

## **Solvent control of optical resolution of 2-amino-1-phenylethanol using dehydroabietic acid**

**Kayoko Taniguchi,<sup>\*a,b</sup> Marie Aruga,<sup>a</sup> Mikio Yasutake<sup>a</sup> and Takuji Hirose<sup>\*a</sup>**

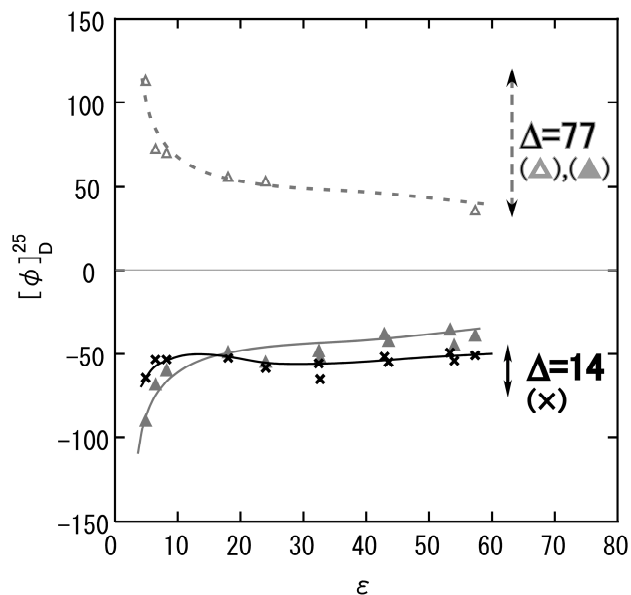
<sup>a</sup> Graduate School of Science and Engineering, Saitama University, Shimo-Ohkubo 255, Sakura-ku, Saitama, Saitama 338-8570, Japan, <sup>b</sup> Eco-Soft Materials Research Unit, RIKEN (The Institute of Physical and Chemical Research), Hirosawa 2-1, Wako, Saitama 351-0198, Japan.

E-mail: [hirose@apc.saitama-u.ac.jp](mailto:hirose@apc.saitama-u.ac.jp); [kytaniguchi@riken.jp](mailto:kytaniguchi@riken.jp)

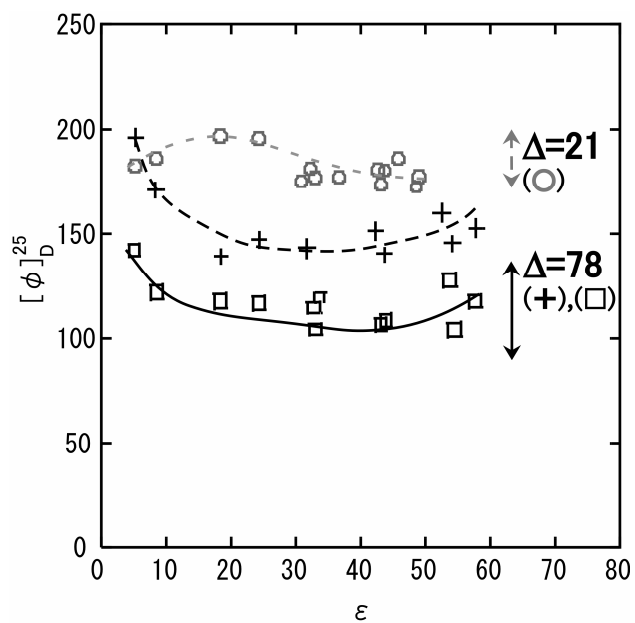
### **Contents:**

1. Solvent dependency of molar rotation of enantiomers and the chiral salts	S2
2. Solvent dependency of molar rotation of diastereomeric salts	S3
3. Hydrogen bonding geometry of diastereomeric salts	S4

