Electronic Supplementary Information

Chiral vanadium(V) complexes with 2-aminoglucose Schiff-base ligands and their solution configurations: Synthesis, structures, and DFT calculations

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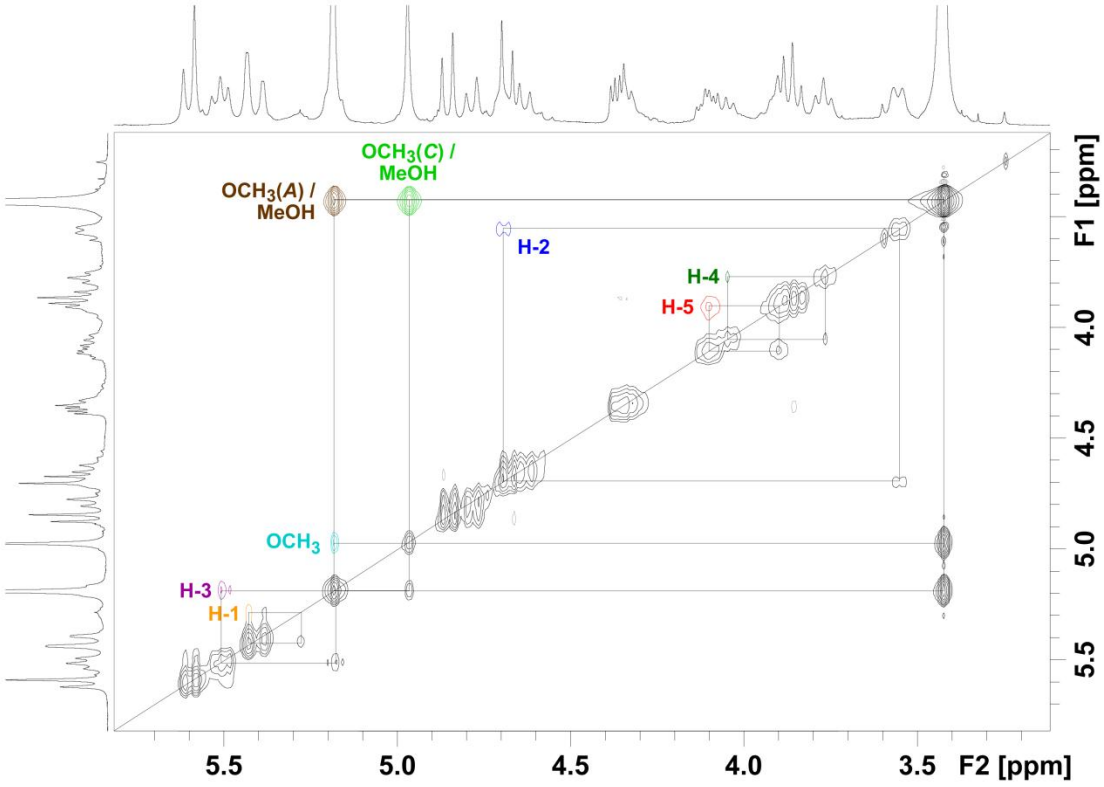

Fig. S1 Aliphatic region of the ^{1}H-^{1}H EXSY spectrum of **1** in a mixture of $CDCl_3$ and CD_3OD.

