112.2(7)
O26	C21	C22	C23	-35.3(7)	C23	C24	C26	N23	-177.6(6)
O35	C31	C32	N31	26.4(7)	C24	N22	C25	N23	0.7(7)

O35	C31	C32	C33	150.9(5)	C25	N22	C24	C23	177.5(5)
O36	C31	C32	N31	-157.6(5)	C25	N22	C24	C26	-0.6(7)
O36	C31	C32	C33	-33.1(7)	C25	N23	C26	C24	0.2(7)
N11	C12	C13	C14	-60.9(7)	C26	N23	C25	N22	-0.6(7)
N12	C14	C16	N13	0.2(6)	C31	C32	C33	C34	173.9(5)
N21	C22	C23	C24	-60.0(7)	C32	C33	C34	N32	-68.9(7)
N22	C24	C26	N23	0.3(7)	C32	C33	C34	C36	110.3(7)
N31	C32	C33	C34	-63.3(7)	C33	C34	C36	N33	-178.2(6)
N32	C34	C36	N33	1.0(7)	C34	N32	C35	N33	1.8(7)
C11	C12	C13	C14	178.0(5)	C35	N32	C34	C33	177.6(5)
C12	C13	C14	N12	-68.6(7)	C35	N32	C34	C36	-1.7(7)
C12	C13	C14	C16	111.6(7)	C35	N33	C36	C34	0.1(7)
C13	C14	C16	N13	-180.0(5)	C36	N33	C35	N32	-1.2(7)
C14	N12	C15	N13	1.3(7)					

**Table S5.** Bond Lengths for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Tc1	O12	1.678(16)	N12	C15	1.34(2)
Tc1	O14	1.752(14)	O15	C11	1.279(19)
Tc1	O13	1.674(15)	C41	C42	1.55(2)
Tc1	O11	1.688(15)	N31	C32	1.48(2)
Tc2	O21	1.711(13)	C11	C12	1.53(2)
Tc2	O22	1.714(14)	N22	C24	1.38(2)
Tc2	O23	1.720(13)	N22	C25	1.32(2)
Tc2	O24	1.698(14)	N21	C22	1.49(2)
Tc3	O31	1.701(13)	C26	N23	1.39(2)
Tc3	O33	1.674(15)	C26	C24	1.38(2)
Tc3	O32	1.71(2)	C46	C44	1.38(2)
Tc3	O34	1.667(16)	C46	N43	1.38(2)
Tc4	O44	1.708(15)	C21	C22	1.52(2)
Tc4	O42	1.698(14)	N23	C25	1.34(3)
Tc4	O43	1.726(14)	N11	C12	1.49(2)
Tc4	O41	1.722(14)	C44	N42	1.39(2)
O36	C31	1.219(18)	C44	C43	1.51(2)
O46	C41	1.24(2)	N41	C42	1.49(2)
O26	C21	1.26(2)	C34	C33	1.48(2)
O25	C21	1.26(2)	C34	C36	1.36(2)
O16	C11	1.216(19)	N42	C45	1.33(2)
O45	C41	1.26(2)	C42	C43	1.53(2)
O35	C31	1.274(17)	C16	N13	1.42(2)
N33	C36	1.38(2)	C24	C23	1.50(2)
N33	C35	1.35(2)	N13	C15	1.29(2)
N32	C34	1.38(2)	C22	C23	1.54(2)
N32	C35	1.33(2)	C31	C32	1.52(2)
C14	N12	1.38(2)	N43	C45	1.30(2)
C14	C16	1.37(2)	C32	C33	1.55(2)
C14	C13	1.49(2)	C13	C12	1.56(2)

**Table S6.** Bond Angles for **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O12	Tc1	O14	108.6(8)	O25	C21	O26	127.5(15)
O12	Tc1	O11	111.0(10)	O25	C21	C22	118.0(15)