### 1. Solvent dependency of molar rotation of enantiomers and the chiral salts

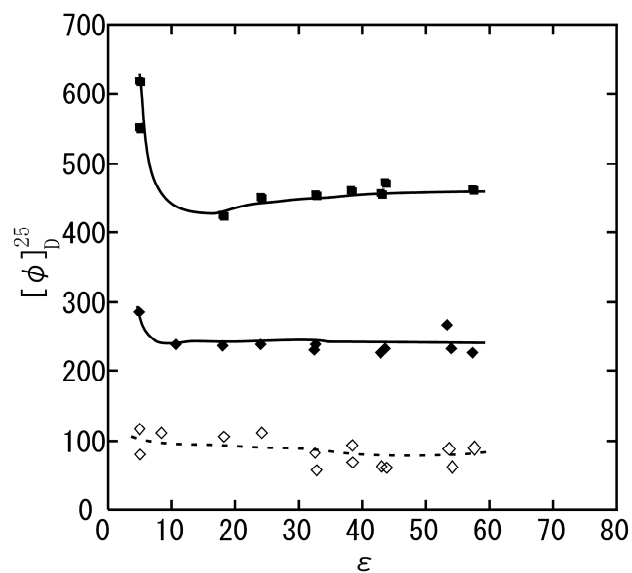


**Fig. S1** Solvent dependency of molar rotation of  $(R)\text{-1}$  and  $(S)\text{-1}$  and the chiral salt with  $\text{CH}_3\text{COOH}$  ( $1/\text{CH}_3\text{COOH}$ ).  $(R)\text{-1}$  ( $\blacktriangle$ ),  $(S)\text{-1}$  ( $\triangle$ ), and  $1/\text{CH}_3\text{COOH}$  ( $\times$ ).



**Fig. S2** Solvent dependency of molar rotation of  $2$  and the chiral salt with  $2\text{-AE}$  ( $2\text{-AE}/2$ ) and  $2\text{-PrNH}_2$  ( $2\text{-PrNH}_2/2$ ).  $2$  ( $\circ$ ),  $2\text{-AE}/2$  ( $+$ ),  $2\text{-PrNH}_2/2$  ( $\square$ ).

## 2. Solvent dependency of molar rotation of diastereomeric salts



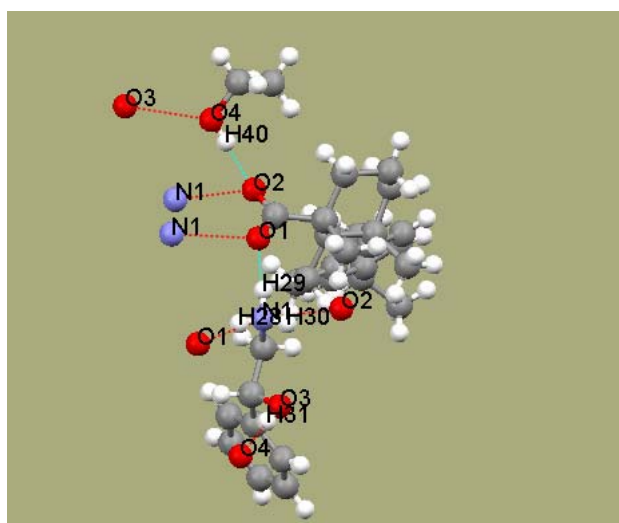
**Fig. S3** Solvent dependence of molar rotation of the diastereomeric salts ((*R*)-**1/2** and (*S*)-**1/2**). (*R*)-**1/2** ( $\diamond$ ), (*S*)-**1/2** (1:1) ( $\blacklozenge$ ), (*S*)-**1/2** (1:2) ( $\blacksquare$ ).

### 3. Hydrogen bonding geometry of the diastereomeric salts

**Table S1** Hydrogen bonding geometry of the (*R*)-1/2 salt.

D-H (Å)	D...A (Å)	H...A (Å)	D-H...A (°)	*Sym.
O4-H40	O4...O2	H40...O2	O4-H40...O2	(1)
0.84	2.709(4)	1.88	170	
N1-H30	N1...O2	H30...O2	N1-H30...O2	(2)
0.91	2.787(5)	1.93	155	
O3-H31	O3...O4	H31...O4	O3-H31...O4	(3)
0.84	2.714(5)	1.88	176	
N1-H28	N1...O1	H28...O1	N1-H28...O1	(4)
0.91	2.789(4)	1.90	166	
N1-H29	N1...O1	H29...O1	N1-H29...O1	(1)
0.91	2.721(5)	1.82	169	

\* (1) +x, +y, +z; (2) +x, -1+y, +z; (3) 1-x, -3/2+y, 1-z; (4) 1-x, -1/2+y, 1-z.