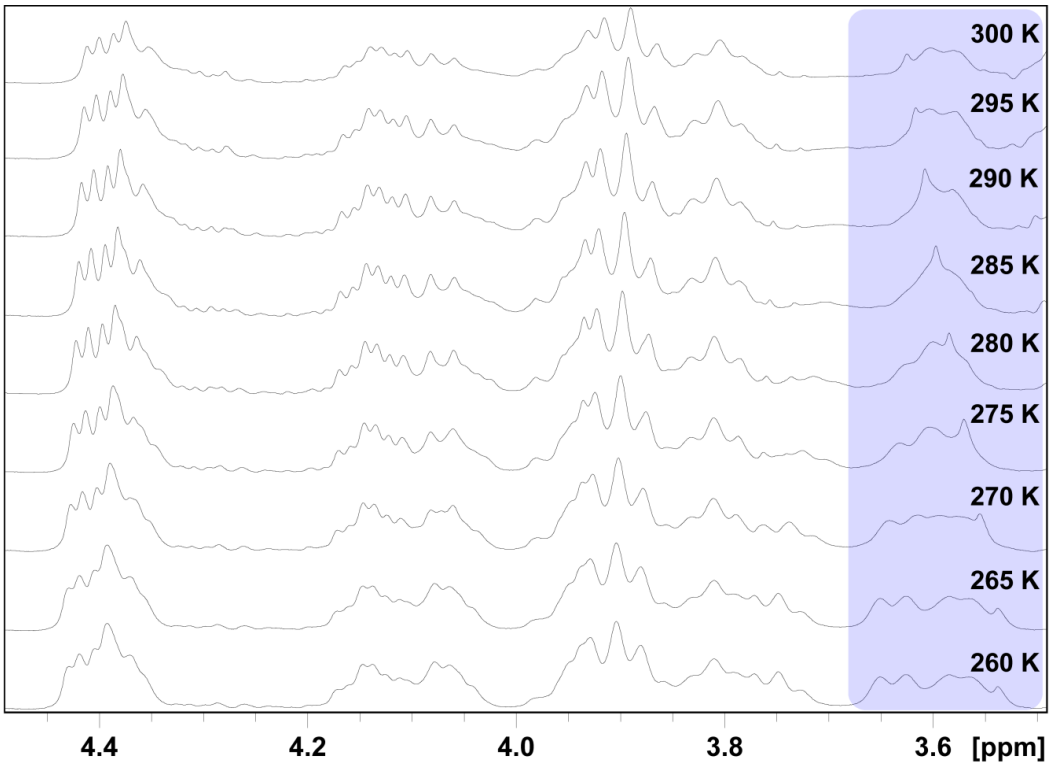

Fig. S2 Variable-temperature ^{1}H NMR spectra of **1** in $CDCl_3$. The region of the H-2 proton is highlighted.

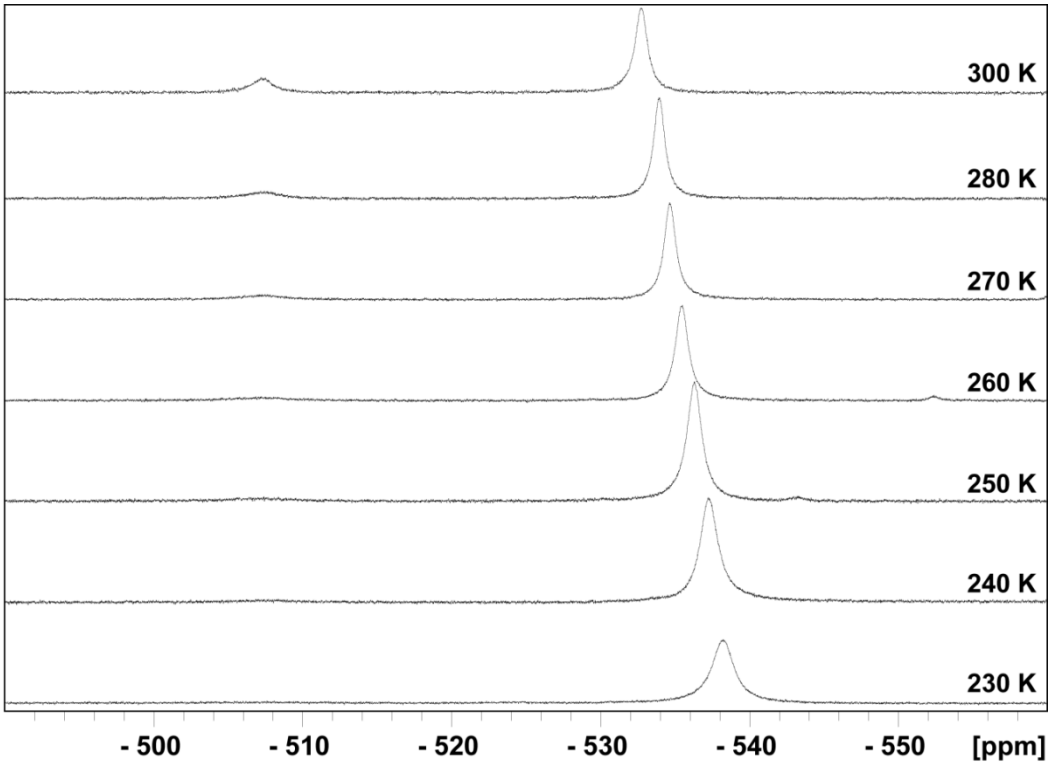

Fig. S3 Variable-temperature ^{51}V NMR spectra of **1** in a mixture of $CDCl_3$ and CD_3OD.

