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Supporting Information

Dirhodium complexes: determination of absolute configuration by exciton chirality method using VCD spectroscopy

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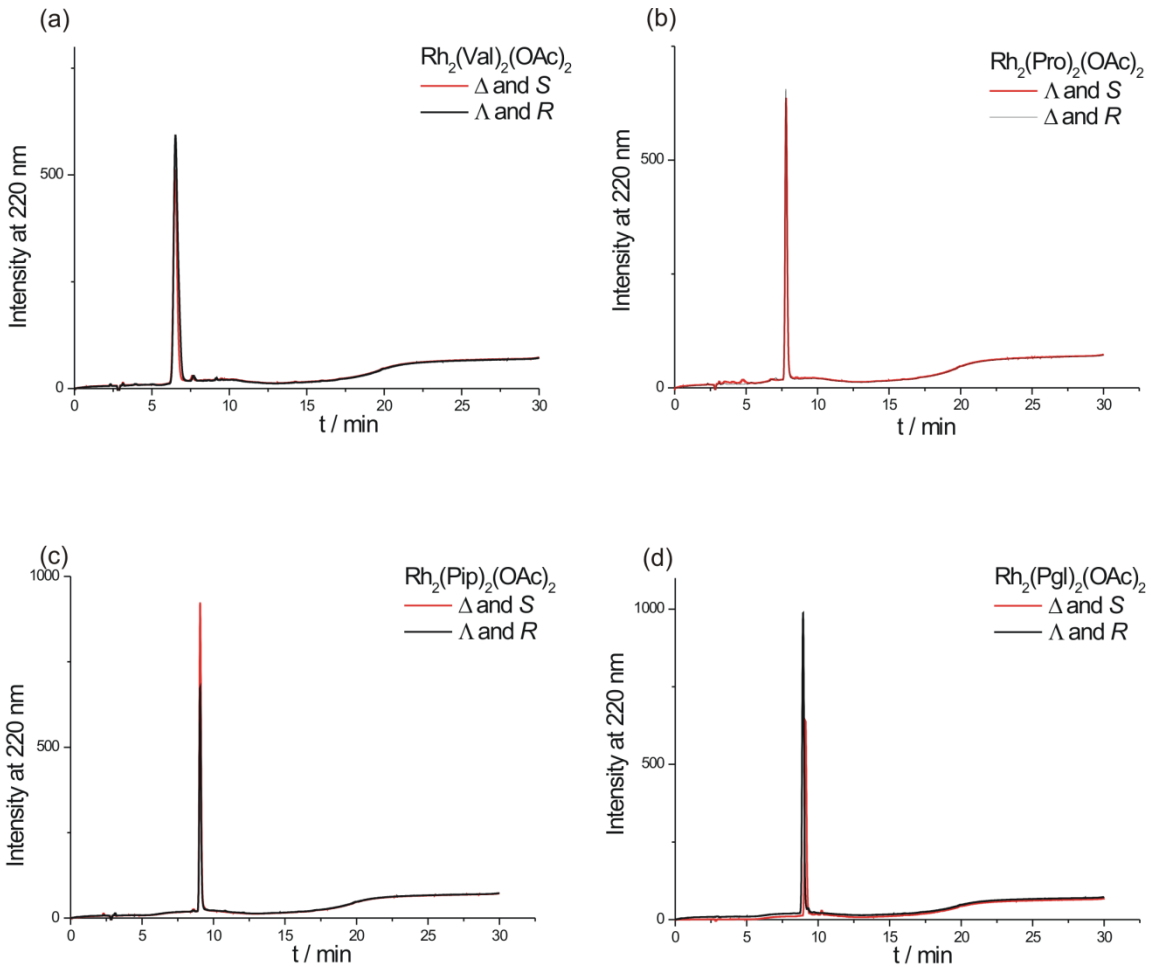

