Supplementary Materials: Assembly of Mn(III) Schiff Base Complexes with Heptacyanorhenate (IV)

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Table S1. Some geometric parameters related to the contacts of the adjacent $[MnSB]^+$ or $[MnSB(Solv)_n]^+$ units.

Compound	d Mn...Mn Å	Mn–O_{Ph} Å	d π–π Å*	∠ π–π °*	shift π–π Å*
$[(Mn^{5Me}Salen)_2OAc]PF_6$,**2**	3.38	2.39	3.86	26.4	0.46
	3.53	2.81	3.71	11.7	1.16
$[Mn_2(salen)_2OAc]ClO_4$ [42]	3.42	2.45	3.62	10.7	1.02
	3.51	2.69	3.78	21.4	0.67
$[(Mn^{3MeO}Salen)_2(H_2O)_2]ClO_4{\cdot}H_2O$,**1** [20]	4.79	4.10	3.76	5.7	1.54
$Mn^{3MeO}Salen(H_2O)_2[Mn^{3MeO}Salen(H_2O)MeCN]$	4.82	4.18			
$(Ph_4B)_2{\cdot}5MeCN$,**6**	8.25	8.06			
$Ph_4P[Mn^{3MeO}Salen(H_2O)_2]_2[Re(CN)_7]{\cdot}6H_2O$,**3**	4.76	4.08			
	6.58	4.07			
$[\{(Mn^{5Me}Salen)_6(H_2O)_2Re(CN)_7\}_2Re(CN)_7]$ $Cl_2{\cdot}PF_6{\cdot}H_2O$, **4**	3.67	2.86	3.80	13.4	1.37
		2.78			
	3.44	2.54			
	5.00	4.34			
		4.19			
$[Mn^{5Me}SalenH_2O(i\text{-}PrOH)][(Mn^{5Me}Salen)_5$ $H_2O(i\text{-}PrOH)_2Re(CN)_7]{\cdot}2PF_6$, **5**	3.42	2.59	3.75	15.4	1.12
	3.42	2.59			
	5.06	4.34	3.88	7.0	1.89

*Parameters of the π–π interactions were found using Olex 2 software [43].

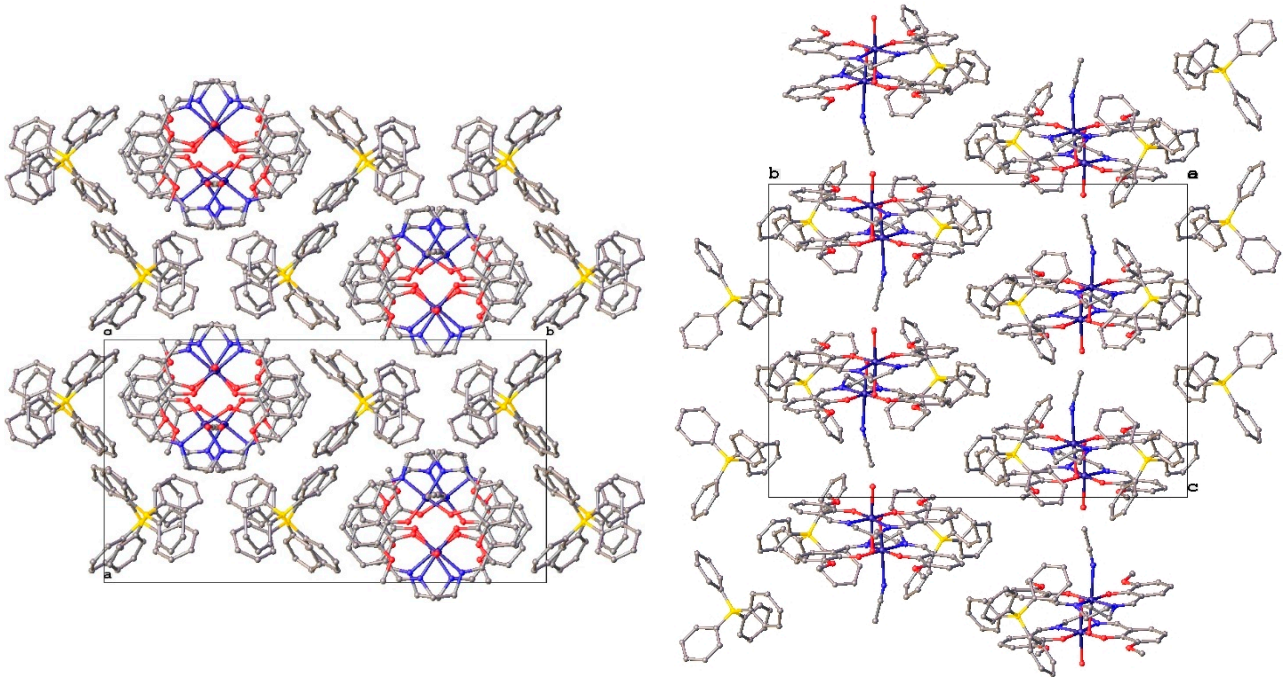

Figure S1. The crystal packing in the compound **6**. View along the axis *c* (left) and *a* (right). Hydrogen atoms are omitted.

