

Supporting Information

Revisiting Homochiral versus Heterochiral Interactions Through a Long Detective Story of a Useful Azobis-nitrile and Puzzling Racemate

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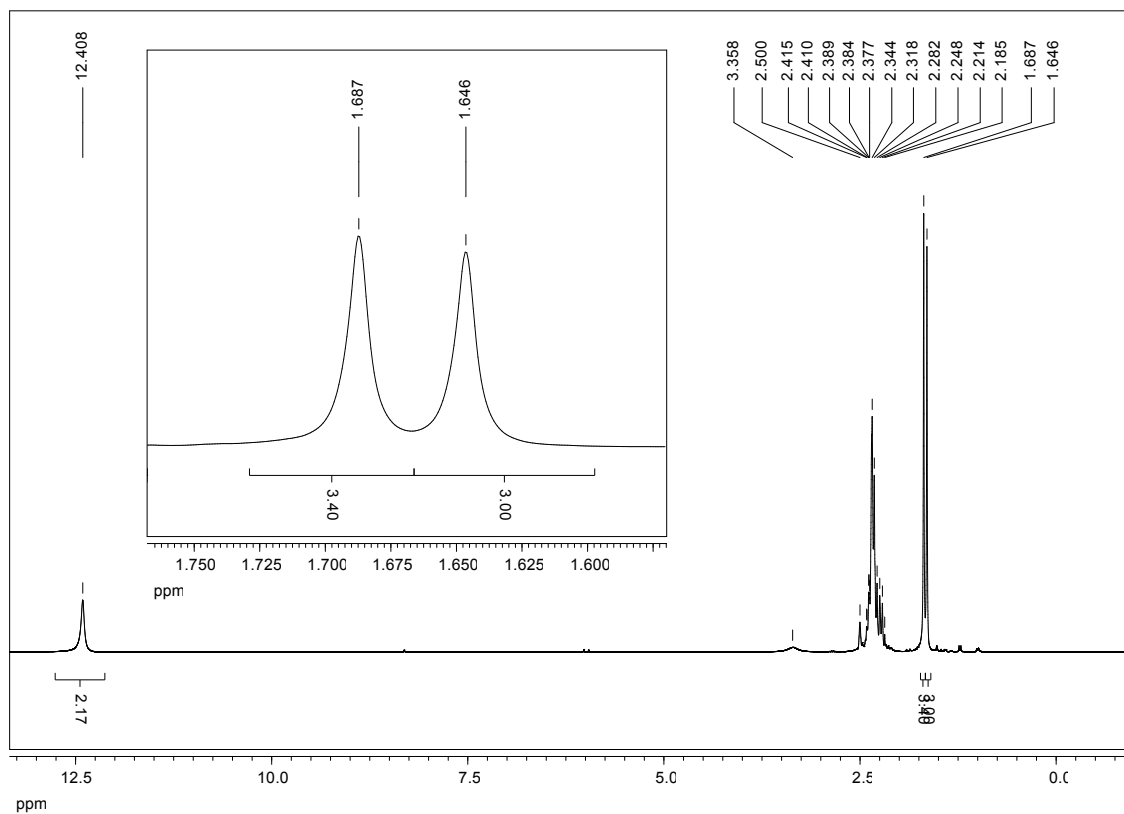


Figure S1. Proton NMR spectrum of ACPA in DMSO- d_6 at 300 MHz. Inset: magnification of diastereotopic methyl groups and signal integration to determine the *meso/d,l* ratio.

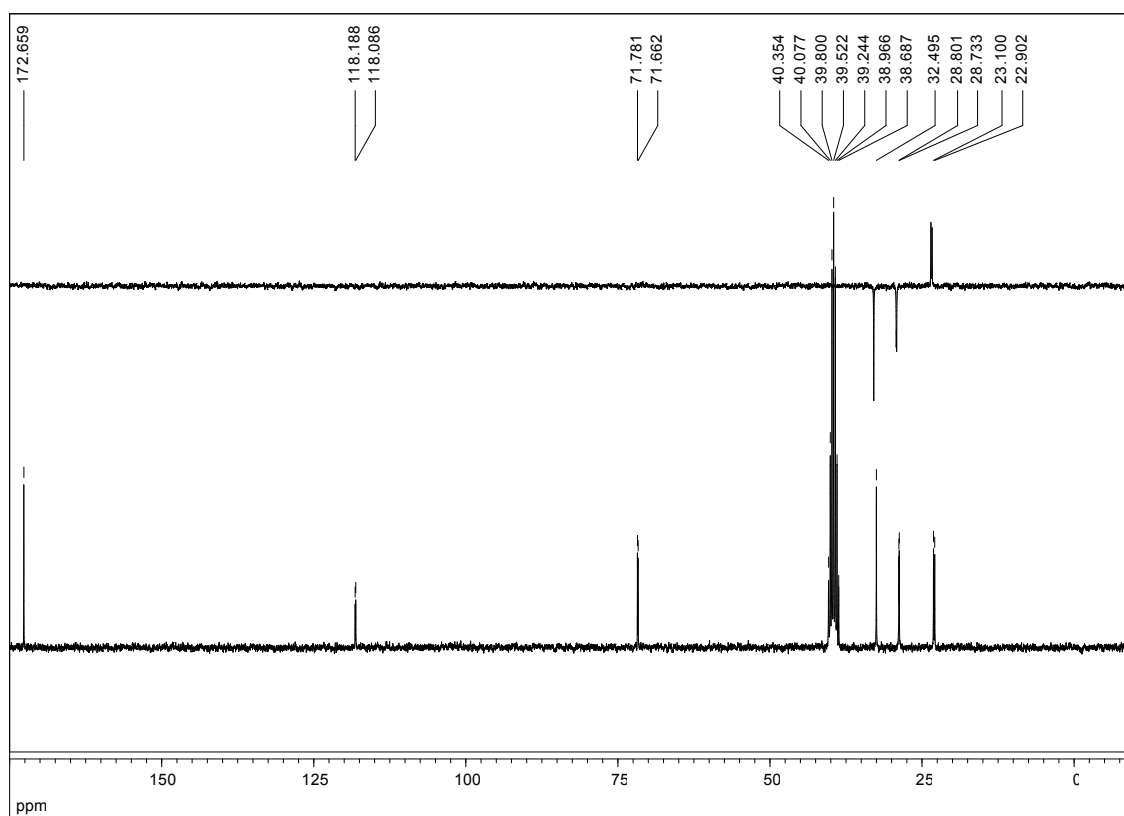


Figure S2. ^{13}C NMR spectrum of ACPA (Aldrich[®]) in DMSO- d_6 at 75 MHz. Top: DEPT experiment of polarization transfer.