Figure S1. The chromatograms of the purified complexes

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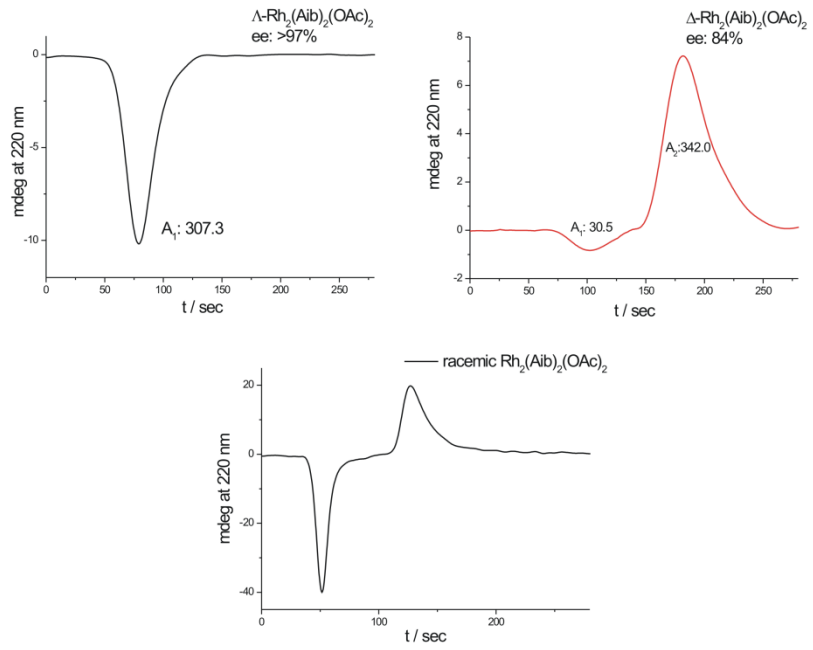

Figure S2. Chiral HPLC-CD separation of the $Rh_2(Aib)_2(OAc)_2$ complex

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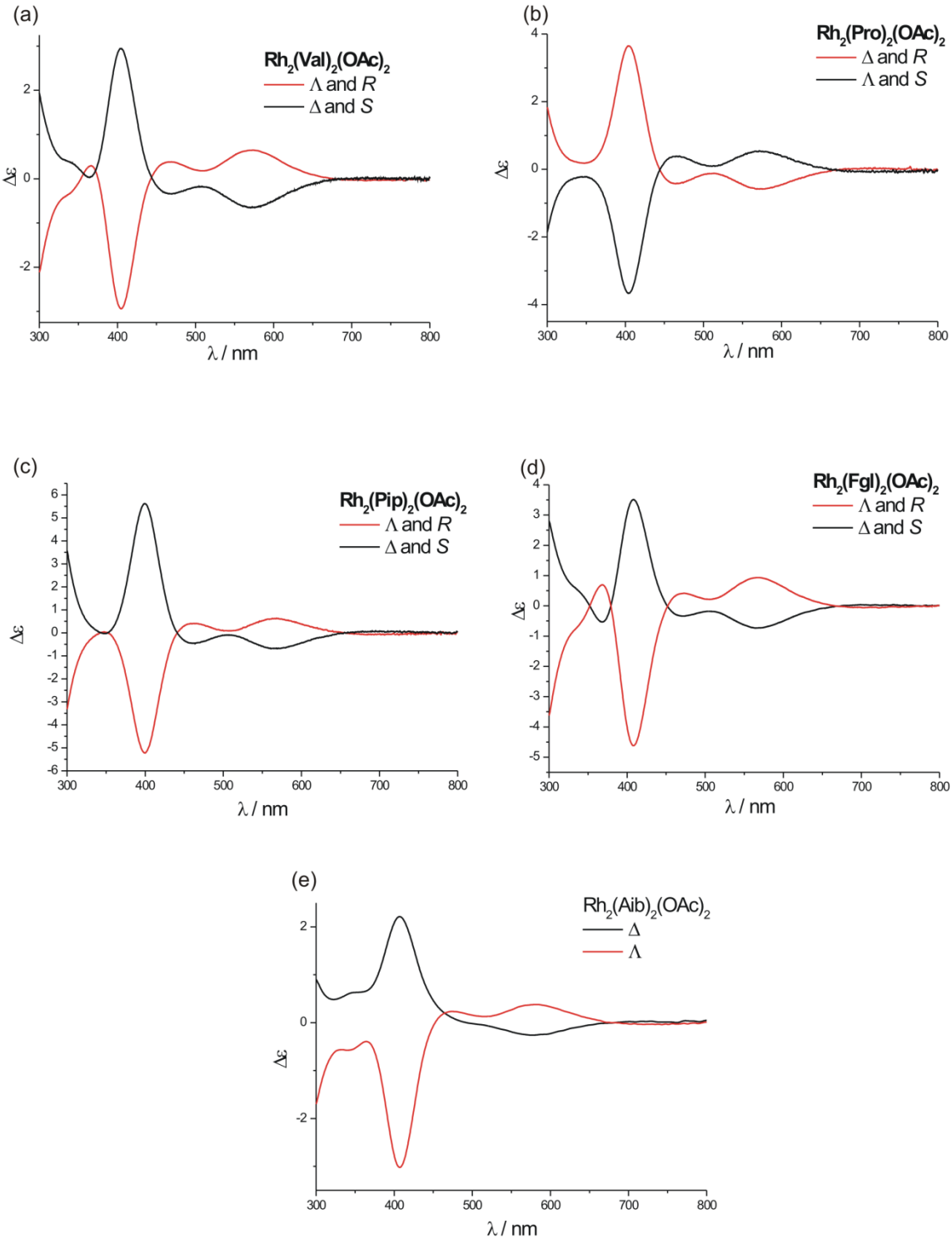