O13	Tc1	O12	108.5(8)	C25	N23	C26	109.1(16)
O13	Tc1	O14	111.4(7)	C46	C44	N42	106.4(16)
O13	Tc1	O11	108.2(10)	C46	C44	C43	130.3(15)
O11	Tc1	O14	109.1(8)	N42	C44	C43	122.7(16)
O21	Tc2	O22	109.6(6)	N32	C34	C33	124.4(15)
O21	Tc2	O23	107.7(6)	C36	C34	N32	105.9(15)
O22	Tc2	O23	111.4(7)	C36	C34	C33	129.7(16)
O24	Tc2	O21	108.0(7)	C45	N42	C44	108.8(16)
O24	Tc2	O22	109.8(6)	N41	C42	C41	111.5(13)
O24	Tc2	O23	110.3(7)	N41	C42	C43	112.7(13)
O31	Tc3	O32	108.2(8)	C43	C42	C41	109.8(13)
O33	Tc3	O31	110.7(7)	C14	C16	N13	105.6(14)
O33	Tc3	O32	109.2(11)	N22	C24	C23	123.0(15)
O34	Tc3	O31	107.5(8)	C26	C24	N22	106.4(15)
O34	Tc3	O33	111.3(11)	C26	C24	C23	130.5(16)
O34	Tc3	O32	109.9(12)	C15	N13	C16	108.7(15)
O44	Tc4	O43	109.1(7)	N21	C22	C21	112.6(14)
O44	Tc4	O41	110.2(7)	N21	C22	C23	111.3(13)
O42	Tc4	O44	110.0(8)	C21	C22	C23	107.4(12)
O42	Tc4	O43	109.4(8)	O36	C31	O35	126.3(14)
O42	Tc4	O41	109.0(8)	O36	C31	C32	116.8(13)
O41	Tc4	O43	109.1(7)	O35	C31	C32	116.8(13)
C35	N33	C36	107.5(14)	C45	N43	C46	110.6(15)
C35	N32	C34	109.8(14)	N31	C32	C31	114.4(12)
N12	C14	C13	123.9(15)	N31	C32	C33	110.7(12)
C16	C14	N12	107.5(13)	C31	C32	C33	109.7(12)
C16	C14	C13	128.6(16)	C34	C33	C32	113.3(13)
C15	N12	C14	107.9(15)	C44	C43	C42	113.8(13)
O46	C41	O45	127.2(15)	C14	C13	C12	114.9(13)
O46	C41	C42	115.4(15)	C24	C23	C22	112.0(13)
O45	C41	C42	117.4(14)	C11	C12	C13	107.8(12)
O16	C11	O15	125.9(14)	N11	C12	C11	112.1(13)
O16	C11	C12	116.9(14)	N11	C12	C13	109.3(13)
O15	C11	C12	117.2(14)	C34	C36	N33	108.1(15)
C25	N22	C24	110.4(15)	N43	C45	N42	108.6(16)
C24	C26	N23	105.9(17)	N22	C25	N23	108.1(17)
C44	C46	N43	105.5(15)	N13	C15	N12	110.3(16)
O26	C21	C22	114.4(15)	N32	C35	N33	108.4(14)

**Table S7.** Hydrogen Bonds for **2**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N33	H33	O42 <sup>1</sup>	0.88	2.26	2.94(2)	134.5
N33	H33	O12 <sup>2</sup>	0.88	2.25	2.81(2)	120.8
N32	H32	O15 <sup>3</sup>	0.88	1.96	2.823(17)	166.9
N12	H12	O45 <sup>1</sup>	0.88	2.08	2.947(19)	170.5
N31	H31A	O25 <sup>1</sup>	0.91	2.09	2.840(17)	138.8
N31	H31B	O46 <sup>1</sup>	0.91	1.93	2.743(17)	147.2
N31	H31C	O22 <sup>3</sup>	0.91	2.01	2.856(19)	153.4
N22	H22	O35	0.88	1.94	2.815(19)	173.8
N21	H21A	O44	0.91	2.00	2.85(2)	154.9
N21	H21B	O45 <sup>3</sup>	0.91	2.22	2.997(17)	142.5
N21	H21C	O16 <sup>4</sup>	0.91	1.92	2.754(18)	151.8
N23	H23	O32 <sup>5</sup>	0.88	1.92	2.69(2)	146.0