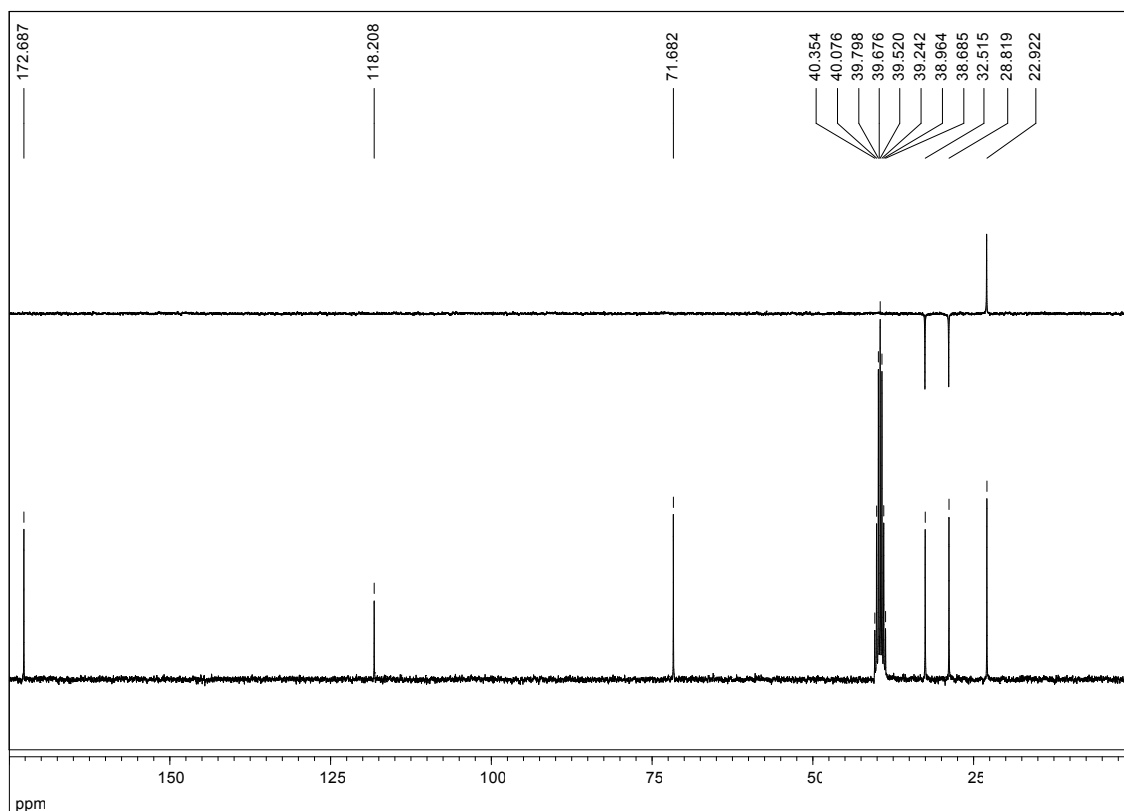


Figure S3. ^{13}C NMR spectrum of racemic-ACPA, (*d,l*)-stereoisomer, in $\text{DMSO-}d_6$ at 75 MHz (bottom); Top: DEPT experiment of polarization transfer.

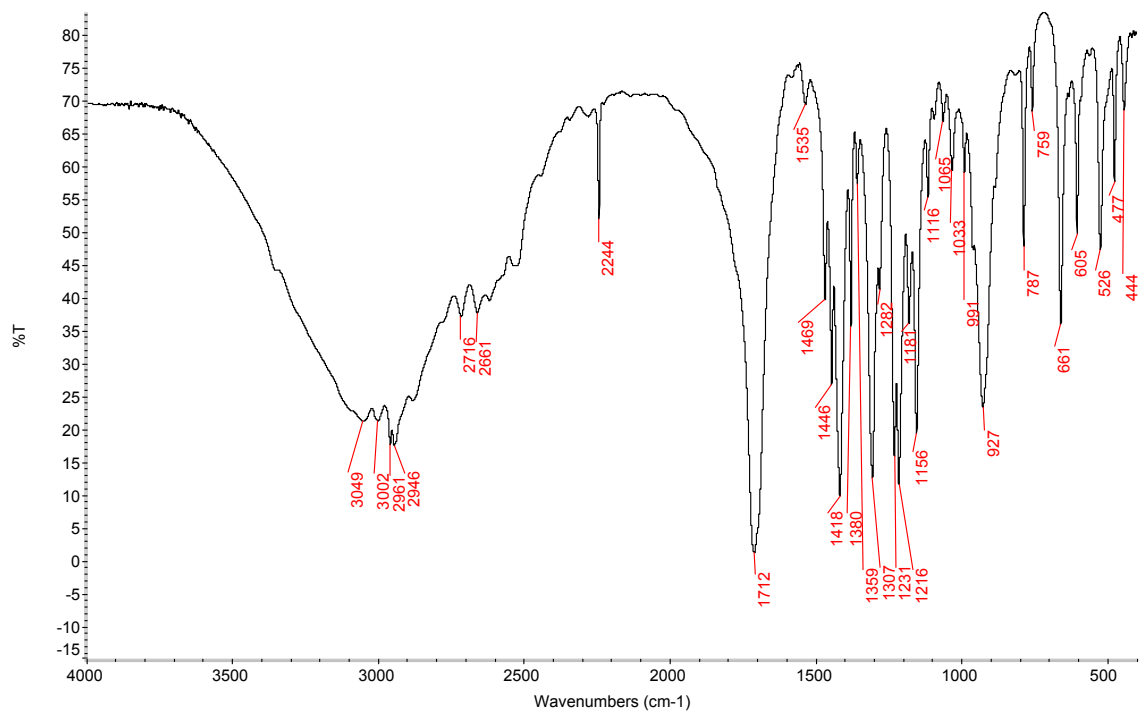


Figure S4. FT-IR spectrum of *meso*-ACPA recorded on a KBr pellet at ambient temperature.

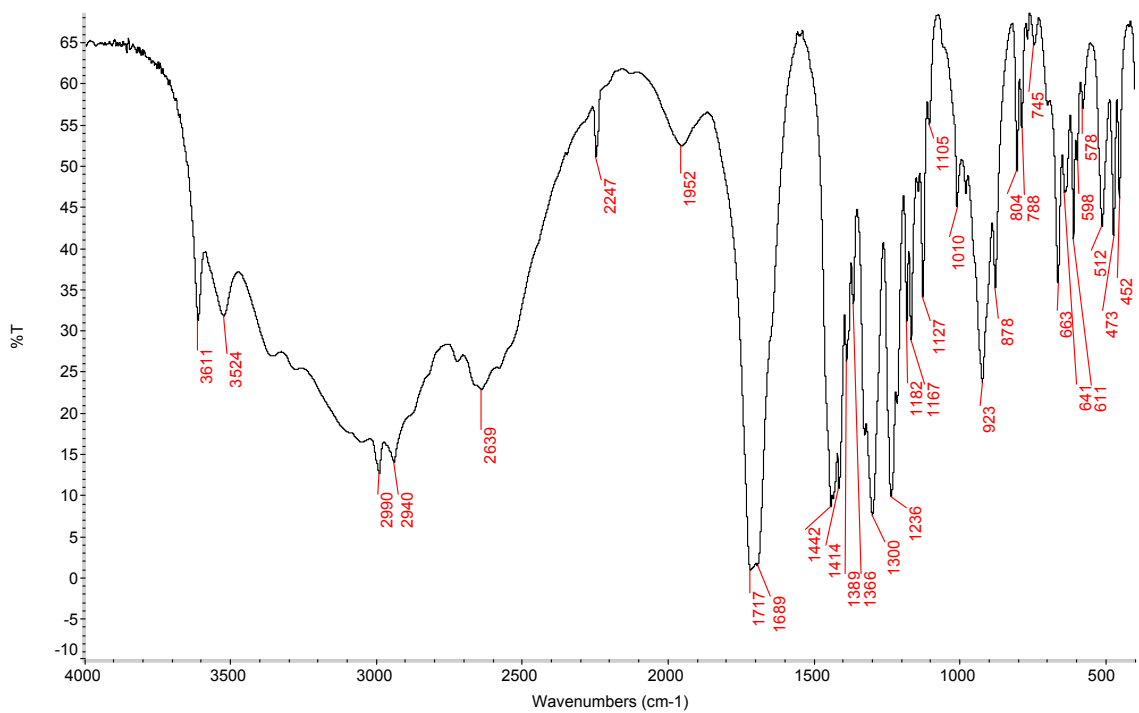


Figure S5. FT-IR spectrum of racemic ACPA (*d,l*-pair) recorded on a KBr pellet at ambient temperature.