Figure S3. ECD spectra of the chiral complexes (solvent: ACN, c: ~0.4 mg/ml, quartz cell of 10 mm).

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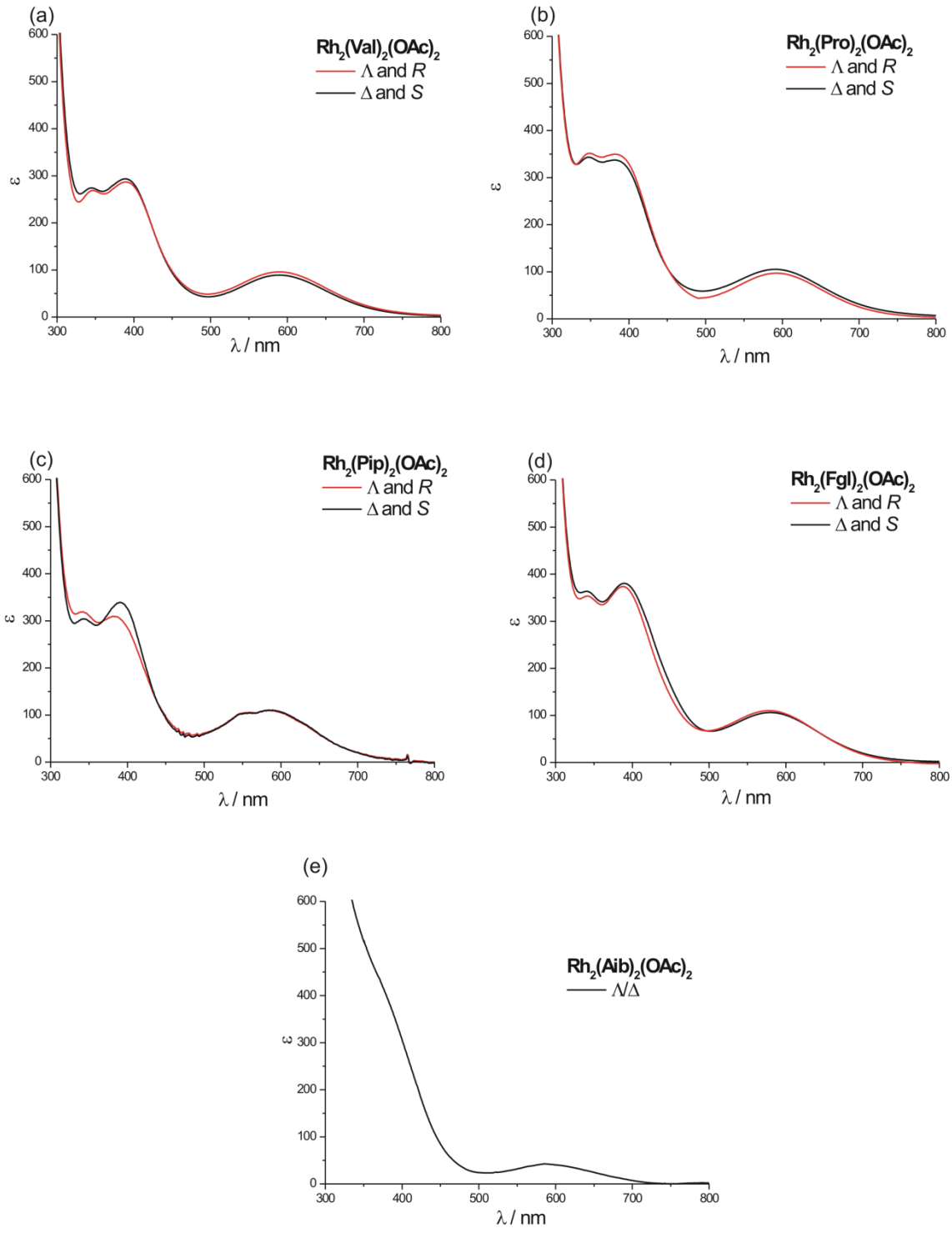