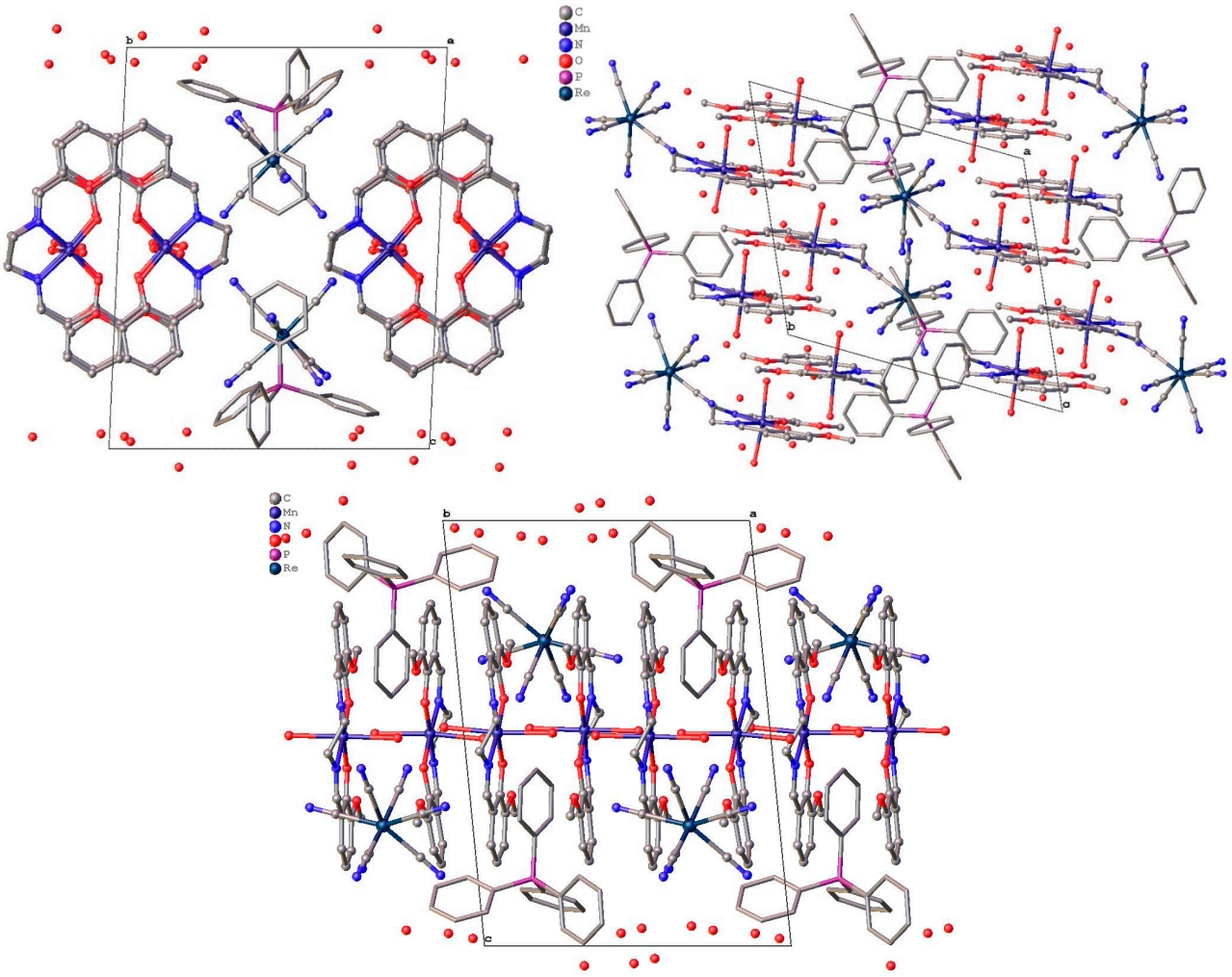

Figure S2. The crystal packing in the compound **6**. View along the three axes. Hydrogen atoms are omitted.

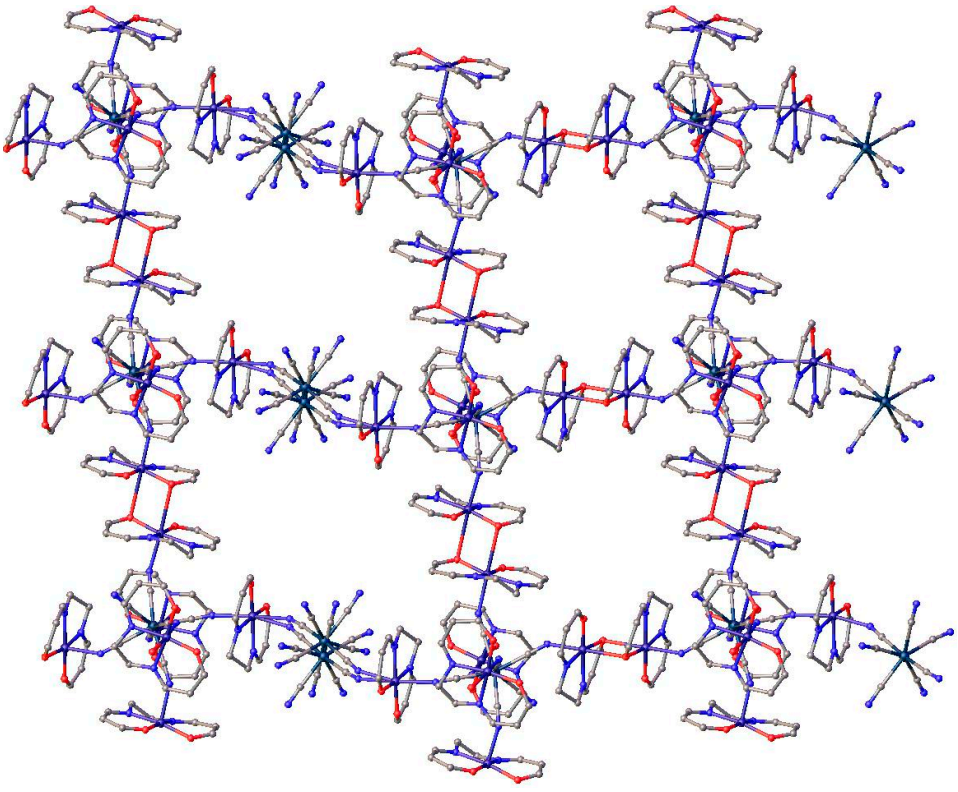

Figure S3. Schematic presentation of a layer in **4**. SB ligand is reduced for clarity.