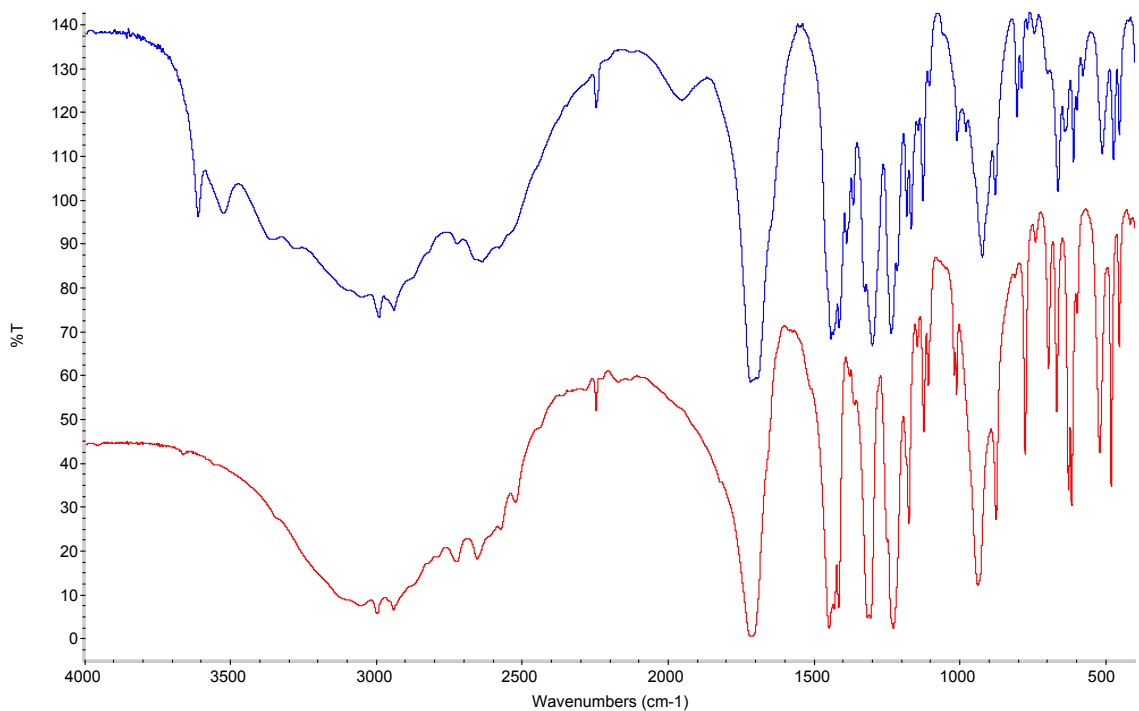


Figure S6. Comparative IR spectra (KBr pellets) of racemic ACPA (top) and a scalemic mixture enriched in the levorotatory enantiomer (bottom).

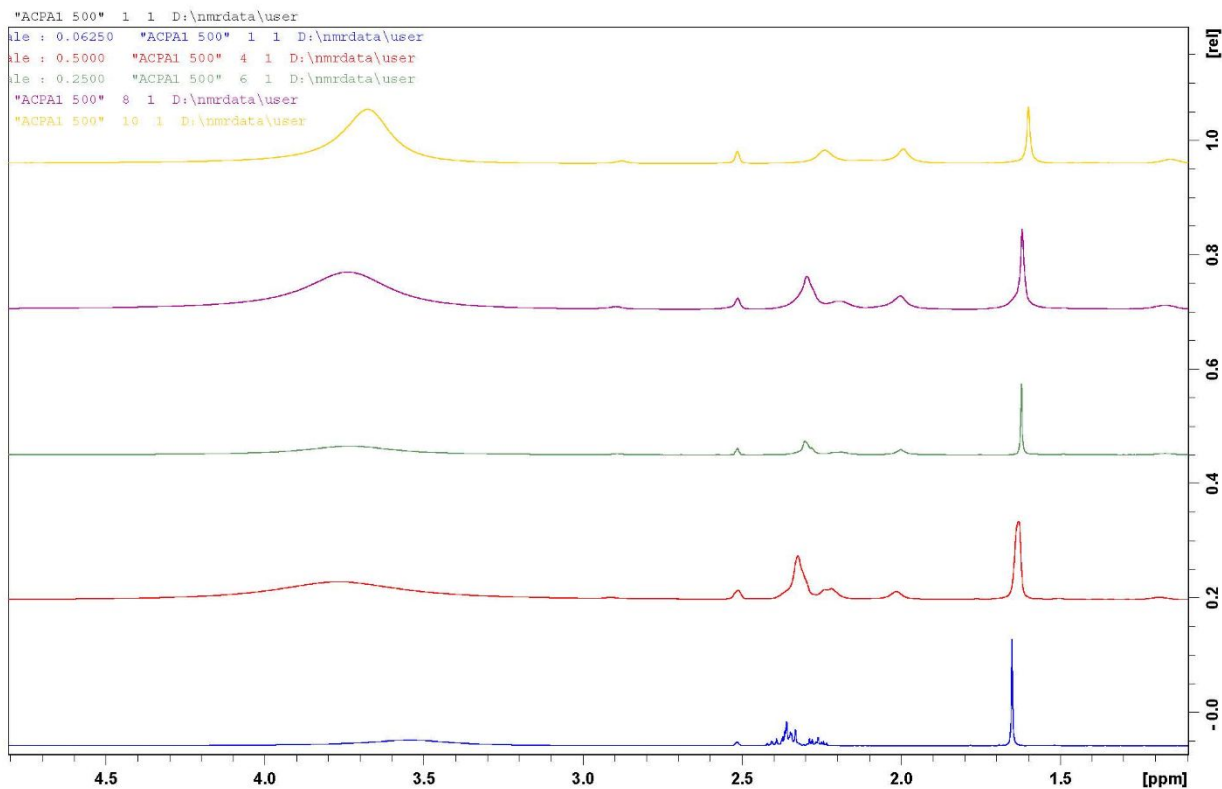


Figure S7. ^1H NMR spectrum of (*d,l*)-ACPA (enantioenriched in the levorotatory enantiomer) in $\text{DMSO-}d_6$ at 500 MHz (bottom), and spectra recorded after successive addition of $\text{Eu}(\text{hfc})_3$ in 0.25:1, 0.5:1, 0.75:1 and 1:1 reagent:substrate molar ratios.

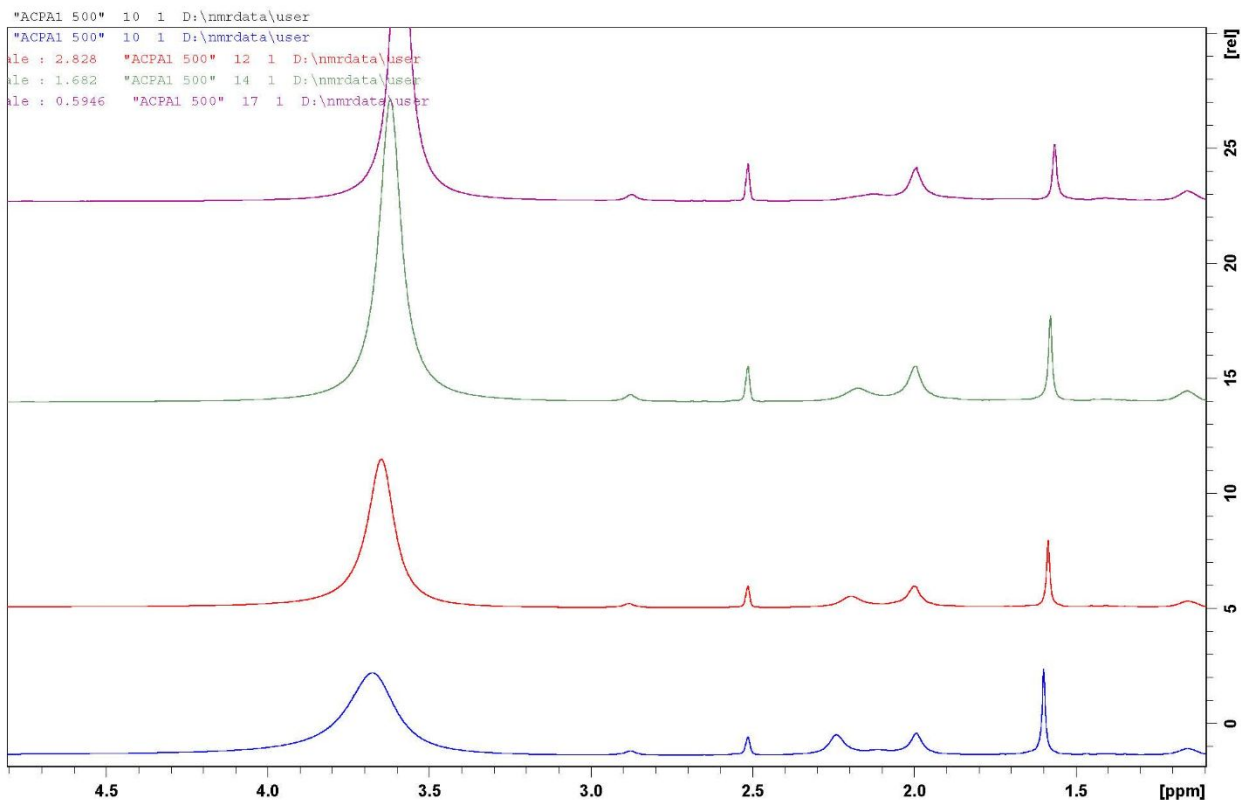


Figure S8. ^1H NMR spectrum of (*d,l*)-ACPA (enantioenriched in the levorotatory enantiomer) in $\text{DMSO-}d_6$ at 500 MHz (bottom), and spectra recorded after successive addition of $\text{Eu}(\text{hfc})_3$ in 1.25:1, 1.5:1, 1.75:1 and 2:1 reagent:substrate molar ratios.