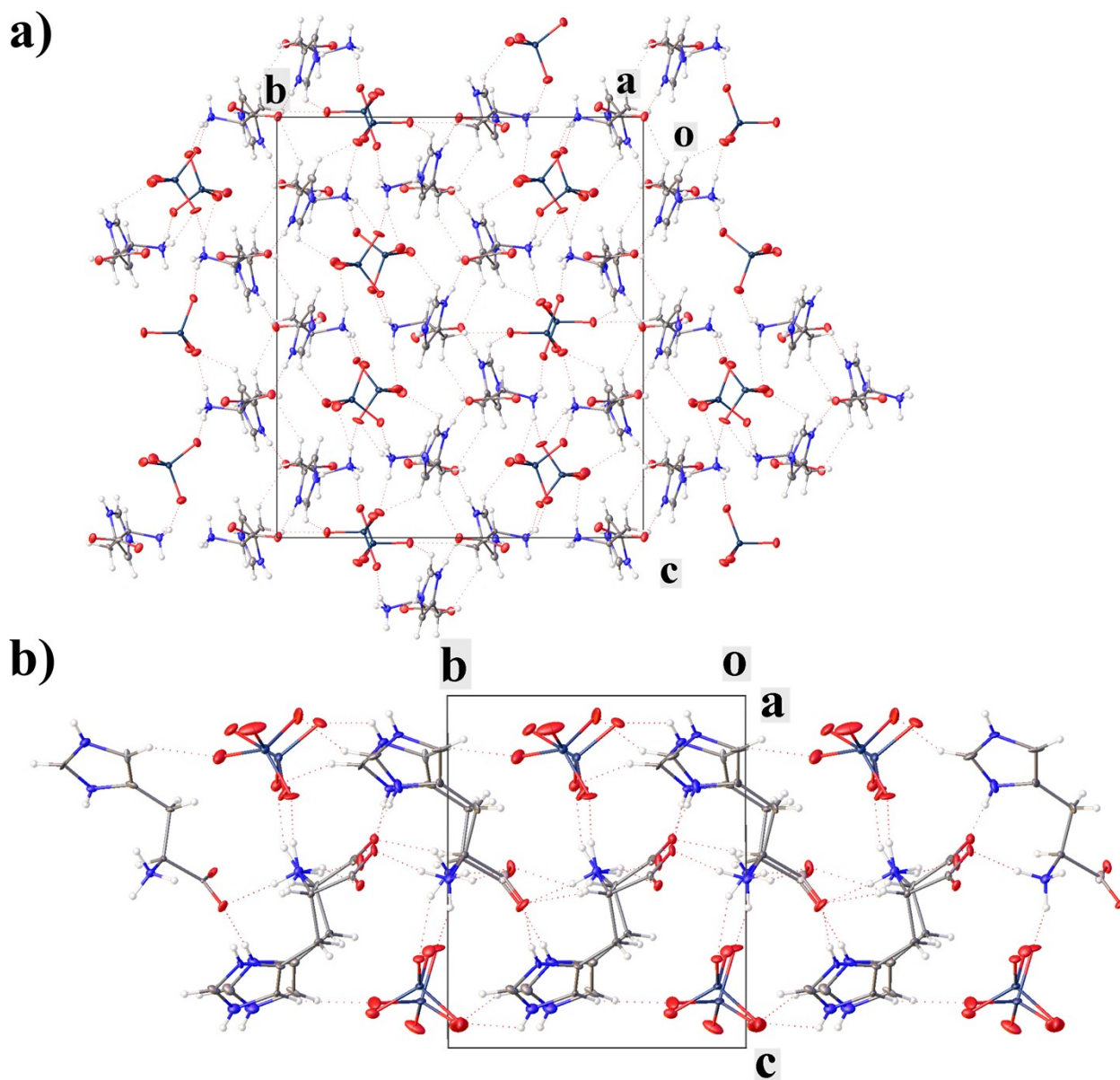
N11	H11A	O31	0.91	2.06	2.859(18)	146.1
N11	H11B	O35	0.91	2.17	3.063(17)	166.1
N11	H11C	O26	0.91	1.88	2.768(19)	164.5
N41	H41A	O15	0.91	2.09	2.920(17)	151.1
N41	H41B	O36 <sup>6</sup>	0.91	1.87	2.751(17)	163.1
N41	H41C	O14	0.91	2.09	2.832(19)	137.6
N42	H42	O26	0.88	2.02	2.78(2)	144.9
C16	H16	O13	0.95	2.38	3.09(2)	131.3
N13	H13	O21 <sup>3</sup>	0.88	2.22	2.845(19)	127.4
N13	H13	O41 <sup>7</sup>	0.88	2.21	3.01(2)	149.9
N43	H43	O23 <sup>8</sup>	0.88	2.22	3.10(2)	174.9
C12	H12A	O46 <sup>1</sup>	1.00	2.49	3.180(19)	125.8
C36	H36	O33	0.95	2.25	3.03(2)	139.5
C45	H45	O34	0.95	2.22	2.90(3)	128.3
C25	H25	O21 <sup>3</sup>	0.95	2.31	3.06(2)	135.7
C35	H35	O44 <sup>1</sup>	0.95	2.53	3.15(2)	123.1

