Electronic Supplementary Material (ESI) for ChemComm.
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Effect of Incarcerated HF on the Exohedral Chemical Reactivity of HF@C_{60}

Supporting Information

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General Methods.

The commercially available reagents and solvents were used without further purification. All solvents were dried according to standard procedures. NMR experiments were recorded on a BRUKER AVANCE-300 in $CDCl_3$, or a BRUKER AVANCE AMX-700 in $CDCl_3$ at 23°C, and referenced to $CDCl_3$; coupling constants (*J*) are reported in Hz and the chemical shifts (δ) in ppm. Mass spectra were reported on a BRUKER-REFLEX (MALDI-TOF). Reactions were monitored by thin-layer chromatography carried out on 0.2 mm TLC-aluminium sheets of silica gel (Merck, TLC Silica gel 60 F_{254}). Flash column chromatographies were performed using silica gel (230-400 mesh). The relative yield and the isolation of some products was carried out in HPLC, columns: 5PYE (4.6 ID x 250mm; toluene/acetonitrile (1:1); 1 ml/min; 320 nm; 25ºC), Buckyprep Waters (4.6 ID x 250mm; toluene/acetonitrile (90:10); 1 ml/min; 320 nm; 25ºC). All these values were monitored in a 320 nm spectrophotometer detector. FTIR spectra were recorded in a Bruker TENSOR FTIR. The spectral range was 4000-550 cm^{-1}.

Experimental Procedures and Characterizations.

Synthesis of α-iminoester 1:

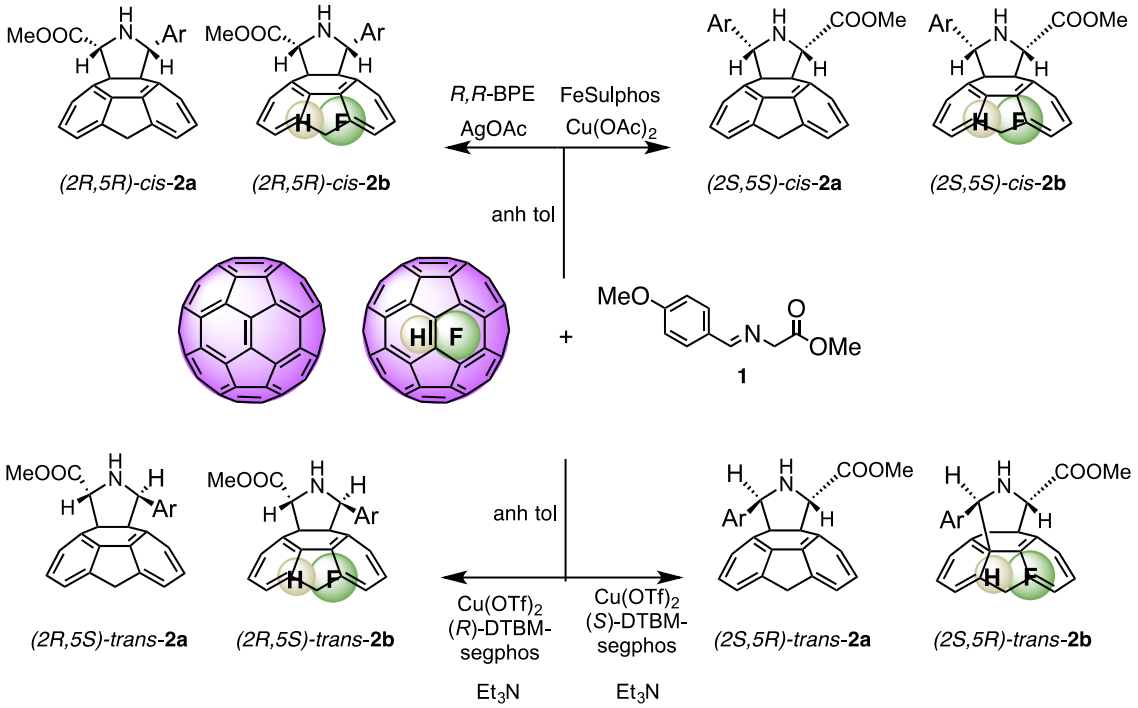
Compound **1** was synthesized according to the method described in literature.[a]

Procedure for catalytic 1,3-dipolar cycloaddition of iminoester 1 and Fullerene.