Table S2. Ideal and observed angles for the complex anion $[Re(CN)_7]^{3-}$.

Re polyhedron / compound	**atoms to define edge 1**	**atoms to define edge 2**	**dihedral angle, deg**
pentagonal bipyramid			54.4; 54.4
capped trigonal prism			0; 0; 41.5
capped octahedron			16.2; 16.2; 16.2
4:3 piano stool			0; 0
3, Re1	C31—C37—C32	C31—C37—C36	54.3
	C31—C36—C34	C31—C36—C37	53.5
	C31—C34—C36	C31—C34—C33	56.4
	C31—C33—C32	C31—C33—C34	47.3
	C31—C32—C33	C31—C32—C37	58.9
	C35—C37—C32	C35—C37—C36	57.2
	C35—C36—C37	C35—C36—C34	56.0
	C35—C34—C36	C35—C34—C33	50.4
	C35—C33—C34	C35—C33—C32	58.7
	C35—C32—C33	C35—C32—C37	50.2
4, Re1	C710—C713—C712	C710—C713—C715	11.1
	C712—C715—C710	C712—C715—C713	10.2
	C713—C714—C715	C713—C714—C716	2.7
	C715—C716—C713	C715—C716—C714	2.7
	C710—C716—C712	C710—C716—C714	16.1
	C712—C714—C710	C712—C714—C716	14.5
	C713—C716—C711	C713—C716—C712	58.6
	C714—C715—C710	C714—C715—C711	18.1
4, Re2	C810—C815—C816	C810—C815—C814	50.2
	C810—C816—C815	C810—C816—C813	59.3
	C810—C812—C816	C810—C812—C813	49.3
	C810—C813—C812	C810—C813—C814	57.9
	C810—C814—C813	C810—C814—C815	51.9
	C811—C814—C815	C811—C814—C813	58.4
	C811—C815—C814	C811—C815—C816	56.5
	C811—C816—C815	C811—C816—C812	46.7
	C811—C812—C816	C811—C812—C813	67.7
	C811—C813—C812	C811—C813—C814	44.7
5, Re01	C00W—C01K—C019	C00W—C01K—C015	70.5
	C00W—C019—C01K	C00W—C019—C00Z	32.4
	C00W—C00Z—C019	C00W—C00Z—C020	72.0
	C00W—C020—C00Z	C00W—C020—C015	39.0
	C00W—C015—C020	C00W—C015—C01K	54.0
	C01C—C01K—C019	C01C—C01K—C015	46.6
	C01C—C019—C01K	C01C—C019—C00Z	70.7
	C01C—C00Z—C019	C01C—C00Z—C020	28.5
	C01C—C020—C00Z	C01C—C020—C015	66.2
	C01C—C015—C020	C01C—C015—C01K	57.0

[a] Dihedral angles for ideal polyhedral were taken from refs [44, 49]

Table S3. Selected bond lengths (Å) and angles (deg) for {Re(CN)$_7$} units.

compound	**Re–C**		**C–Re–C**		**C–Re–C**	
3, Re1	Re1--C31	2.099(4)	C31--Re1--C32	85.62(14)	C31--Re1--C35	175.46(15)
	Re1--C32	2.108(4)	C31--Re1--C33	95.21(15)	C32--Re1--C36	145.46(14)
	Re1--C33	2.105(4)	C31--Re1--C34	90.64(15)	C33--Re1--C36	143.43(14)
	Re1--C34	2.108(4)	C31--Re1--C36	89.33(14)	C34--Re1--C32	142.67(15)
	Re1--C35	2.102(4)	C31--Re1--C37	86.85(14)	C37--Re1--C33	143.51(14)
	Re1--C36	2.108(4)	C33--Re1--C32	71.11(14)	C37--Re1--C34	144.20(15)
	Re1--C37	2.101(4)	C33--Re1--C34	72.28(15)		
			C34--Re1--C36	71.40(15)		
			C35--Re1--C32	93.03(14)		
			C35--Re1--C33	88.45(15)		
			C35--Re1--C34	93.05(15)		
			C35--Re1--C36	89.33(14)		
			C37--Re1--C32	72.75(14)		
			C37--Re1--C35	88.61(14)		
			C37--Re1--C36	72.87(14)		
4*, Re1	Re1--C710	2.082(9)	C711--Re1--C713	86.0(3)	C710--Re1--C711	129.6(3)
	Re1--C711	2.125(8)	C712--Re1--C710	71.3(3)	C710--Re1--C713	125.9(3)
	Re1--C712	2.051(8)	C712--Re1--C713	78.7(3)	C710--Re1--C716	127.6(2)
	Re1--C713	2.125(8)	C712--Re1--C716	78.8(2)	C712--Re1--C711	159.1(3)
	Re1--C714	2.054(8)	C714--Re1--C710	72.0(3)	C712--Re1--C714	110.4(3)
	Re1--C715	2.065(6)	C714--Re1--C711	81.0(3)	C712--Re1--C715	113.2(2)
	Re1--C716	2.106(6)	C714--Re1--C716	79.8(2)	C714--Re1--C713	162.1(2)
			C715--Re1--C710	72.0(3)	C714--Re1--C715	108.4(2)
			C715--Re1--C711	77.6(2)	C715--Re1--C716	160.3(2)
			C715--Re1--C713	80.4(2)		
			C716--Re1--C711	86.4(2)		
			C716--Re1--C713	87.2(2)		
5, Re1	Re01--C00W	2.00(3)	C0W--Re01--C00Z	79.5(9)	C0W--Re01--C01C	178.1(9)
	Re01--C00Z	2.13(3)	C0W--Re01--C01K	81.0(10)	C01K--Re01--C00Z	138.3(9)
	Re01--C01C	2.05(2)	C0W--Re01--C015	92.5(11)	C15--Re01--C00Z	141.7(11)
	Re01--C01K	2.11(3)	C0W--Re01--C019	98.9(10)	C19--Re01--C015	149.2(11)
	Re01--C015	2.08(3)	C0W--Re01--C020	100.4(9)	C019--Re01--C020	130.3(10)
	Re01--C019	2.05(3)	C1C--Re01--C00Z	102.2(9)	C020--Re01--C01K	150.0(8)
	Re01--C020	2.11(3)	C1C--Re01--C01K	97.2(9)		
			C1C--Re01--C015	86.4(10)		
			C1C--Re01--C019	81.3(9)		
			C1C--Re01--C020	80.9(9)		
			C15--Re01--C01K	75.4(11)		
			C15--Re01--C020	74.6(11)		
			C19--Re01--C00Z	68.9(9)		
			C19--Re01--C01K	78.3(10)		
			C020--Re01--C00Z	70.3(9)		