Figure S4. UV-vis spectra of the complexes (ACN, quartz cell of 10 mm, Jasco V-660 spectrophotometer)

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Table S1. UV-vis spectroscopic data of the complexes

Complex	**λ_{max} / nm (ε / $dm^3 \cdot mol^{-1} \cdot cm^{-1}$)**		
$Rh_2(Val)_2(OAc)_2$	589 (89)	389 (291)	346 (272)
$Rh_2(Pro)_2(OAc)_2$	593 (101)	382 (342)	349 (345)
$Rh_2(Pip)_2(OAc)_2$	582 (108)	388 (318)	342 (310)
$Rh_2(Fgl)_2(OAc)_2$	579 (107)	390 (376)	341 (357)
$Rh_2(Aib)_2(OAc)_2$	587 (43)	shoulder	shoulder

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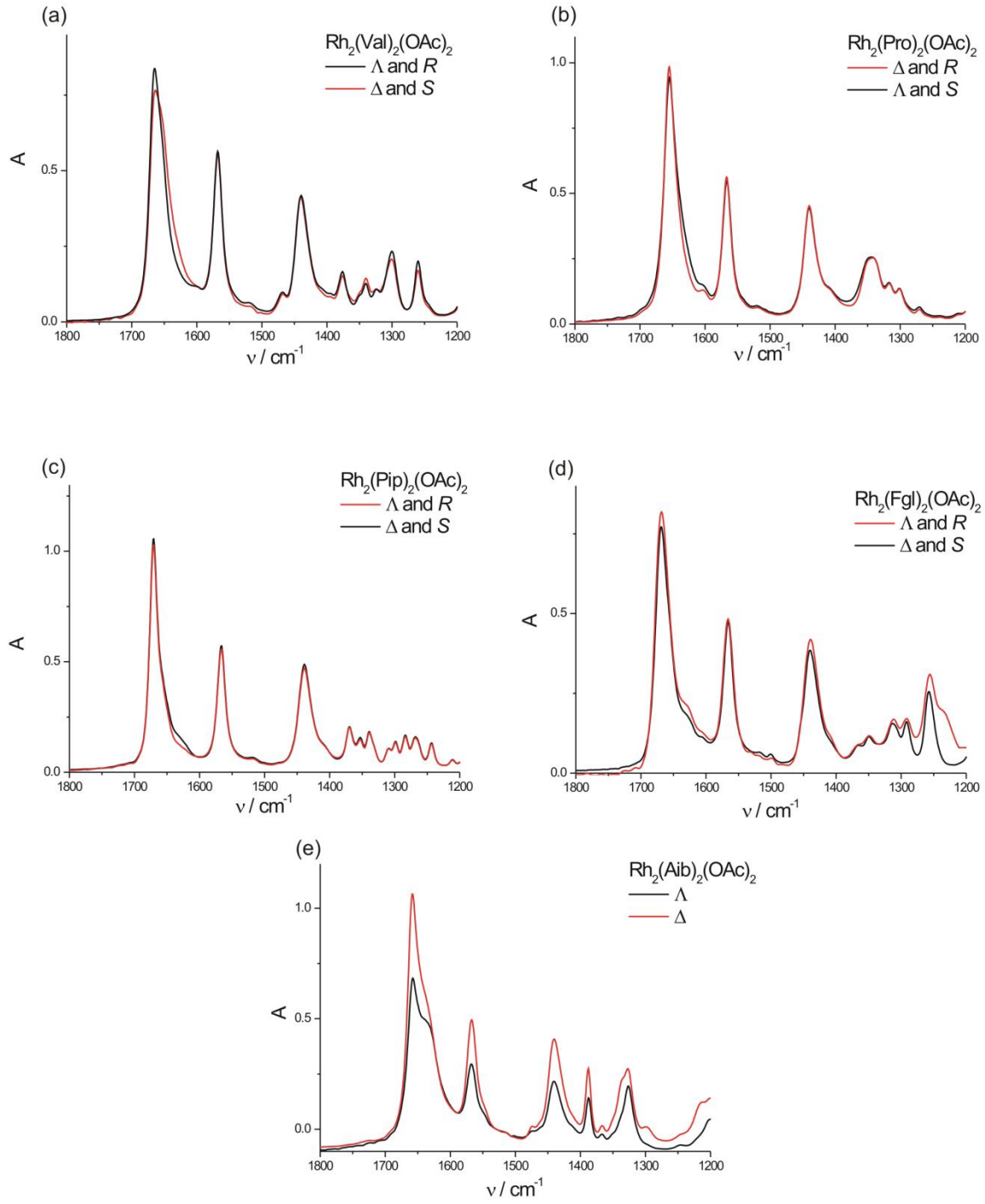