Chiral ligand (0.0028 mmol) and metal salt (0.0025 mmol) were dissolved in toluene (7 mL). The solution was stirred for 1h (at room temperature for *trans*-isomers, or 0ºC for *cis*-isomers), the mixture was cooled to the indicated reaction temperature, and then, a solution of **1** (0.028 mmol) in toluene (1.5 mL) was added. Finally, a small amount of Et_3N (in the case of the *trans*-isomers) and a sample composed by C_{60}:HF@C_{60} (12:88) (0.025 mmol) were added. The reaction mixture was stirred for 2 hours and afterwards, it was quenched with a saturated ammonium chloride solution (40 mL). The mixture was extracted with toluene (3 x 20 mL), and the combined extracts were washed with brine (30 mL). The organic layer was dried over $MgSO_4$ and concentrated in vacuum. The crude product was purified by silica gel flash chromatography, eluent: CS_2 to remove the unreacted fullerenes and chloroform to isolate compound **2a,b**.

Synthesis of compounds 2ab:

NOTE: The characterization is exclusively referred to compound **2b** since the starting sample is 88% HF@C_{60}. The signals corresponding to empty C_{60} derivatives (**2a**) are too small to be detectable in the spectra.



Chiral ligand/metal salt pair for the synthesis of (2*R*,5*R*)-*cis*-**2b**: R,R-BPE/ AgOAc

Chiral ligand/metal salt pair for the synthesis of (2*S*,5*S*)-*cis*-**2b**: FeSulphos/ $Cu(OAc)_2$