*Due to disorder of $[Re(CN)_7]^{3-}$ units for Re2, bond lengths Re2–C, C–N and 'angle distances' Re2···N were restrained to be 2.10, 1.16 and 3.25 Å respectively with default corresponding standard deviations.

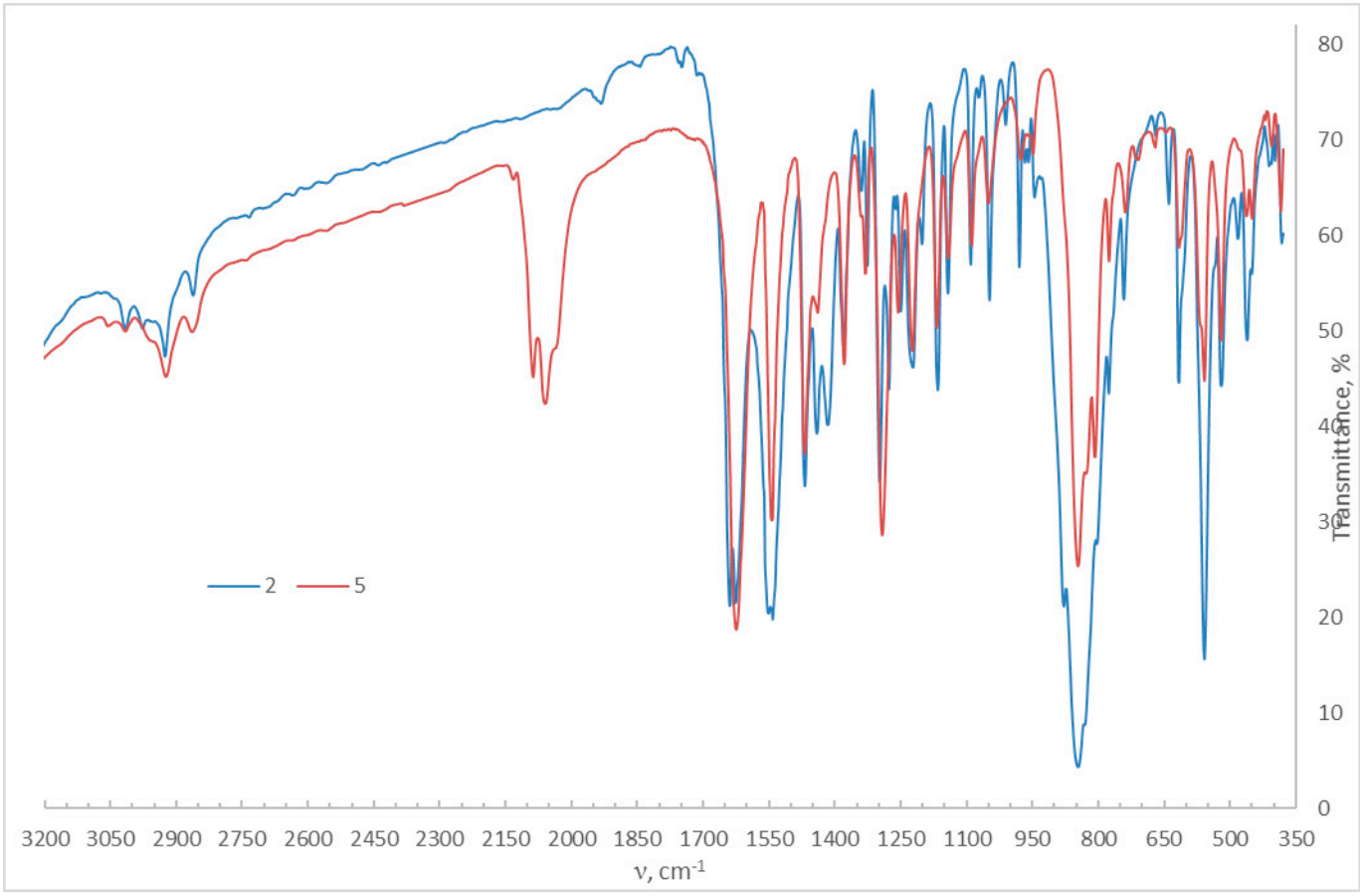

Figure S4. IR spectra of the compound **5** and its precursor **2** registered in KBr pellets.