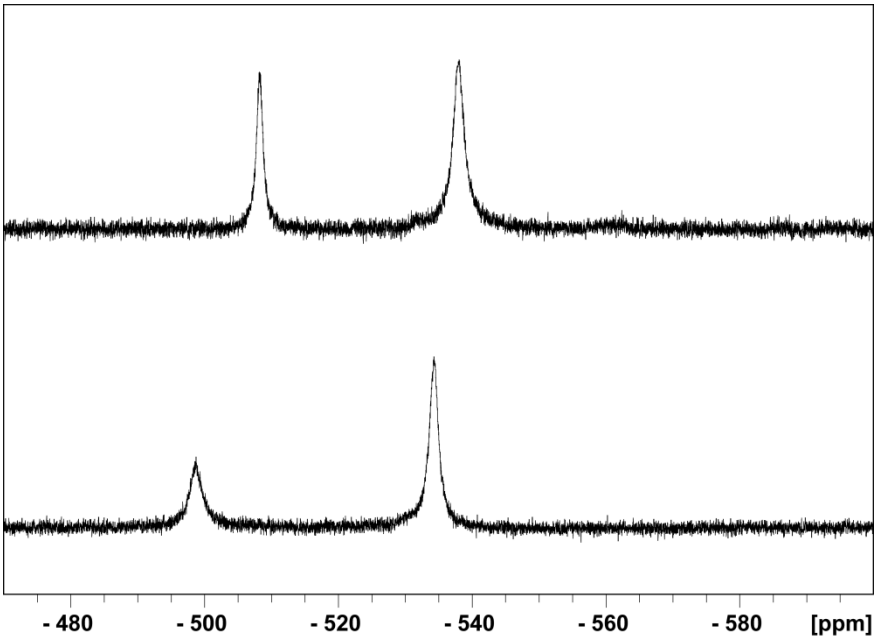

Fig. S4 ^{51}V NMR spectra of **1** in $CDCl_3$ (top) and with added pyridine (bottom).