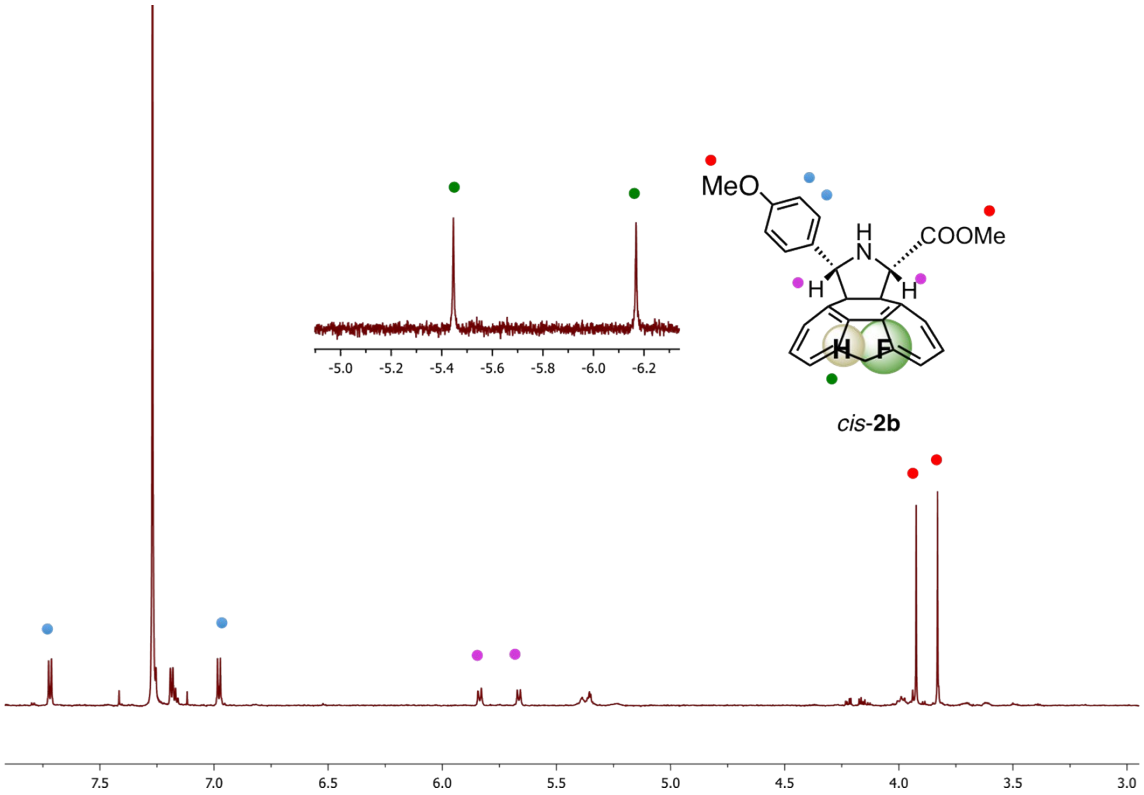


Figure S1. ^{1}H NMR (700 MHz, 298 K, $CDCl_3$) of compound ***cis*-2b**.

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.72 (d, J = 8.7 Hz, 2H), 6.98 (d, J = 8.7 Hz, 2H), 5.84 (d, J = 10.2 Hz, 1H), 5.66 (d, J = 9.6 Hz, 1H), 3.92 (s, 3H), 3.83 (s, 3H), -5.81 (d, J = 505.8 Hz, 1H) ppm.