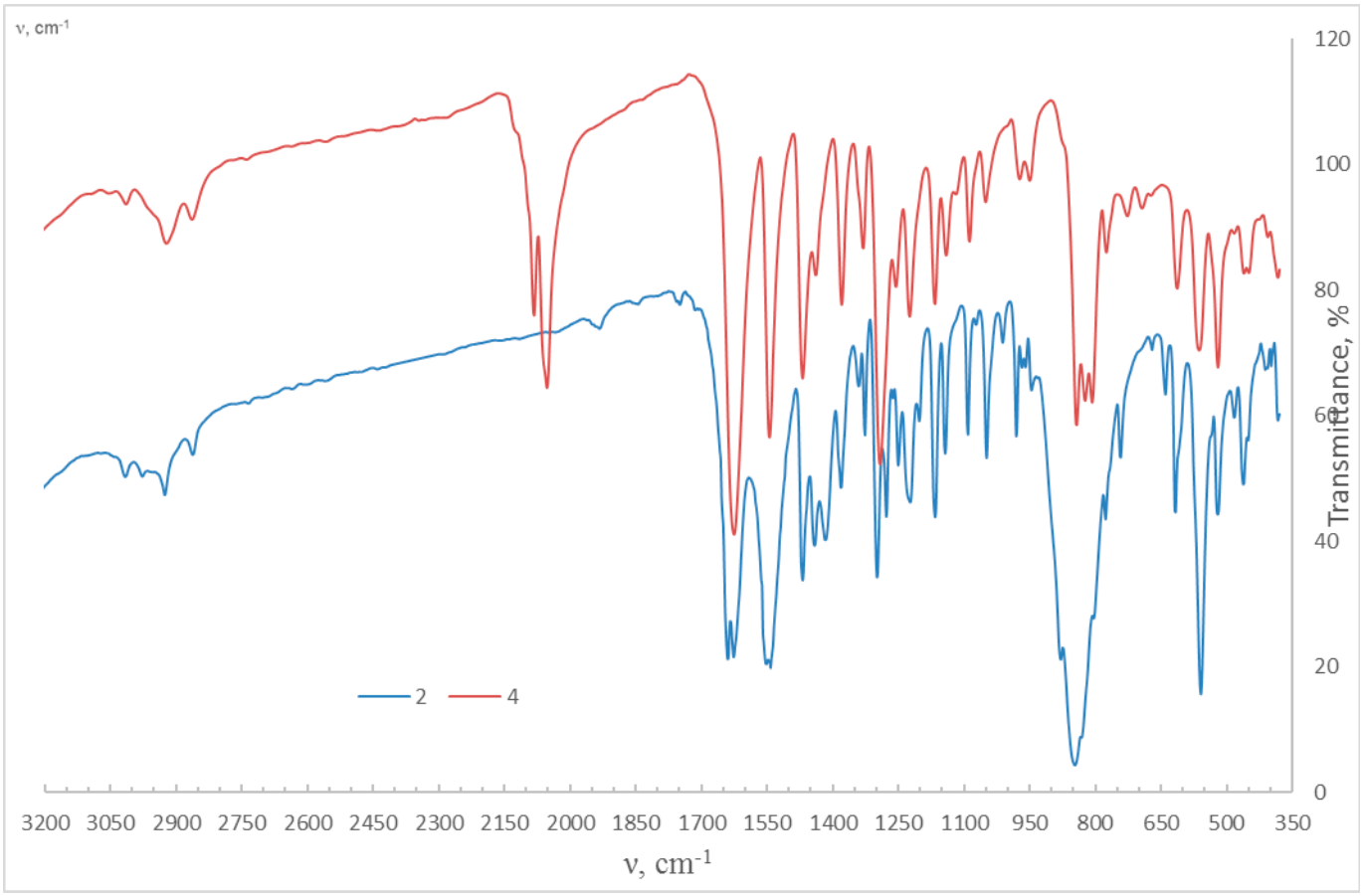

Figure S5. IR spectra of the compound **4** and its precursor **2** registered in KBr pellets.