Figure S5. The FT-IR spectra of the chiral complexes (c: 14 mg/ml, ACN-d_3, BaF_2 cell of 0.207 mm).

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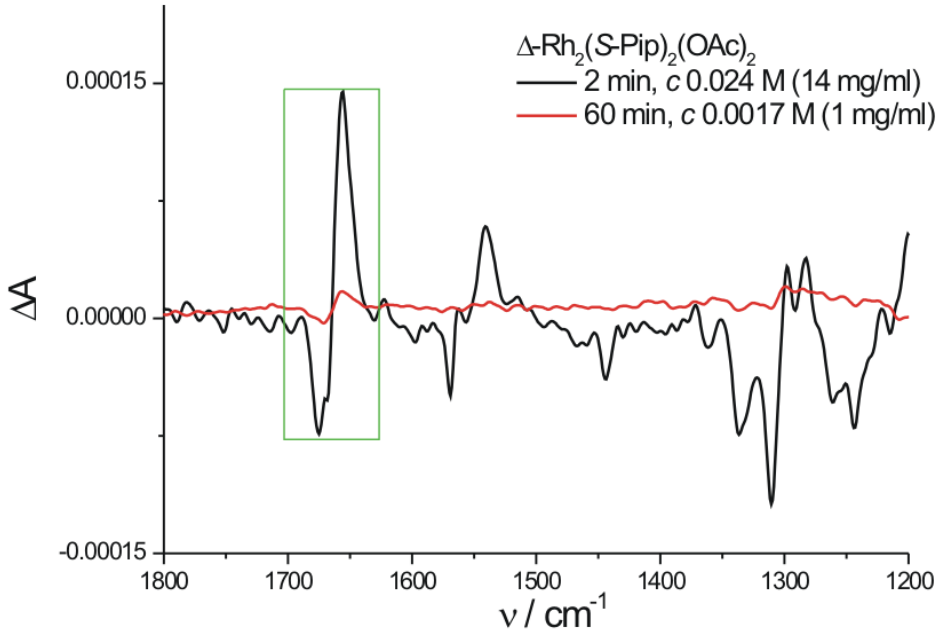
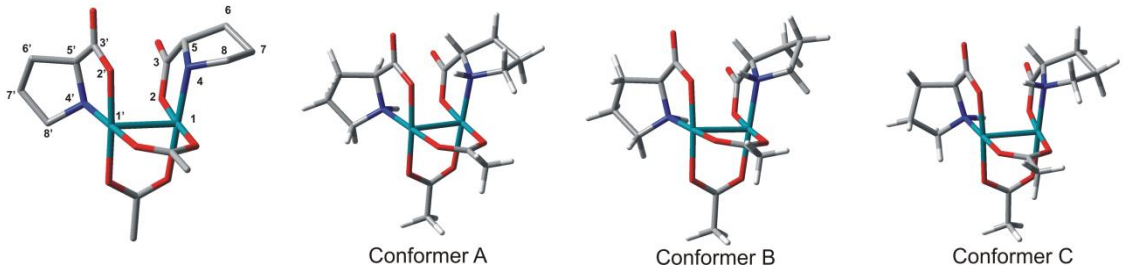