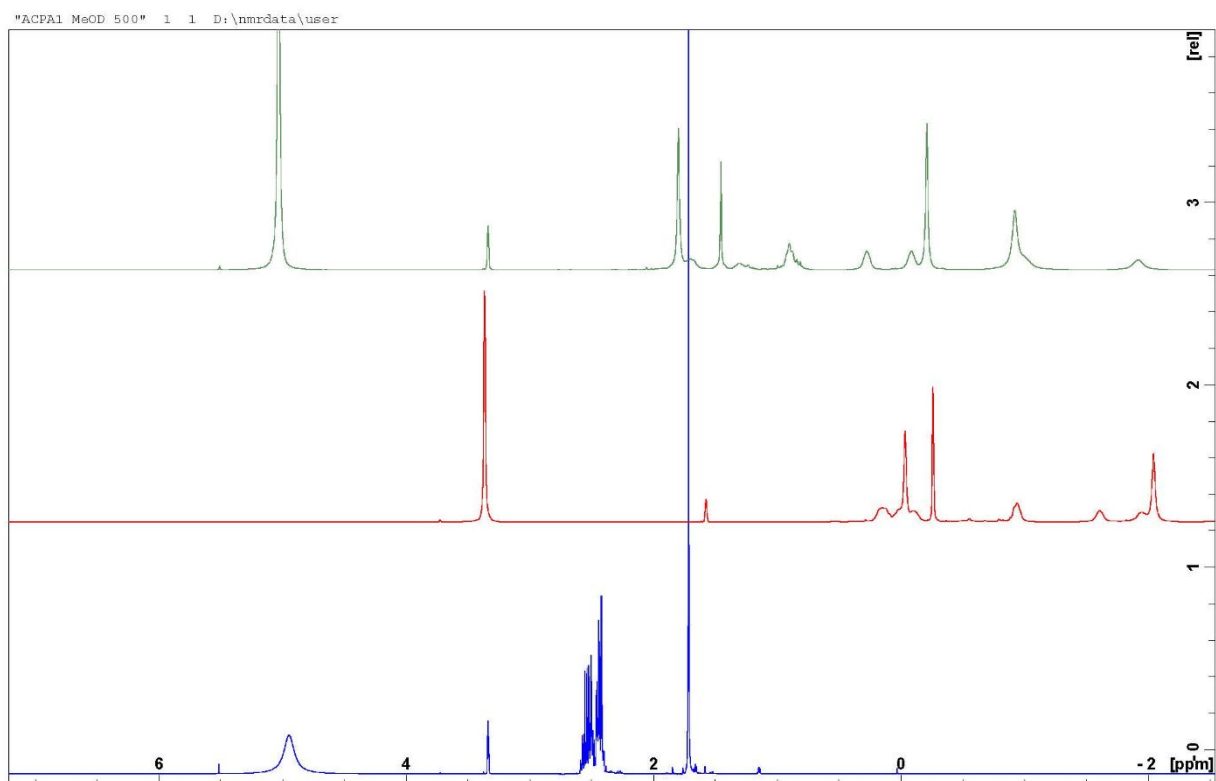


Figure S9. ^1H NMR spectrum of (*d,l*)-ACPA (enantioenriched in the levorotatory enantiomer) in CD_3OD at 500 MHz (bottom), and spectra recorded after successive addition of $\text{Eu}(\text{hfc})_3$ in 1:1 and 2:1 reagent:substrate molar ratios.

Crystallographic Information

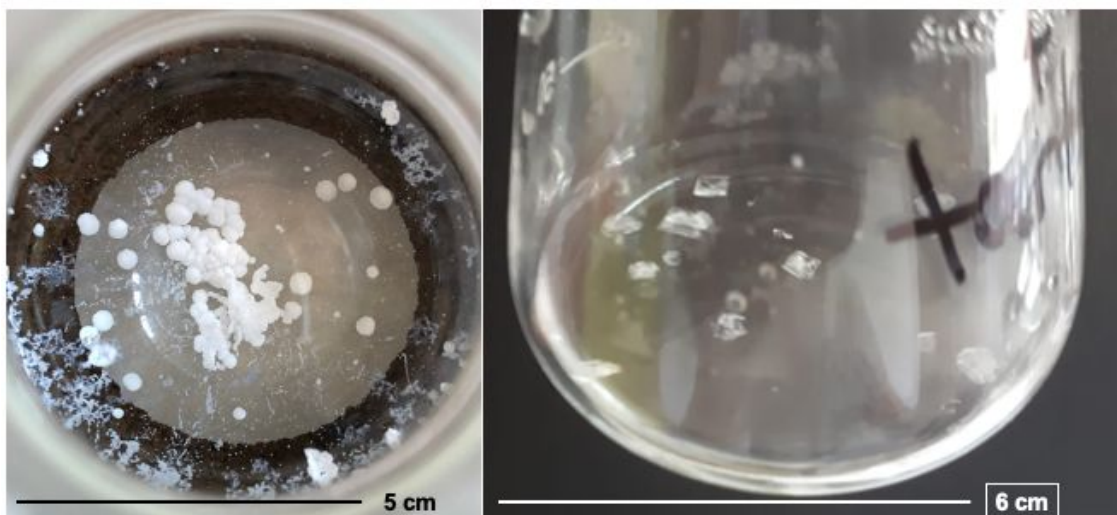


Figure S10. Left image: spherical aggregates of tiny ACPA crystals (*d,l*-racemate). Right image: larger (mm-sized) prismatic crystals of ACPA showing enantioenrichment.

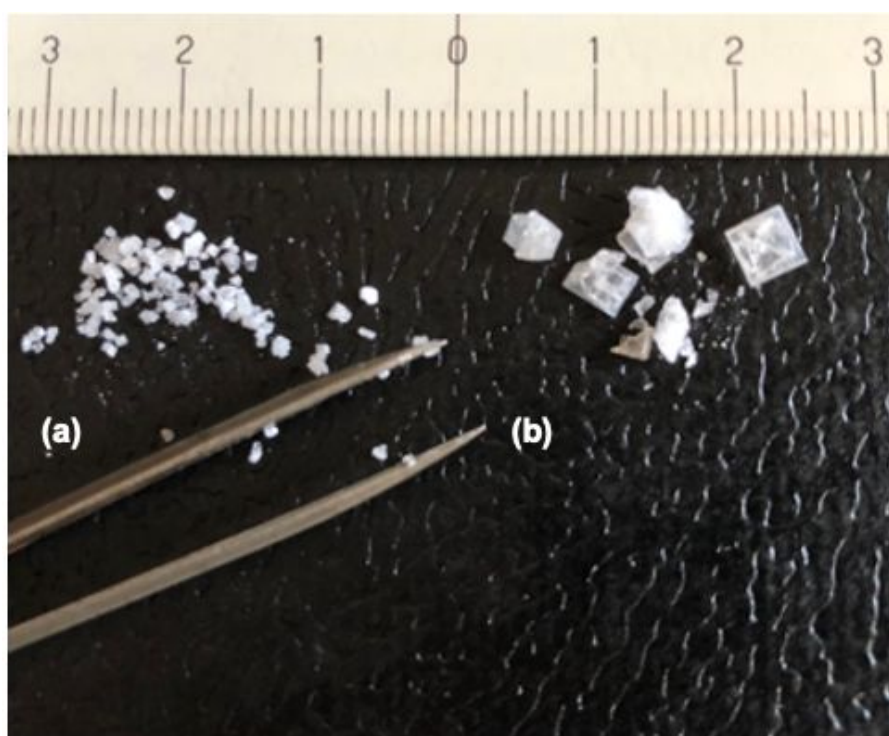


Figure S11. ACPA-crystals of arbitrary handedness, small and low *ees* (a) and large and high *ees* (b) obtained by spontaneous resolution of the *d,l*-racemate.