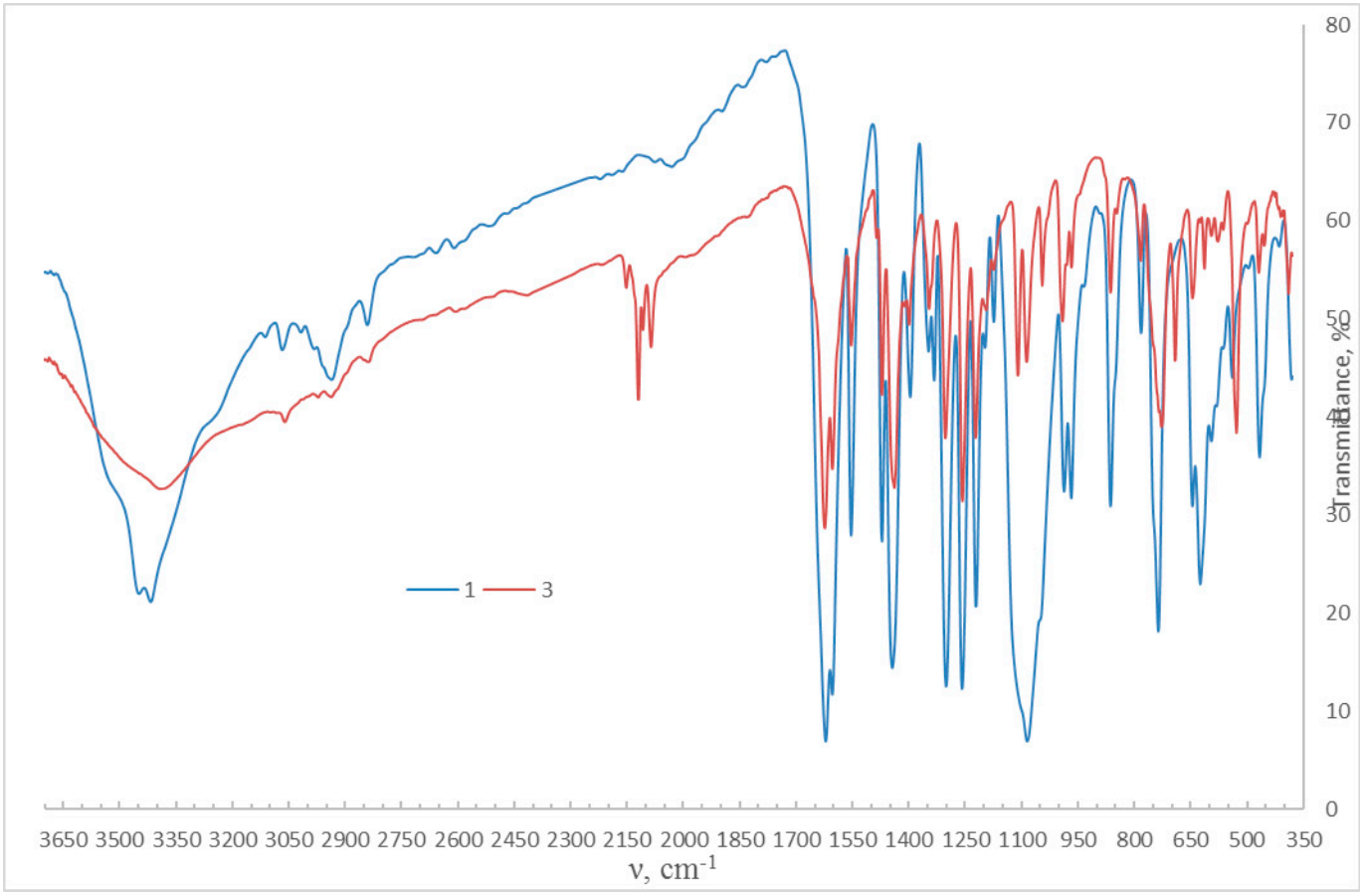

Figure S6. IR spectra of the compound **3** and its precursor **1** registered in KBr pellets.

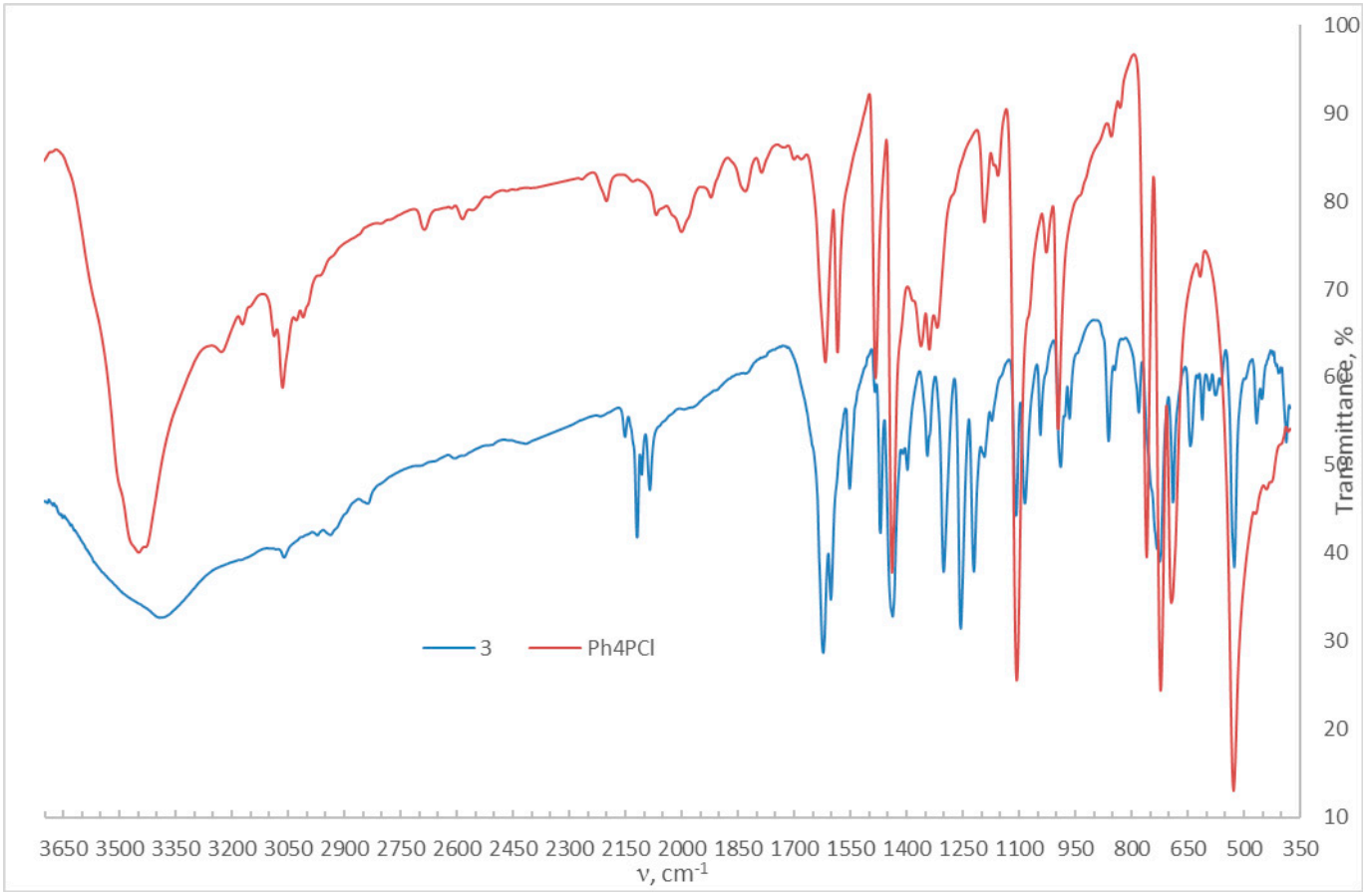

Figure S7. IR spectra of the compound **3** and Ph4PCl registered in KBr pellets.