Figure S6. Application of the VCD exciton chirality method for a short and a low-concentration measurement (ACN-d_3, BaF_2 cell of 0.207 mm).

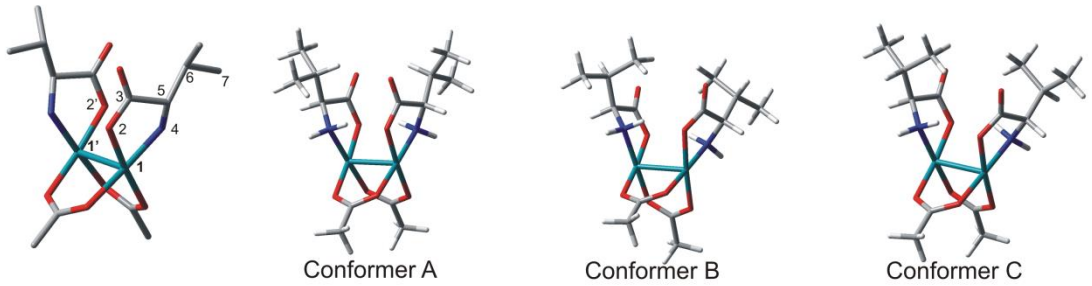
Table S2. Results of population analysis

Compound	Conformer	ΔG(kcal/mol)	Population
Δ-Rh_2(*S*-Val)$_2$(OAc)$_2$	A	0.000	0.811
	B	0.948	0.163
	C	2.021	0.026
Λ-Rh_2(*S*-Pro)$_2$(OAc)$_2$	A	0.000	0.528
	B	0.319	0.307
	C	0.689	0.164
Δ-Rh_2(*S*-Pip)$_2$(OAc)$_2$	A	0.000	1
Δ-Rh_2(*S*-Pgl)$_2$(OAc)$_2$	A	0.000	0.947
	B	1.695	0.053
Δ- Rh_2(Aib)$_2$(OAc)$_2$	A	0.000	1



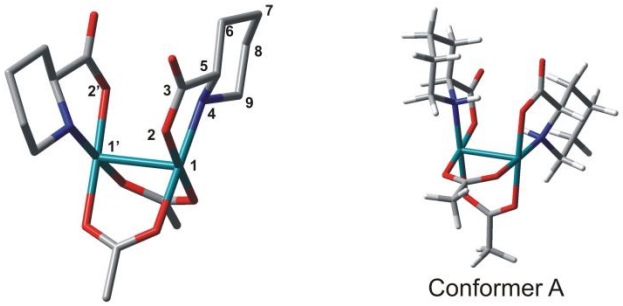
Complex	Conformer	Torsion Angle						
		α(2,1,1',2')	β(4,5,3,2), β'	γ(1,4,5,6),γ'	δ(4,5,6,7), δ'	ε(5,6,7,8), ε'	ζ(6,7,8,4), ζ'	η(7,8,4,5), η'
Λ-Rh_2(*S*-Pro)$_2$(OAc)$_2$	A	-82	-8, -8	-113, -116	+13, -32	-33, +30	+41, -34	-33, +14
	B	-81	-7	-115	-32	+40	-34	+14
	C	-81	-10	-111	+12	-33	+41	-34

Figure S7. Conformers of **Λ**-Rh_2(*S*-Pro)$_2$(OAc)$_2$ complex and their relevant torsion angles