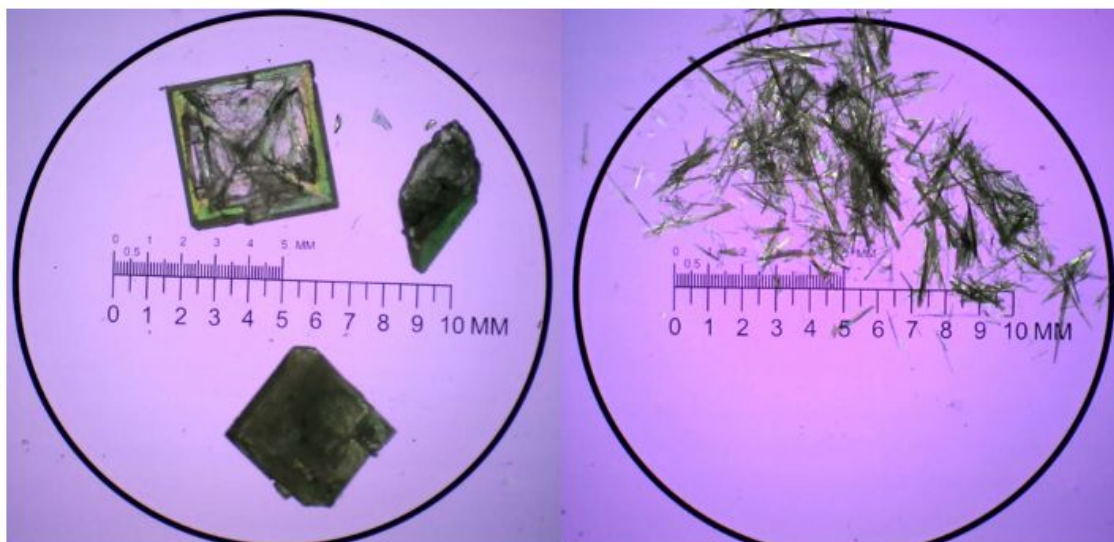


Figure S12. Observation under polarizing light (polarizer turned counterclockwise) of an entioenriched mixture of ACPA prismatic crystals (left) and large thin crystals of the *meso*-stereoisomer (right), shown at 16.7x magnification.

Table S1: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for the (*R,R*)-configured ACPA enantiomer. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}

Atom	X	y	z	U_{eq}
O1	3519.7(12)	1360.9(12)	5297.7(3)	30.7(3)
O2	5065.3(11)	2525.7(10)	4907.6(3)	22.4(2)
O3	10706.8(10)	4522.9(10)	5714.8(3)	20.8(2)
O4	9554.8(12)	2965.0(12)	5321.2(3)	31.2(3)
N1	4102.1(12)	6421.9(13)	6205.7(4)	25.3(3)
N2	5642.8(11)	3401.0(12)	6585.8(3)	16.6(2)
N3	6477.1(11)	4342.3(12)	6626.8(3)	16.1(2)
N4	7927.5(13)	1233.4(13)	6943.9(4)	25.0(3)
C1	4381.2(14)	2257.5(14)	5270.0(4)	17.6(3)
C2	4792.3(14)	3143.2(14)	5648.6(4)	18.2(3)
C3	3870.6(13)	2924.2(14)	6045.8(4)	17.1(3)
C4	4250.6(13)	3833.3(13)	6438.0(4)	16.0(3)
C5	4194.5(13)	5300.7(14)	6312.3(4)	18.8(3)
C6	3293.8(14)	3564.9(16)	6826.5(4)	22.6(3)
C7	7883.5(14)	2389.8(14)	6874.0(4)	17.6(3)
C8	8111.2(15)	4677.7(15)	7214.6(4)	21.7(3)
C9	7851.5(13)	3887.6(13)	6788.4(4)	15.9(3)
C10	8907.4(13)	4264.3(14)	6434.5(4)	17.4(3)
C11	8630.0(13)	3536.6(14)	6002.5(4)	17.4(3)
C12	9745.8(14)	3730.5(14)	5671.3(4)	18.5(3)

Table S2: Anisotropic Displacement Parameters ($\times 10^4$) for (*R,R*)-configured ACPA enantiomer. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2} \times U_{11} + \dots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	32.0(6)	36.7(6)	23.5(5)	-11.9(5)	6.4(4)	-16.3(5)
O2	29.4(6)	20.9(5)	17.0(4)	-2.8(4)	1.7(4)	-4.6(4)
O3	19.3(5)	24.2(5)	19.0(4)	-0.4(4)	3.0(4)	-4.2(4)
O4	32.7(6)	40.9(7)	19.8(5)	-9.6(5)	9.8(4)	-16.7(5)
N1	18.7(6)	21.8(6)	35.2(7)	-1.5(5)	-0.1(5)	2.1(5)
N2	15.1(5)	19.5(6)	15.0(5)	-1.8(4)	-1.0(4)	-1.0(4)
N3	14.2(5)	19.3(5)	14.8(5)	-2.4(4)	1.9(4)	-0.7(4)
N4	27.5(7)	23.4(7)	24.0(6)	1.2(5)	-0.9(5)	0.0(5)
C1	16.1(6)	18.5(6)	18.2(6)	-1.2(5)	-1.8(5)	2.9(5)
C2	16.9(6)	19.5(6)	18.2(6)	-3.0(5)	-1.1(5)	-1.7(5)
C3	14.9(6)	18.0(6)	18.4(6)	-2.4(5)	-2.0(5)	-0.4(5)
C4	12.5(6)	17.1(6)	18.5(6)	-1.7(5)	-0.7(5)	0.1(5)
C5	14.0(6)	21.9(7)	20.4(6)	-4.7(5)	0.3(5)	0.6(5)
C6	18.4(6)	29.4(7)	19.8(6)	-2.9(6)	3.7(5)	-3.0(6)
C7	15.7(6)	23.6(7)	13.6(6)	-1.1(5)	-0.6(5)	-1.1(5)
C8	23.7(7)	23.5(7)	17.7(6)	-2.8(5)	-1.0(5)	-4.7(6)
C9	14.8(6)	17.0(6)	15.9(6)	-0.2(5)	-1.0(5)	-1.5(5)
C10	13.9(6)	20.8(7)	17.3(6)	0.7(5)	0.7(5)	-2.1(5)
C11	15.1(6)	21.3(6)	15.7(6)	1.1(5)	0.3(5)	-1.7(5)
C12	19.4(6)	20.1(6)	15.9(6)	0.8(5)	0.2(5)	0.4(5)

Table S3: Bond Lengths in Å for (*R,R*)-configured ACPA enantiomer

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.2160(18)	C2	C3	1.5252(18)
O2	C1	1.3190(16)	C3	C4	1.5363(17)
O3	C12	1.2224(18)	C4	C5	1.4831(19)
O4	C12	1.3180(17)	C4	C6	1.5327(18)
N1	C5	1.1449(19)	C7	C9	1.4848(19)
N2	N3	1.2334(16)	C8	C9	1.5342(18)
N2	C4	1.4922(16)	C9	C10	1.5379(17)
N3	C9	1.4962(17)	C10	C11	1.5228(17)
N4	C7	1.1489(19)	C11	C12	1.4982(18)
C1	C2	1.4986(18)			

Table S4: Bond Angles in ° for (R,R)-configured ACPA enantiomer

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N3	N2	C4	114.89(11)	N4	C7	C9	178.90(16)
N2	N3	C9	113.83(11)	N3	C9	C8	106.21(11)
O1	C1	O2	123.42(13)	N3	C9	C10	107.30(10)
O1	C1	C2	123.10(12)	C7	C9	N3	111.64(11)
O2	C1	C2	113.47(11)	C7	C9	C8	109.97(11)
C1	C2	C3	112.06(11)	C7	C9	C10	110.18(11)
C2	C3	C4	113.41(11)	C8	C9	C10	111.47(11)
N2	C4	C3	107.02(10)	C11	C10	C9	112.27(11)
N2	C4	C6	105.76(10)	C12	C11	C10	113.41(11)
C5	C4	N2	112.63(11)	O3	C12	O4	123.71(13)
C5	C4	C3	110.27(11)	O3	C12	C11	124.32(12)
C5	C4	C6	110.06(11)	O4	C12	C11	111.96(12)
C6	C4	C3	111.01(11)				
N1	C5	C4	177.13(15)				