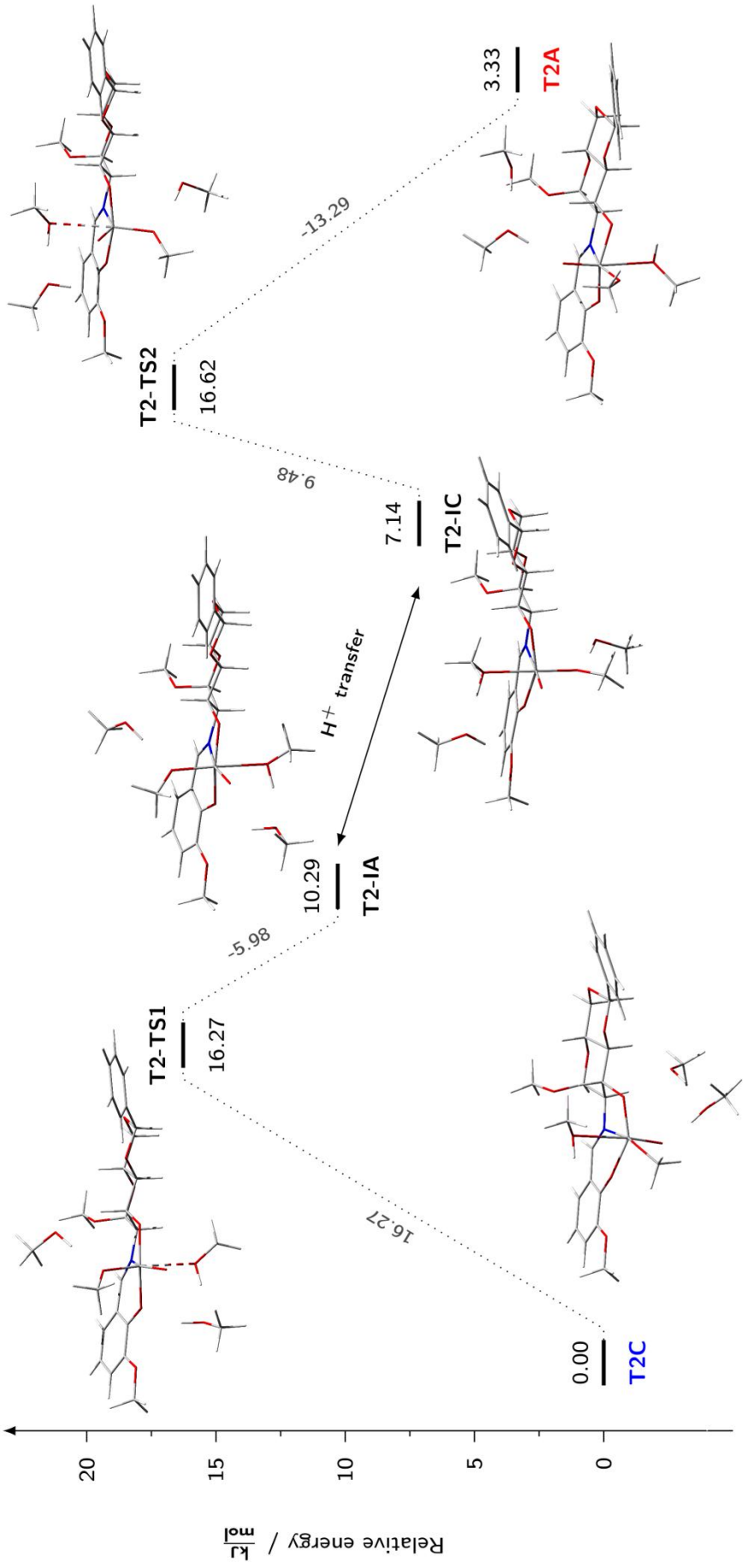

Fig. S5 Scheme for a possible isomerisation mechanism between the *A*- and *C*-configured diastereomers of **2**.

Table S1 Selected bond lengths (pm) and angles (°) for the optimized geometries from DFT calculations of the *A*- and *C*-configured diastereomers of complexes **1** and **2** as well as their methanol adducts **1–MeOH** and **2–MeOH**; for the atom labelling see Fig. 1

	1		**1–MeOH**		**2**		**2–MeOH**	
	A	*C*	*A*	*C*	*A*	*C*	*A*	*C*
V–O1	159.1	159.7	161.0	161.5	159.2	159.7	161.1	161.6
V–O2	191.0	189.6	190.3	192.4	190.4	189.1	189.5	191.7
V–O3	185.7	184.5	187.0	182.8	186.1	184.8	187.5	182.7
V–O4	177.5	178.2	179.0	180.2	177.7	178.5	179.2	180.4
V–N	222.0	221.3	221.8	221.1	221.4	220.5	221.1	219.9
V–O1M	–	–	250.3	256.8	–	–	250.9	262.7
O1–V–O2	104.11	108.10	100.73	100.17	104.20	107.57	100.99	100.51
O1–V–O3	104.63	109.69	100.99	104.75	104.52	109.65	100.93	105.05
O1–V–O4	109.27	104.71	104.35	101.51	109.19	104.85	104.33	102.05
O1–V–N	96.86	93.76	93.14	96.91	97.49	94.44	93.27	97.56
O2–V–O3	144.65	136.86	150.02	148.93	144.82	137.53	149.90	148.64
O2–V–O4	94.68	94.26	98.05	93.41	94.87	94.22	103.51	92.68
O2–V–N	80.10	80.78	81.47	81.63	80.00	80.64	81.36	81.54
O3–V–O4	94.86	95.62	96.32	99.42	94.49	95.39	95.91	99.35
O3–V–N	76.44	76.75	76.94	77.25	76.52	76.84	77.03	77.41
O4–V–N	153.82	161.49	162.23	161.51	153.25	160.69	162.06	160.26