Complex	Conformer	Torsion Angle			
		α(2,1,1',2')	β(4,5,3,2)	γ(1,4,5,6)	δ(4,5,6,7)
Δ-Rh_2(*S*-Val)$_2$(OAc)$_2$	A	+74	+34	-164	-43
	B	+72	+28	-169	63
	C	+73	+29	-172	-161

Figure S8. Conformers of **Δ**-Rh_2(*S*-Val)$_2$(OAc)$_2$ complex and their relevant torsion angles



Complex	Conformer	Torsion Angle							
Δ-Rh_2(*S*-Pip)$_2$(OAc)$_2$		α(2,1,1',2')	β(4,5,3,2)	γ(1,4,5,6)	δ(4,5,6,7)	ε(5,6,7,8)	ζ(6,7,8,9)	η(7,8,9,4)	θ(8,9,4,5)
	A	+75	+33	-165	-57	+53	-52	54	-59

Figure S9. Conformer A of **Δ**-Rh_2(*S*-Pip)$_2$(OAc)$_2$ complex and its relevant torsion angles

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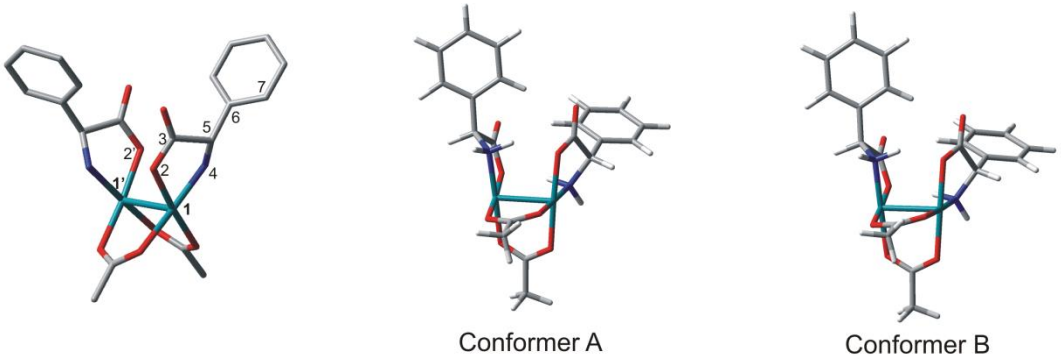
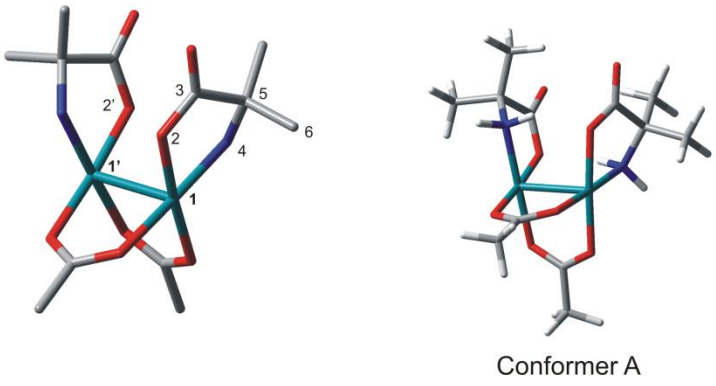


Complex	Conformer	Torsion Angle			
		α(2,1,1',2')	β(4,5,3,2)	γ(1,4,5,6)	δ(4,5,6,7)
Δ-Rh_2(*S*-Pgl)$_2$(OAc)$_2$	A	+69	+35	-172	-113
	B	+66	+33	-172	-111

Figure S10. Conformers of **Δ**-Rh_2(*S*-Pgl)$_2$(OAc)$_2$ complex and their relevant torsion angles



Complex	Conformer	Torsion Angle		
		α(2,1,1',2')	β(4,5,3,2)	γ(1,4,5,6)
Δ-Rh_2(Aib)$_2$(OAc)$_2$	A	+74	+28	+83

Figure S11. Conformer A of **Δ**-Rh_2(Ai*b*)$_2$(OAc)$_2$ complex and its relevant torsion angles