Table S5: Torsion Angles in ° for (R,R)-configured ACPA enantiomer

Atom	Atom	Atom	Atom	Angle/°
O1	C1	C2	C3	-8.13(19)
O2	C1	C2	C3	173.27(11)
N2	N3	C9	C7	-1.43(16)
N2	N3	C9	C8	-121.29(12)
N2	N3	C9	C10	119.38(12)
N3	N2	C4	C3	128.92(12)
N3	N2	C4	C5	7.59(16)
N3	N2	C4	C6	-112.65(12)
N3	C9	C10	C11	-61.64(14)
C1	C2	C3	C4	-179.12(11)
C2	C3	C4	N2	-64.88(13)
C2	C3	C4	C5	57.94(15)
C2	C3	C4	C6	-179.83(11)
C4	N2	N3	C9	178.23(10)
C7	C9	C10	C11	60.09(14)
C8	C9	C10	C11	-177.53(12)
C9	C10	C11	C12	-172.06(11)
C10	C11	C12	O3	-8.67(19)
C10	C11	C12	O4	172.71(12)

Table S6: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for (*R,R*)-configured ACPA enantiomer. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}

Atom	X	y	z	U_{eq}
H2	4826.64	1973.63	4710.83	34
H4	10182.06	3117.97	5139.28	47
H2A	4748.73	4117.5	5559.15	22
H2B	5752.14	2934.74	5730.12	22
H3A	3925.36	1951.01	6135.87	21
H3B	2909.96	3115.31	5961.02	21
H6A	3339.45	2594.13	6907.68	34
H6B	2351.48	3799.82	6744.53	34
H6C	3578.6	4129.15	7075.84	34
H8A	8042.09	5664.29	7158.36	32
H8B	9030.36	4462.41	7324.16	32
H8C	7426.91	4411.21	7433.44	32
H10A	8887.49	5267.48	6386.12	21
H10B	9835.69	4017.01	6538.84	21
H11A	8516.05	2544.09	6059.42	21
H11B	7758.18	3883.1	5879.03	21

Table S7: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for *meso*-ACPA crystal. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}

Atom	X	y	z	U_{eq}
O1	2187.8(14)	5427.0(10)	737.1(7)	27.4(2)
O2	-96.3(13)	3678.0(10)	1144.5(7)	25.7(2)
N1	9530.5(17)	6236.1(12)	3891.2(9)	25.6(3)
N2	4739.1(15)	4559.4(10)	4635.5(8)	18.4(2)
C1	1670.3(18)	4442.6(13)	1334.9(10)	19.5(3)
C2	2964.4(18)	3966.4(13)	2360.7(10)	19.2(3)
C3	4909.6(18)	4918.3(13)	2610.0(9)	18.5(3)
C4	6230.3(17)	4488.7(12)	3687.5(9)	17.4(3)
C5	8065.2(18)	5495.9(12)	3836.6(9)	18.5(3)
C6	7108.6(19)	2973.7(13)	3658.5(10)	20.8(3)

Table S8: Anisotropic Displacement Parameters ($\times 10^4$) for *meso*-ACPA crystal. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2} \times U_{11} + \dots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	24.9(5)	33.1(5)	23.5(5)	6.8(4)	-8.8(4)	-5.6(4)
O2	21.1(4)	35.8(5)	19.7(4)	2.8(4)	-6.1(3)	-7.0(4)
N1	23.4(5)	31.2(6)	21.9(5)	5.3(4)	-3.3(4)	-4.2(5)
N2	18.6(5)	22.2(5)	14.0(5)	-0.5(3)	-1.9(4)	0.2(4)
C1	17.1(5)	24.6(6)	16.9(6)	-4.3(5)	-0.7(4)	1.3(4)
C2	17.3(6)	23.1(6)	16.9(6)	-1.1(5)	-2.3(4)	0.4(5)
C3	17.5(6)	23.4(6)	14.5(5)	0.1(4)	-2.2(4)	-0.3(4)
C4	16.0(5)	21.8(6)	14.1(6)	-1.1(4)	-1.0(4)	-1.2(4)
C5	19.1(6)	23.5(6)	12.6(5)	2.0(4)	-2.1(4)	1.8(5)
C6	21.2(6)	22.6(6)	18.4(6)	-0.9(5)	-2.0(4)	1.1(5)

Table S9: Bond Lengths in \AA for *meso*-ACPA crystal

Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA
O1	C1	1.2199(15)	N2	N2 ¹	1.2335(19)
O2	C1	1.3234(14)	N2	C4	1.4897(15)
N1	C5	1.1458(16)	C1	C2	1.4996(16)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C2	C3	1.5230(16)	C4	C6	1.5294(16)
C3	C4	1.5446(15)	----		
C4	C5	1.4873(16)			¹ 1-x,1-y,1-z

Table S10: Bond Angles in ° for *meso*-ACPA crystal

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2 ¹	N2	C4	114.10(12)	C5	C4	N2	112.25(9)
O1	C1	O2	123.47(10)	C5	C4	C3	107.93(9)
O1	C1	C2	123.77(10)	C5	C4	C6	109.08(9)
O2	C1	C2	112.76(10)	C6	C4	C3	113.77(9)
C1	C2	C3	111.98(10)	N1	C5	C4	175.67(13)
C2	C3	C4	113.27(9)	----			
N2	C4	C3	106.88(9)				¹ 1-x,1-y,1-z
N2	C4	C6	107.00(9)				

Table S11: Torsion Angles in ° for *meso*-ACPA crystal

Atom	Atom	Atom	Atom	Angle/°
O1	C1	C2	C3	3.91(16)
O2	C1	C2	C3	-176.23(10)
N2 ¹	N2	C4	C3	-117.35(13)
N2 ¹	N2	C4	C5	0.80(16)
N2 ¹	N2	C4	C6	120.43(13)
C1	C2	C3	C4	177.87(9)
C2	C3	C4	N2	-58.90(12)
C2	C3	C4	C5	-179.84(9)
C2	C3	C4	C6	58.97(13)

¹1-x,1-y,1-z

Table S12: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for *meso*-ACPA crystal. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}

Atom	X	y	z	U_{eq}
H2	-830(30)	4000(20)	486(19)	61(6)
H2A	3463.54	2981.27	2246.41	23
H2B	2033.87	3969.68	3016.79	23

Atom	X	y	z	<i>U_{eq}</i>
H3A	4407.61	5908.54	2691.33	22
H3B	5859.43	4886.55	1962.14	22
H6A	8056.56	2807.35	4326.16	31
H6B	7926.24	2843.35	2978.65	31
H6C	5905.81	2299.74	3651.97	31

Computational Data

Cartesian coordinates and thermochemistry for the optimizations of (E,R,R); (Z,R,R); (E,R,S) and (Z,R,S) azobis-nitrile.

(E,R,S)

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.....  
::                      THERMODYNAMIC                      ::  
.....  
:: total free energy          -65.308665626804 Eh  ::  
.....  
:: total energy              -65.532680279407 Eh  ::  
:: zero point energy         0.274325782245 Eh  ::  
:: G(RRHO) w/o ZPVE         -0.050311129642 Eh  ::  
:: G(RRHO) contrib.         0.224014652603 Eh  ::  
.....
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O	-4.719638245	-1.058929886	-0.035163401
H	-4.988215882	-1.908615999	0.337338557
O	-2.652165821	-1.869871271	0.091046064
N	-1.989323871	0.240408547	2.470691324
N	0.533669951	0.952973827	0.405162380
C	-3.410792585	-0.983622366	-0.228189769
C	-3.020522352	0.300216825	-0.919771530
H	-3.532192263	1.132512928	-0.433200581
H	-3.426693808	0.230154943	-1.931975258
C	-1.507871978	0.504392834	-0.991025810
H	-1.263439117	1.140544345	-1.842969198
H	-1.026922595	-0.462457992	-1.156413588
C	-0.921362494	1.157044699	0.274182144
C	-1.518648576	0.623689668	1.497287595
C	-1.102179250	2.683769129	0.260695060
H	-2.158614868	2.935657138	0.211395922
H	-0.593916160	3.090827973	-0.610748544
H	-0.669820328	3.118764546	1.159774804
O	0.360772172	-2.290402112	-1.381451824
O	0.009275946	-2.262542120	0.820456532

H	-0.938902737	-2.357415861	0.560331639
N	3.418327645	1.054809766	1.819498966
N	1.069267444	0.592190382	-0.657724796
C	0.779716514	-2.197597860	-0.251453893
C	2.244326891	-2.003924146	0.075943235
H	2.360031882	-1.689361294	1.114490239
H	2.727395045	-2.976019262	-0.044466165
C	2.888876382	-1.008820238	-0.894201068
H	3.974205006	-1.109513523	-0.860896102
H	2.552028477	-1.227695887	-1.910561049
C	2.526763064	0.451269208	-0.560292026
C	3.017753067	0.794157580	0.776229611
C	3.119897866	1.410556448	-1.599226831
H	2.723775656	1.162952273	-2.581520547
H	2.844740077	2.434277740	-1.353957827
H	4.203375073	1.321591574	-1.614324305