<sup>1</sup>+X,1+Y,+Z; <sup>2</sup>+X,1+Y,-1+Z; <sup>3</sup>-1+X,1+Y,+Z; <sup>4</sup>-1+X,+Y,+Z; <sup>5</sup>-1+X,+Y,1+Z; <sup>6</sup>1+X,-1+Y,+Z; <sup>7</sup>+X,+Y,1+Z; <sup>8</sup>+X,+Y,-1+Z

**Table S8.** Torsion Angles for **2**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O36	C31	C32	N31	173.6(12)	C46	C44	N42	C45	0(2)
O36	C31	C32	C33	-61.4(16)	C46	C44	C43	C42	148.7(19)
O46	C41	C42	N41	159.2(14)	C46	N43	C45	N42	2(2)
O46	C41	C42	C43	-75.0(18)	C21	C22	C23	C24	-178.9(14)
O26	C21	C22	N21	161.3(14)	N23	C26	C24	N22	1(2)
O26	C21	C22	C23	-75.8(17)	N23	C26	C24	C23	-177.0(18)
O25	C21	C22	N21	-18(2)	C44	C46	N43	C45	-1(2)
O25	C21	C22	C23	104.6(17)	C44	N42	C45	N43	-1(2)
O16	C11	C12	N11	165.1(14)	N41	C42	C43	C44	-57.9(19)
O16	C11	C12	C13	-74.7(18)	C34	N32	C35	N33	5(2)
O45	C41	C42	N41	-19.4(19)	N42	C44	C43	C42	-41(3)
O45	C41	C42	C43	106.3(17)	C16	C14	N12	C15	1(2)
O35	C31	C32	N31	-6.0(18)	C16	C14	C13	C12	133.6(19)
O35	C31	C32	C33	119.1(15)	C16	N13	C15	N12	-2(2)
N32	C34	C33	C32	-56(2)	C24	N22	C25	N23	-1(2)
N32	C34	C36	N33	-0.9(19)	C24	C26	N23	C25	-1(2)
C14	N12	C15	N13	1(2)	C31	C32	C33	C34	175.4(13)
C14	C16	N13	C15	2(2)	N43	C46	C44	N42	1(2)
C14	C13	C12	C11	174.7(14)	N43	C46	C44	C43	172.1(18)
C14	C13	C12	N11	-63.3(19)	C33	C34	C36	N33	-178.8(17)
N12	C14	C16	N13	-2.0(19)	C43	C44	N42	C45	-172.0(17)
N12	C14	C13	C12	-47(2)	C13	C14	N12	C15	-178.1(16)
O15	C11	C12	N11	-11.6(19)	C13	C14	C16	N13	177.0(17)
O15	C11	C12	C13	108.6(16)	C36	N33	C35	N32	-6(2)
C41	C42	C43	C44	177.0(14)	C36	C34	C33	C32	121.6(19)
N31	C32	C33	C34	-57.4(17)	C25	N22	C24	C26	0(2)
N22	C24	C23	C22	-52(2)	C25	N22	C24	C23	178.1(17)
N21	C22	C23	C24	-55.2(18)	C35	N33	C36	C34	4(2)
C26	N23	C25	N22	2(2)	C35	N32	C34	C33	175.5(16)
C26	C24	C23	C22	125(2)	C35	N32	C34	C36	-3(2)

## 2. Non-valent interactions details

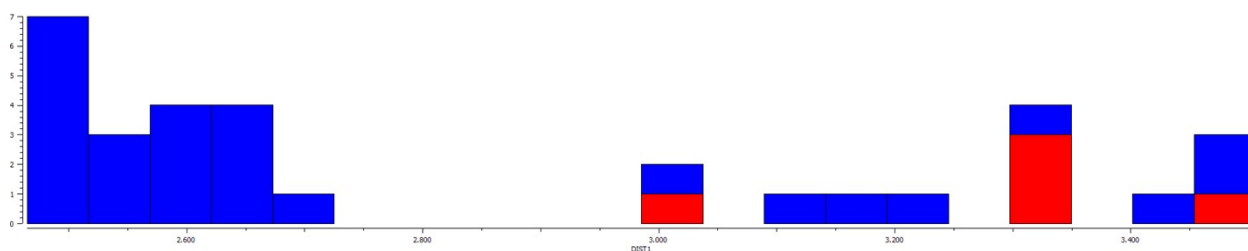


**Figure S1.** Crystal packing of **1** (a) and **2** (b) showing cationic and anionic columns.

**Table S9.**  $M \cdots O$  ( $M = \text{Mn}, \text{Re}$ ) distances and formulas of compounds containing  $\text{C}-\text{O} \cdots \text{M}$  interactions.