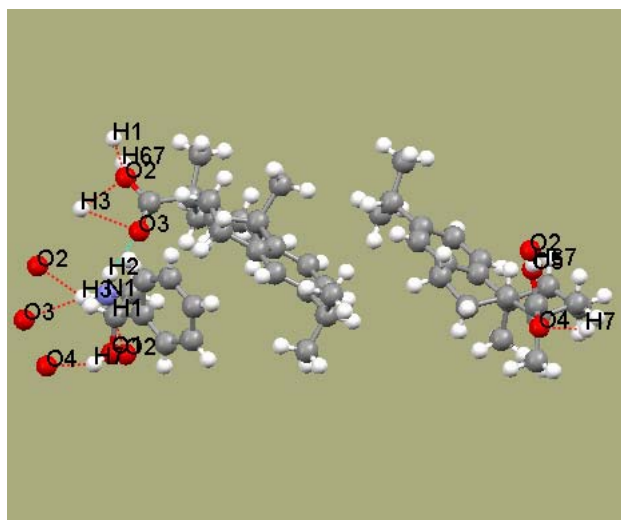


**Fig. S4** Hydrogen bonding geometry of the (*R*)-1/2 salt.

**Table S2** Hydrogen bonding geometry of the (*S*)-1/2 (1:2) salt.

D-H (Å)	D...A (Å)	H...A (Å)	D-H...A (°)	*Sym.
N1-H1	N1...O2	H1...O2	N1-H1...O2	(1)
0.91	2.788(5)	1.88	172	
N1-H2	N1...O3	H2...O3	N1-H2...O3	(2)
0.91	2.655(6)	1.87	144	
O5-H67	O5...O2	H67...O2	O5-H67...O2	(3)
0.84	2.582(5)	1.75	173	
O1-H7	O1...O4	H7...O4	O1-H7...O4	(5)
0.84	2.695(6)	1.91	155	
N1-H3	N1...O2	H3...O2	N1-H3...O2	(4)
0.91	3.049(5)	2.29	141	

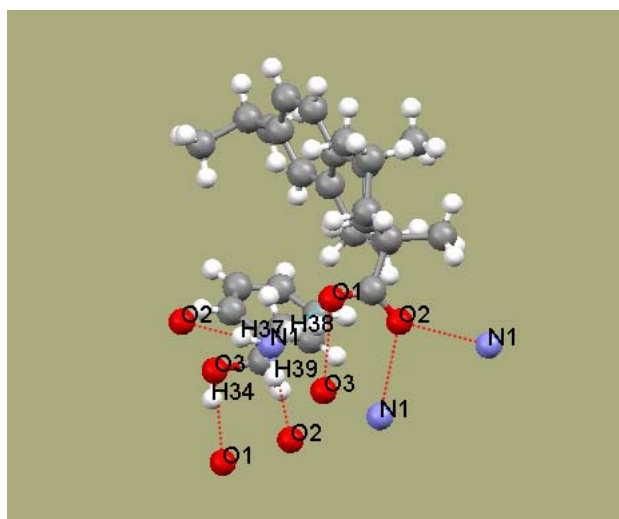
\*(1) 1+ x, +y, +z; (2) +x, +y, +z; (3) -x, -1/2+y, 1/2-z; (4) 1/2+x, 3/2-y, -z; (5) 3/2-x, 1-y, -1/2+z.

**Fig. S5** Hydrogen bonding geometry of the (*S*)-1/2 (1:2) salt.

**Table S3** Hydrogen bonding geometry of the (*S*)-1/2 (1:1) salt.

D-H (Å)	D··A (Å)	H··A (Å)	D-H··A (°)	*Sym.
N1-H38	N1··O1	H38··O1	N1-H38··O1	(1)
0.91	2.729(3)	1.82	174	
N1-H39	N1··O2	H39··O2	N1-H39··O2	(2)
0.91	2.764(3)	1.86	170	
N1-H37	N1··O2	H37··O2	N1-H37··O2	(3)
0.91	2.744(3)	1.84	175	
O3-H34	O3··O1	H34··O1	O3-H34··O1	(2)
0.84	2.884(3)	2.09	159	

\*(1) +x, +y, +z; (2) 1-x, -1/2+y, 1-z; (3) +x, -1+y, +z.

**Fig. S6** Hydrogen bonding geometry of the (*S*)-1/2 (1:1) salt.