(Z,R,S)

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:::
::
THERMODYNAMIC
::
:::
:: total free energy          -65.293794817632 Eh  ::
:::
:: total energy                -65.519510128456 Eh  ::
:: zero point energy           0.274622735165 Eh   ::
:: G(RRHO) w/o ZPVE           -0.048907424341 Eh   ::
:: G(RRHO) contrib.           0.225715310824 Eh   ::
:::

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O	-0.833269664	2.832983552	0.141675665
H	-1.745276102	2.572115069	0.397280252
O	-0.209628717	1.445759840	1.775484714
N	3.024039218	-2.148722037	-0.435440875
N	0.588384294	0.319421227	-1.104893027
C	0.065968736	2.177016719	0.854028028

C	1.485575033	2.452674636	0.406914684
H	1.912323343	3.164730476	1.117006160
H	1.481630398	2.916299037	-0.579514297
C	2.322347675	1.170925458	0.440937944
H	2.131551123	0.653684458	1.383726639
H	3.382337290	1.427143491	0.405573411
C	2.025041910	0.231654599	-0.751606118
C	2.534466453	-1.111729478	-0.515674386
C	2.743790593	0.739019932	-2.017868263
H	2.397880608	1.742925114	-2.254027232
H	2.517631870	0.083253288	-2.856063119
H	3.819460136	0.758098876	-1.858525770
O	-2.953651932	1.116286673	0.090910239
O	-3.456260490	-0.061626574	-1.733973871
H	-3.695222839	0.790754824	-2.121297784
N	1.464215289	-1.433357970	2.217165537
N	-0.340620061	-0.345081350	-0.672019091
C	-3.068037635	0.050044266	-0.468831070
C	-2.875127899	-1.291714774	0.193985894
H	-3.756313146	-1.438826877	0.824398725
H	-2.871348820	-2.077982766	-0.560442545
C	-1.637974898	-1.339703444	1.093059994
H	-1.611616662	-0.432952866	1.704440499
H	-1.713341719	-2.200368724	1.759228700
C	-0.304409842	-1.445857005	0.308609660
C	0.738428972	-1.414074015	1.326277237
C	-0.229098338	-2.748168881	-0.503619773
H	-0.445898068	-3.596312343	0.141945043
H	-0.955268401	-2.718180957	-1.312705761
H	0.762094313	-2.870558627	-0.933306250

(E,R,R)

```

:~::~:
:~:                THERMODYNAMIC                :~:
:~::~:

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:: total free energy          -65.303641516938 Eh  ::
::.....::
:: total energy              -65.530072058529 Eh  ::
:: zero point energy         0.274552549109 Eh  ::
:: G(RRHO) w/o ZPVE         -0.048122007518 Eh  ::
:: G(RRHO) contrib.         0.226430541591 Eh  ::
::.....::

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O	-1.723271497	-0.951046627	-1.684872196
O	-3.223522603	-0.869380168	-0.031414591
H	-2.996755692	-1.819674442	0.094388832
O	1.723329605	0.950527072	-1.685367056
N	1.539553462	2.845985628	0.804336611
N	-0.593994033	0.185155263	0.705631505
N	0.593705921	-0.184886245	0.705304101
N	-1.539647717	-2.845492732	0.804862839
C	-2.466146219	-0.318799637	-0.971801927
C	-2.652720232	1.179793476	-1.068700504
H	-3.438991146	1.503175500	-0.387409530
H	-2.956909839	1.413041372	-2.090725853
C	-1.334381346	1.912210759	-0.791341497
H	-1.491026812	2.985974813	-0.900682360
H	-0.585582243	1.593214466	-1.522611380
C	-0.768787430	1.639118191	0.621649413
C	0.514558545	2.331718434	0.738677690
C	-1.716110381	2.061651887	1.747261628
H	-2.599344783	1.426197209	1.735960137
H	-2.014471746	3.099040482	1.617766968
H	-1.217353349	1.949114925	2.707870403
C	-0.514557921	-2.331579708	0.739417236
C	1.716140658	-2.060574508	1.747930851
H	1.217357553	-1.947583110	2.708471763
H	2.599274508	-1.424985583	1.736285301
H	2.014662386	-3.097987402	1.619015001
C	0.768688587	-1.638854947	0.622103616
C	1.334314493	-1.912571853	-0.790750182

H	1.491051328	-2.986372254	-0.899601297
H	0.585514116	-1.593966609	-1.522188335
C	2.652607914	-1.180171842	-1.068386726
H	3.438916179	-1.503328849	-0.387031352
H	2.956758874	-1.413745319	-2.090349886
C	2.466056172	0.318462397	-0.971986547
O	3.223318706	0.869325005	-0.031651546
H	2.996755078	1.819693657	0.093661306

(Z,R,R)

```

:~::~:
::
:~::~:
:: total free energy          -65.294207277843 Eh  ::
:~::~:
:: total energy              -65.519654157044 Eh  ::
:: zero point energy         0.275015030643 Eh    ::
:: G(RRHO) w/o ZPVE         -0.049568151442 Eh    ::
:: G(RRHO) contrib.         0.225446879201 Eh    ::
:~::~:

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O	-3.753690401	-1.339300826	1.391328540
H	-3.677166976	-2.299206890	1.470640212
O	-2.896904415	-1.636026805	-0.646548470
N	-1.116354642	1.641765100	-2.132558491
N	-0.765123215	-0.212487262	0.912214491
C	-3.350655983	-0.906585055	0.199376145
C	-3.553550925	0.581323938	0.034978104
H	-4.556471259	0.827181923	0.386619351
H	-3.474960399	0.831786271	-1.024028353
C	-2.540803598	1.390577026	0.857157002
H	-2.627818504	1.120241240	1.911748598
H	-2.771309506	2.451557953	0.750581247
C	-1.076797730	1.144354527	0.419144561
C	-1.019048643	1.383355048	-1.016298082

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O	1.50493321137313	1.48820972572350	-4.49031047236237
O	1.29190869401211	0.97408313695026	-2.32925498539064
H	2.25175258864006	0.87143499394668	-2.33467247799413
O	-7.55398605767029	2.56640442967335	-0.28813042290520
N	-3.76009627982888	1.03555159067992	-5.33842921595359
N	-3.29291423007407	1.37429855105582	-2.07054324043950
N	-3.24069270552903	2.50180869546707	-2.59679807034122
N	-3.66455694264311	5.79528477863956	-2.95862346446583
C	0.81053744576109	1.29887532077555	-3.52187096317250
C	-0.69469810451023	1.41384470667393	-3.53095350189108
H	-1.02385631947873	1.57369482612424	-4.56046739631539
H	-0.96299373375913	2.30075213200703	-2.94702217286605
C	-1.37246776158126	0.18046131704264	-2.93470567560221
H	-1.07912065731702	0.05807405969777	-1.89145642297999
H	-1.07514346988690	-0.71674504796997	-3.47936987725346
C	-2.90790288515629	0.29790464836228	-2.99345060061292
C	-3.35830798823637	0.66269257449736	-4.33117586681964
C	-3.58335271701358	-0.98657640753615	-2.51856062163297
H	-3.27358542194132	-1.19288214523565	-1.49775034180532
H	-3.29715411018743	-1.82104762465475	-3.15429537154482
H	-4.66591127852360	-0.86930098114395	-2.54169698498153
C	-3.63851993532445	4.81514257985126	-2.36389877783263
C	-2.51251517557860	3.61017055356612	-0.55493424934817
H	-1.55144425657713	3.85520099009654	-1.00480322319015
H	-2.44449850610540	2.63379172162341	-0.08167543802394
H	-2.75972971631629	4.36157467140918	0.19026926959014
C	-3.60116818709932	3.55449815124930	-1.62858888757695
C	-4.97684447781115	3.22687668288878	-1.02254067117225
H	-4.86165855589290	2.36087936766097	-0.36908361405545
H	-5.31441855060942	4.06577725991226	-0.41076164077417
C	-6.01271511580047	2.90972940435701	-2.09988374607198
H	-6.15527352927127	3.76192422455848	-2.77555726873760
H	-5.70161271077120	2.04902955644932	-2.70211170832623
C	-7.34998146242589	2.57220197268722	-1.49153480223701