Table S2 Selected ^{1}H, ^{13}C, and ^{51}V NMR chemical shifts from DFT calculations for the *A*- and *C*-configured diastereomers of complex **1** and its methanol adduct **1–MeOH** and their comparison with experimental data

	A configuration			*C* configuration				
	1A	**1A–MeOH**	Exp.	**1C**	**1C–MeOH**	Exp.	Δ(DFT)[a]	Δ(Exp.)[b]
V	–623	–594	–538	–587	–566	–508	32	30
H-2	3.36	3.37	3.54	5.06	4.75	4.72	1.54	1.18
H-3	5.64	5.43	5.53	5.32	5.38	5.20	0.19	0.33
H-4	3.55	3.39	3.76	3.97	3.84	4.10	0.44	0.34
C2	80.4	79.5	73.1	80.8	81.8	75.1	1.4	2.0
C3	90.0	88.4	81.6	97.0	94.5	85.7	6.6	4.1

[a] Average difference between the NMR chemical shifts of the diastereomers: $\Delta(\mathrm{DFT}) = |\,[\delta(\mathbf{1A}) - \delta(\mathbf{1C}) + \delta(\mathbf{1A–MeOH}) - \delta(\mathbf{1C–MeOH})]/2\,|$. [b] $\Delta = |\,\delta_A - \delta_C\,|$.

Table S3 Selected ^{1}H, ^{13}C, and ^{51}V NMR chemical shifts from DFT calculations for the *A*- and *C*-configured diastereomers of complex **2** and its methanol adduct **2–MeOH** and their comparison with experimental data

	A configuration			*C* configuration				
	2A	**2A–MeOH**	Exp.	**2C**	**2C–MeOH**	Exp.	Δ(DFT)[a]	Δ(Exp.)[b]
V	–621	–591	–530	–587	–559	–502	33	28
H-2	3.31	3.37	3.52	5.04	4.76	4.62	1.56	1.10
H-3	5.70	5.52	5.45	5.36	5.34	5.19	0.26	0.26
H-4	3.47	3.41	3.75	3.96	3.83	3.98	0.45	0.23
C2	79.0	79.2	72.9	80.8	81.7	75.1	2.2	2.2
C3	90.9	88.1	81.3	97.0	94.5	85.5	6.2	4.2

[a] Average difference between the NMR chemical shifts of the diastereomers: $\Delta(\mathrm{DFT}) = |\,[\delta(\mathbf{2A}) - \delta(\mathbf{2C}) + \delta(\mathbf{2A–MeOH}) - \delta(\mathbf{2C–MeOH})]/2\,|$. [b] $\Delta = |\,\delta_A - \delta_C\,|$.

Table S4 Selected bond lengths (pm) and angles (°) for the optimized geometries from DFT calculations of the intermediate structures and transition states for the isomerization mechanisms depicted in Figs. 8 and S5

	T1				T2			
	IA	**IC**	**TS1**	**TS2**	**IA**	**IC**	**TS1**	**TS2**
V–O1	160.3	160.3	159.6	159.8	160.5	160.5	159.9	160.2
V–O2	197.2	195.9	195.2	190.5	195.6	191.9	194.5	193.0
V–O3	183.8	183.6	182.8	185.5	184.1	185.2	183.3	182.9
V–N	228.5	232.4	221.4	221.0	228.3	230.5	222.8	224.0
V–OMe	181.7	183.5	180.7	180.3	182.2	184.4	181.2	181.3
V–OHMe	233.0	226.4	315.8	366.0	232.6	225.5	282.0	286.4
O1–V–O2	97.60	98.28	93.87	94.32	98.08	101.83	94.91	93.20
O1–V–O3	101.80	102.67	100.17	97.33	101.61	99.79	100.48	100.29
O1–V–N	163.52	173.69	140.85	141.57	163.66	175.73	145.01	146.23
O2–V–O3	155.56	152.58	156.88	154.28	155.44	151.35	156.79	154.90
O2–V–N	80.01	80.81	80.29	79.74	79.88	80.43	80.15	79.91
O3–V–N	77.16	76.42	77.22	76.87	77.09	76.93	77.26	76.90