NAME	DIST $M \cdots O$	formula
NAPWEK	3.329	$\text{C}_5 \text{H}_{12} \text{N}_1 \text{O}_2 1+, \text{O}_4 \text{Re} 1-, \text{H}_2 \text{O} 1$
YATVEY	3.237	$4(\text{K} 1+), 6(\text{Na} 1+), n(\text{C}_{48} \text{H}_{24} \text{Cu}_8 \text{Mn}_{13} \text{O}_{80} 9-), 0.5(\text{C}_1 \text{H}_1 \text{O}_2 1-), 0.5(\text{C}_2 \text{H}_3 \text{O}_2 1-), 19.5(\text{H}_2 \text{O} 1)$
YATVEY	2.512	$4(\text{K} 1+), 6(\text{Na} 1+), n(\text{C}_{48} \text{H}_{24} \text{Cu}_8 \text{Mn}_{13} \text{O}_{80} 9-), 0.5(\text{C}_1 \text{H}_1 \text{O}_2 1-), 0.5(\text{C}_2 \text{H}_3 \text{O}_2 1-), 19.5(\text{H}_2 \text{O} 1)$
YATVEY	2.465	$4(\text{K} 1+), 6(\text{Na} 1+), n(\text{C}_{48} \text{H}_{24} \text{Cu}_8 \text{Mn}_{13} \text{O}_{80} 9-), 0.5(\text{C}_1 \text{H}_1 \text{O}_2 1-), 0.5(\text{C}_2 \text{H}_3 \text{O}_2 1-), 19.5(\text{H}_2 \text{O} 1)$
YATVEY	2.563	$4(\text{K} 1+), 6(\text{Na} 1+), n(\text{C}_{48} \text{H}_{24} \text{Cu}_8 \text{Mn}_{13} \text{O}_{80} 9-), 0.5(\text{C}_1 \text{H}_1 \text{O}_2 1-), 0.5(\text{C}_2 \text{H}_3 \text{O}_2 1-), 19.5(\text{H}_2 \text{O} 1)$

YATVEY	2.474	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),19.5(H2 O1)
YATVEY	3.138	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),19.5(H2 O1)
YATVEY	2.55	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),19.5(H2 O1)
YATVEY	2.651	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),19.5(H2 O1)
YATVEY	2.499	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),19.5(H2 O1)
YATVEY	2.609	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),19.5(H2 O1)
YATVIC	3.193	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),22.4(H2 O1)
YATVIC	2.521	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),22.4(H2 O1)
YATVIC	2.5	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),22.4(H2 O1)
YATVIC	2.475	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),22.4(H2 O1)
YATVIC	2.499	4(K1 1+),6(Na1 1+),n(C48 H24 Cu8 Mn13 O80 9-),0.5(C1 H1 O2 1-),0.5(C2 H3 O2 1-),22.4(H2 O1)
AVAYAY	2.571	(C48 H24 Mn3 N6 O12)n
AVAYAY	2.571	(C48 H24 Mn3 N6 O12)n
CUFFAM	3.495	(C24 H28 Mn3 N2 O22)n
CUFFAM	3.495	(C24 H28 Mn3 N2 O22)n
DEGXEV	3.506	C12 H12 N2 Np1 O15 Re2
DEGXEV	3.036	C12 H12 N2 Np1 O15 Re2
HEBMIM	2.594	(C43 H34 Mn3 N2 O15)n,2n(H2 O1)
JUVWUU	3.422	(C16 H15 Mn1 N1 O5)n
KUGTAK	2.656	C66 H66 Mn2 O34 P2 Ti6
KUGTAK	2.656	C66 H66 Mn2 O34 P2 Ti6
NAFCAB	3.334	C3 H8 N1 O2 1+,O4 Re1 1-
PAPKIB	3.318	(C96 H48 Mn6 N12 O25 2-),2n(H1 1+),2.5n(H2 O1)
POMKUY	3.347	C2 H5 N1 O2,C2 H6 N1 O2 1+,O4 Re1 1-
YELTUH	2.679	(C14 H10 Mn1 N2 Ni1 O10)n
ZEVVUU	2.673	(C14 H10 Co1 Mn1 N2 O10)n
IYOHUC	3.037	2(H12 Mn1 O6 2+),H8 Mn1 O4 2+,2(C30 H54 Au3 Co2 N6 O12 S6 3-)



**Figure S2.** Diagram showing the distribution of M...O distances (Å) in C-O...M interactions in structures with rhenium (red) and manganese (blue).