O	-8.26748269449652	2.28030878121095	-2.37582455001153
H	-9.13049907055041	2.08825329635250	-1.90697839843860
O	-2.24697235538007	12.31224497069999	-9.73640279861825
O	-0.09863550924031	12.82796413124659	-9.41560865948592
H	-0.39786438723046	13.77081637082896	-9.51942845595639
O	-0.00976192066986	6.11317479293287	-8.36070302055304
N	-3.55857156260517	6.85169473727441	-10.65361913827728
N	-0.72795838311874	8.60913639136552	-11.59888526164806
N	-0.11985674198660	7.70523186306759	-10.99389367213299
N	1.70647262809154	9.15115391634626	-13.47984678519319
C	-1.09208672123400	11.98185200177054	-9.59298851600217
C	-0.61578121557102	10.54666972816239	-9.58151900032547
H	-0.00867412408983	10.41239296877288	-8.68404600815286
H	0.05693504100278	10.42193346541400	-10.43465933272660
C	-1.75542088676345	9.52438124533282	-9.60443629727683
H	-2.67106243440847	9.97406906459054	-9.20642115704150
H	-1.47776838273512	8.68879198380840	-8.95977305073255
C	-2.04402301273882	8.94092012588948	-11.00390720556303
C	-2.86373535950757	7.74708847441745	-10.82318502193121
C	-2.75973592091099	9.91067754406193	-11.94617674608013
H	-2.78696974875500	9.49804058401480	-12.95562009930295
H	-2.22508059329793	10.85690773610364	-11.97901066517999
H	-3.77992358796221	10.09903142311425	-11.60438321776553
C	1.51372931067432	8.45088844061902	-12.59088971627882
C	1.43757916981398	6.09552597105305	-11.98195886586063
H	0.90066575737091	5.95739509821038	-12.91969352404971
H	1.05582577233057	5.38970437762543	-11.24734313894287
H	2.49314332926008	5.90321268689519	-12.15140524349230
C	1.24740551241092	7.52876392994533	-11.48282635775261
C	2.19285837059609	7.87979500565844	-10.31483770495510
H	3.21356399808092	7.86504481100224	-10.69593240601292
H	1.97215630840966	8.89465849621038	-9.97449033649193
C	2.11556055568427	6.91541635654092	-9.12407216755433
H	2.26829870384452	5.88491722782760	-9.44293022898947
H	2.91388354710257	7.18510035969901	-8.43229319354532
C	0.81514930775606	7.01149952858059	-8.36976684232135

O	0.66725806187579	8.13225039091964	-7.71129351761182
H	-0.18428433913844	8.14179494185556	-7.16132272440158
O	-1.59574268732021	-2.18283917981730	-11.69848543608820
O	-1.99929446047913	-2.69066411370976	-9.57959824298135
H	-2.77473655036468	-3.21172188976760	-9.97987595872276
O	-0.95697126752000	4.16865131184199	-4.64839786917506
N	-2.54220441268699	-0.34898750985784	-7.63807213444828
N	0.76191158430484	0.42244706519780	-7.84725920818825
N	0.15524675225369	1.23680974239616	-8.56641947394507
N	-0.34886133983916	3.96365943066452	-10.43607297206343
C	-1.28127341061736	-2.13802846109961	-10.509712111636086
C	-0.01810467519185	-1.45009045891813	-10.06740945418094
H	-0.17994082025539	-0.36632659020090	-10.14967066687163
H	0.74599655903103	-1.69999049665333	-10.80484789695640
C	0.45668836809344	-1.82362839710857	-8.66219591937762
H	1.54653747051752	-1.85666149169362	-8.64987708207195
H	0.08527818946939	-2.81066777711161	-8.38128919171307
C	0.02143347912616	-0.81287600051415	-7.58229731396403
C	-1.41729187444538	-0.57293342978613	-7.62067473808560
C	0.45169191916632	-1.29121991723884	-6.19548739834304
H	1.52850315838631	-1.43996756587601	-6.19168857681213
H	-0.04090396529174	-2.22599749610600	-5.94470079543507
H	0.20107686646469	-0.53989044372753	-5.45042408145560
C	0.25219592501194	3.29482770965461	-9.72252511536118
C	2.32350339522796	2.03241569660781	-9.41356695286428
H	2.94955631368455	2.90735633111395	-9.56939197006724
H	2.15655644934981	1.53614397477515	-10.36785868026301
H	2.82694502713133	1.34195820319600	-8.74101462369735
C	0.98645583132079	2.44272445068908	-8.79450350581411
C	1.17877597117961	3.16486651810088	-7.44391046344988
H	1.79755273011627	2.53047286360618	-6.80633142466148
H	1.70398967585116	4.10631626061484	-7.61469536705388
C	-0.16937989397953	3.41066466393830	-6.77034538925165
H	-0.84287547495037	3.92161268554999	-7.46849638993780
H	-0.63410954490469	2.45854611594569	-6.50351443163871
C	-0.13524826782428	4.27676262740676	-5.53131203037142

O	0.82074477049834	5.18543246051675	-5.52827483197070
H	0.80020330392004	5.71390925493919	-4.69071167563456
O	-4.01806330731880	-4.00917136805618	-10.59795797754649
O	-3.22928599382049	-4.00384983044581	-12.68118765515742
H	-2.54233621885788	-3.35706037486051	-12.32083743570810
O	-13.17238790352775	-1.50629669937872	-13.86931579963777
N	-5.20864080972312	-1.60595062266859	-12.89054189382657
N	-7.53672395239343	-3.92330040836977	-12.51323792179005
N	-8.70099699412282	-3.97205836836757	-12.93887628423354
N	-9.28579406008107	-2.55710000946718	-9.95072666442112
C	-4.07061626415991	-4.38444277541962	-11.75962037638055
C	-5.11127283215742	-5.36059190688284	-12.24111851634933
H	-5.90021408294748	-5.44205543021361	-11.49211245519906
H	-4.61434778825737	-6.32966159379769	-12.31557891457308
C	-5.68472933132289	-5.00312812726567	-13.61322369317435
H	-6.32055010315721	-5.82186406377956	-13.95082875127099
H	-4.87639886844927	-4.87479857626261	-14.33462730873633
C	-6.54720922955292	-3.72651259062399	-13.58887325045629
C	-5.76968315745085	-2.55729870055683	-13.19551401131596
C	-7.18199502033405	-3.47147679616663	-14.95788428634617
H	-6.39871247782147	-3.32204380868933	-15.69709918532054
H	-7.82183428932242	-2.58938973797417	-14.92402088585805
H	-7.78394098752169	-4.33062049614427	-15.24231950838238
C	-9.47292317531909	-3.32702011678845	-10.78064163633930
C	-9.42169041158737	-5.70175311710895	-11.39470233742355
H	-10.13154355014293	-5.97187815885565	-10.61736049994266
H	-8.40781612406743	-5.77469823297838	-11.00602051907470
H	-9.52801017736657	-6.38485659951836	-12.23356214730538
C	-9.67885293231311	-4.27011639182329	-11.87281560433469
C	-11.07862201684232	-4.11131336246032	-12.48124475923981
H	-11.19677543524065	-4.87113284873874	-13.25464116762564
H	-11.83369413395187	-4.28530045954274	-11.71329005823922
C	-11.25362517429048	-2.72213649222555	-13.09891804747554
H	-11.16254539092062	-1.93639123517404	-12.34355777150553
H	-10.47082384846298	-2.55872848106775	-13.84886254606253
C	-12.57687229982846	-2.55494975800235	-13.81013686233582

O	-12.99831905559134	-3.66962192561456	-14.387744441974702
H	-13.83282604021058	-3.56428494846233	-14.86024992996787
O	-1.03064320840250	-4.16882384358644	-6.64773356261733
O	-2.53316543681041	-5.54389712171760	-5.74796035109766
H	-1.77841195050074	-6.12840702673978	-5.60302291838317
O	-9.82065357860511	-0.12215626363503	-5.86097688108518
N	-4.93430127229917	-1.31126813331341	-9.34485192369838
N	-6.19840962630408	-2.60256658943268	-6.58321156711866
N	-6.20607205891426	-3.35777128252906	-5.59461146128404
N	-6.62457003924740	-0.26381805314256	-4.20017275742032
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RS-RS

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RR-RS

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RR-SS

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