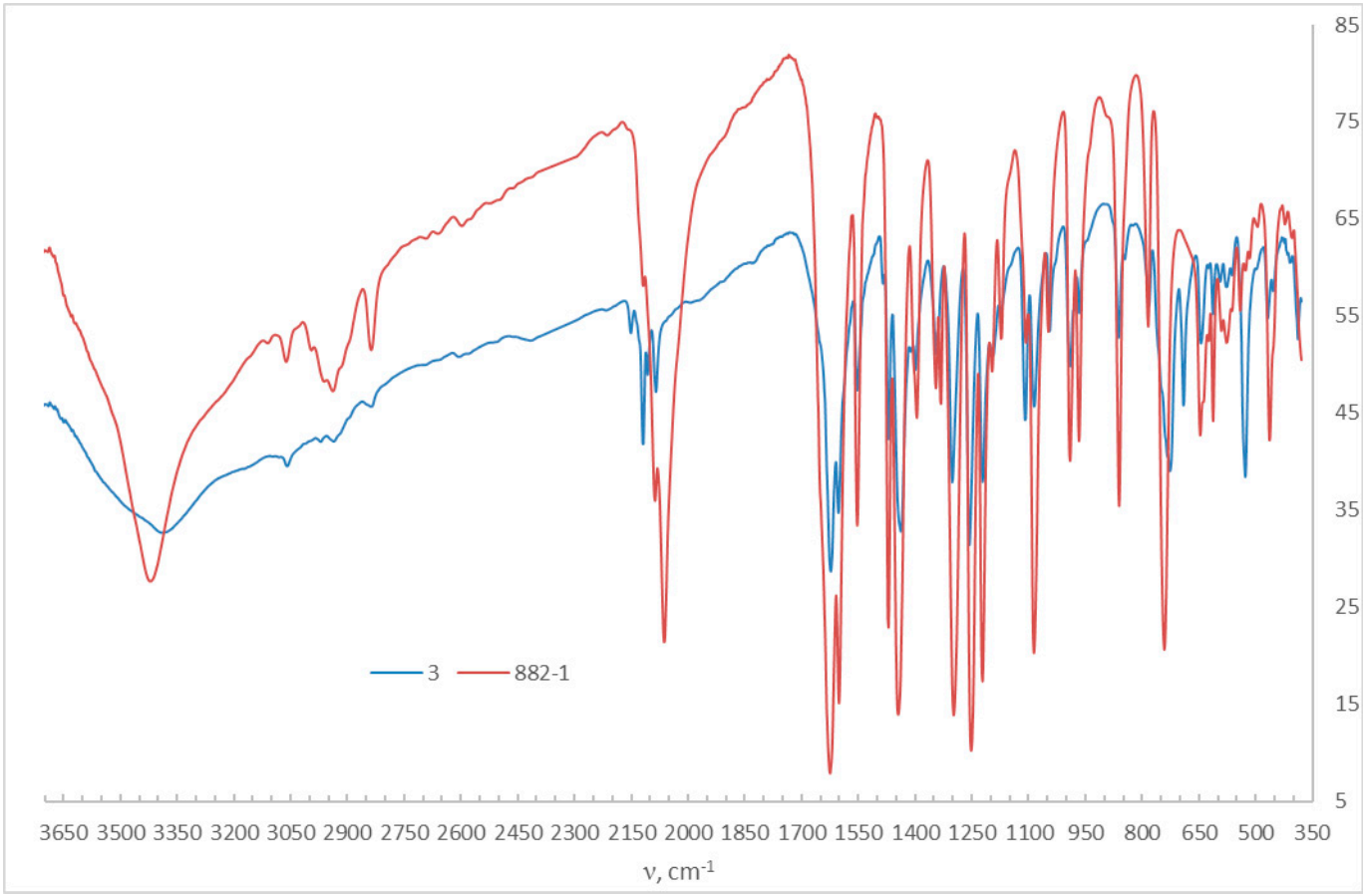

Figure S8. IR spectra of the compound **3** and $[Mn^{3MeO}SalenH_2O)_4Re(CN)_7]ClO_4(CH_3CN)_{1,5}(H_2O)_{6,5}$ (882-1) in KBr pellets.

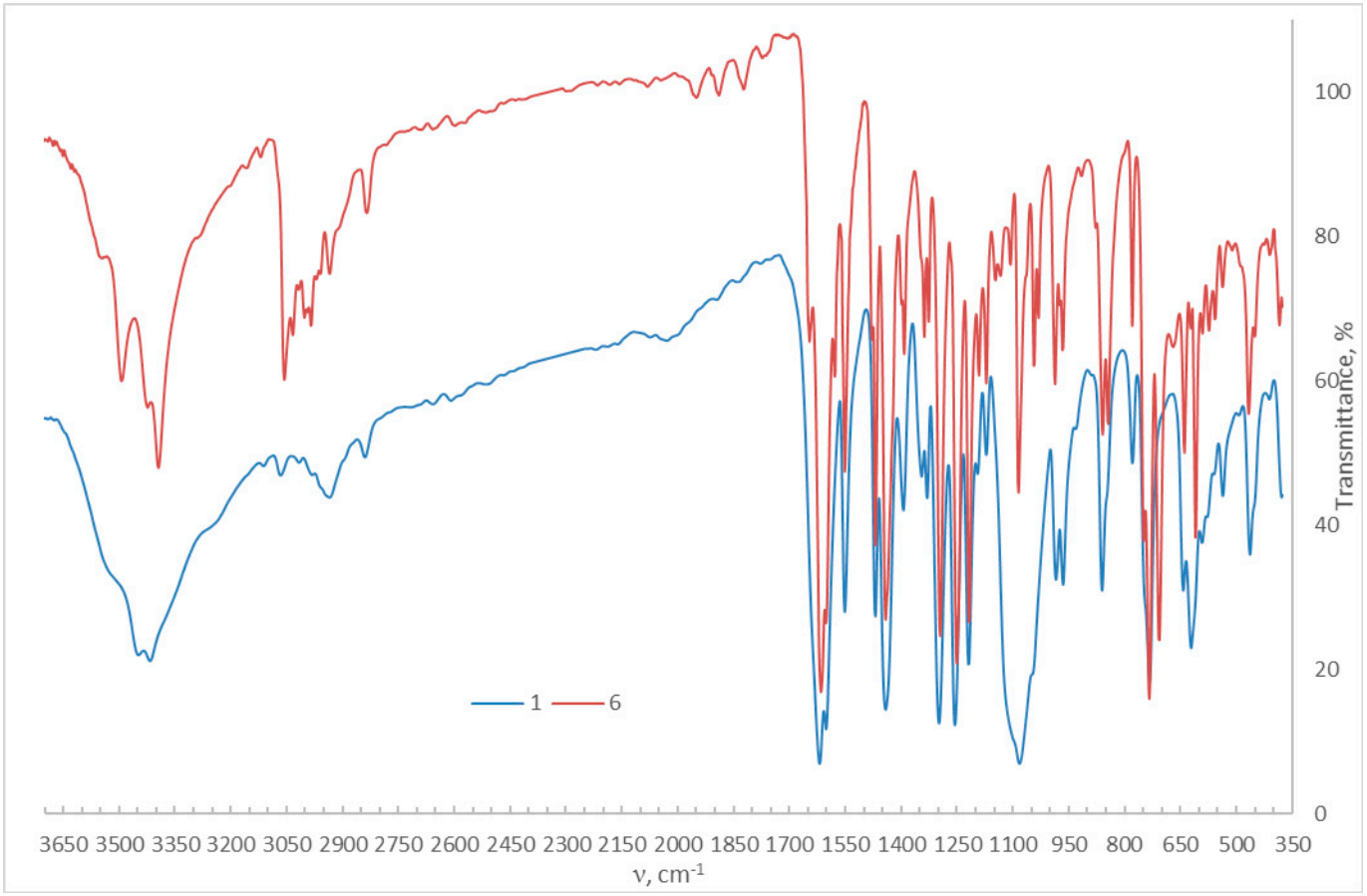

Figure S9. IR spectra of the compound **6** and its precursor **1** registered in KBr pellets.

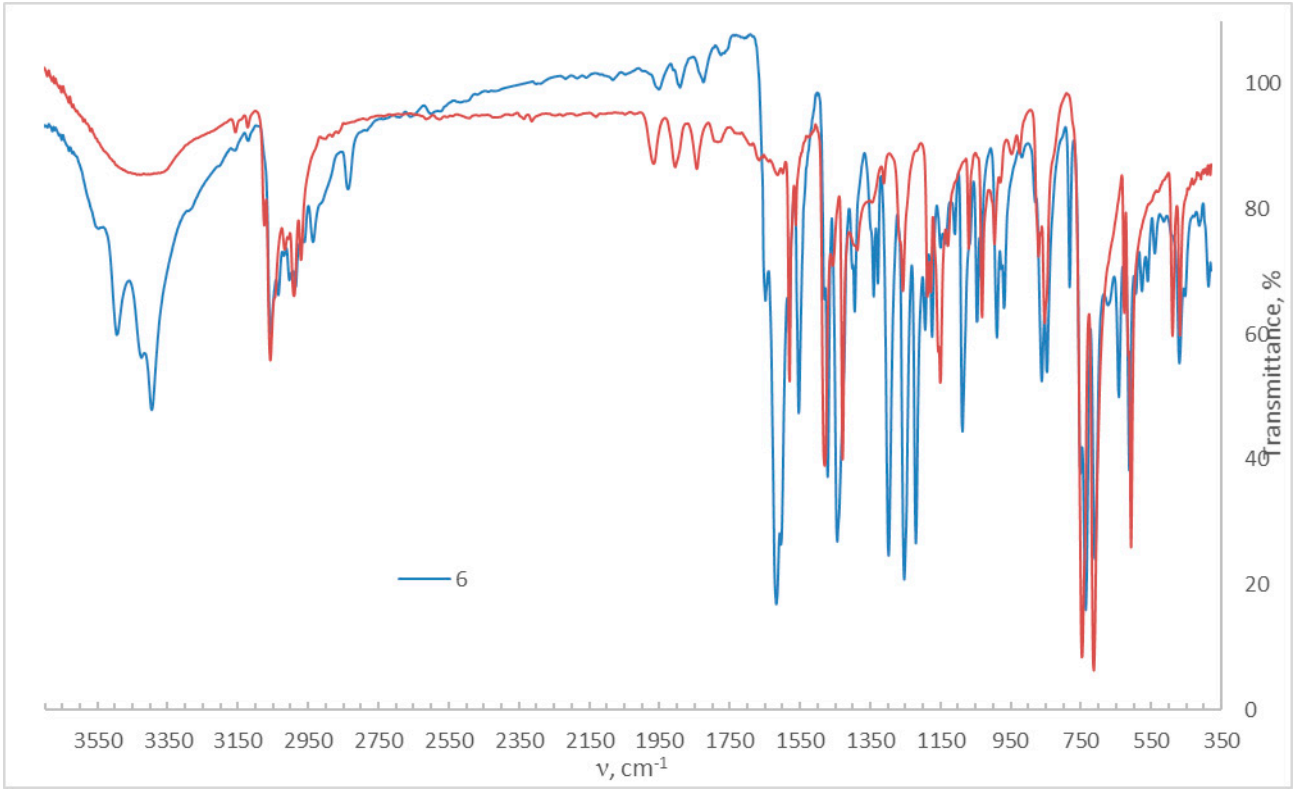

Figure S10. IR spectra of the compound **6** and $NaPh_4B$ registered in KBr pellets.