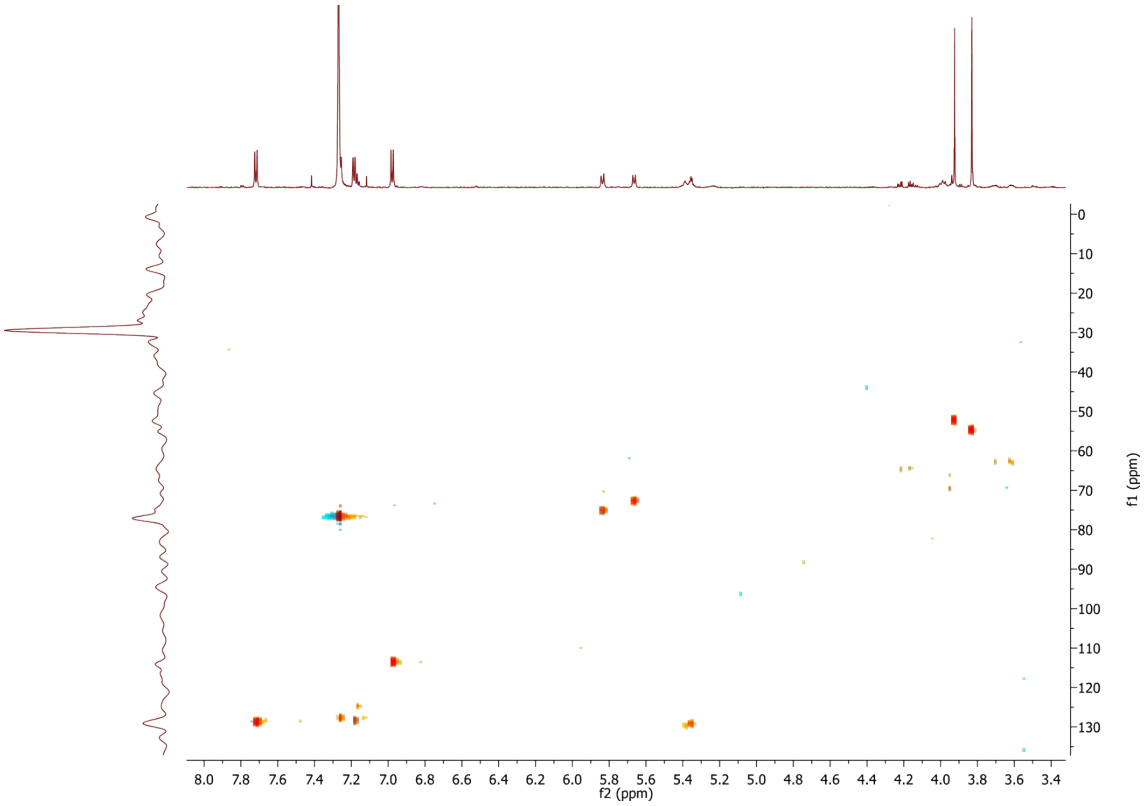


Figure S2. HSQC-NMR (700 MHz, 298 K, $CDCl_3$) of compound ***cis*-2b**.

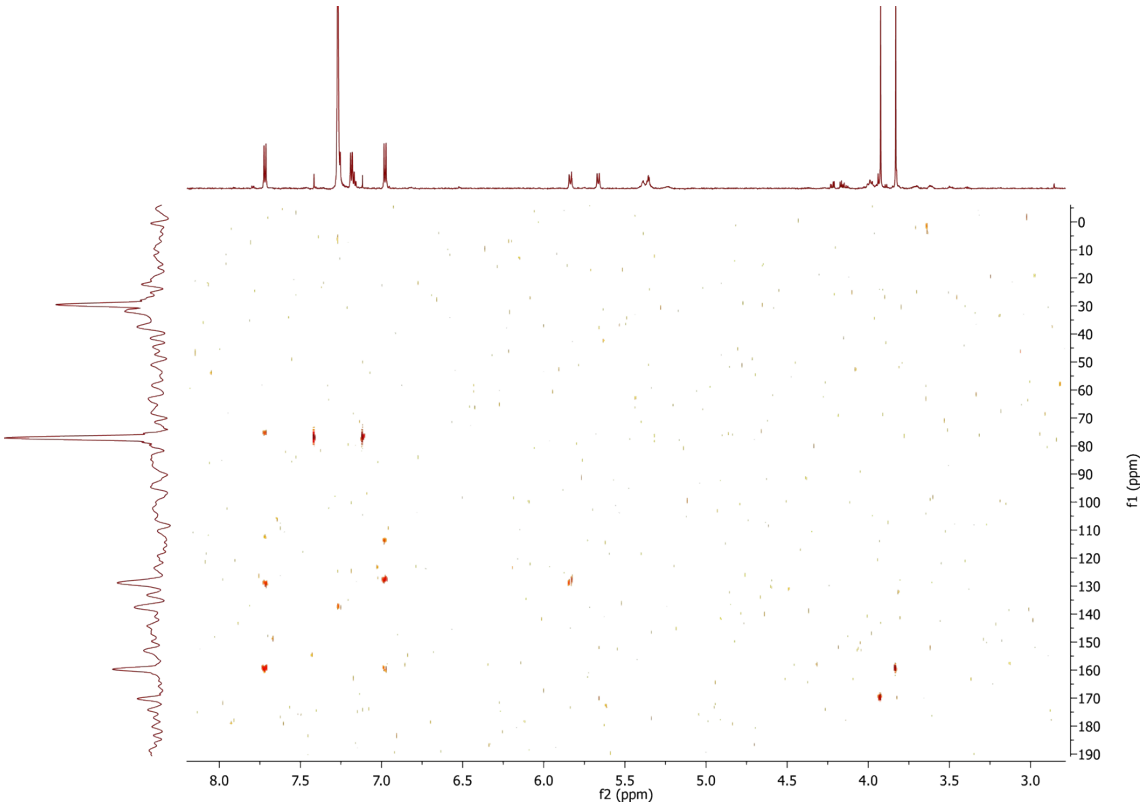


Figure S3. HMBC-NMR (700 MHz, 298 K, $CDCl_3$) of compound ***cis*-2b**.

HRMS (MALDI TOF) of compound *cis*-2b: theoretical: 947.0958 m/z, found: 948.1031 [M+].

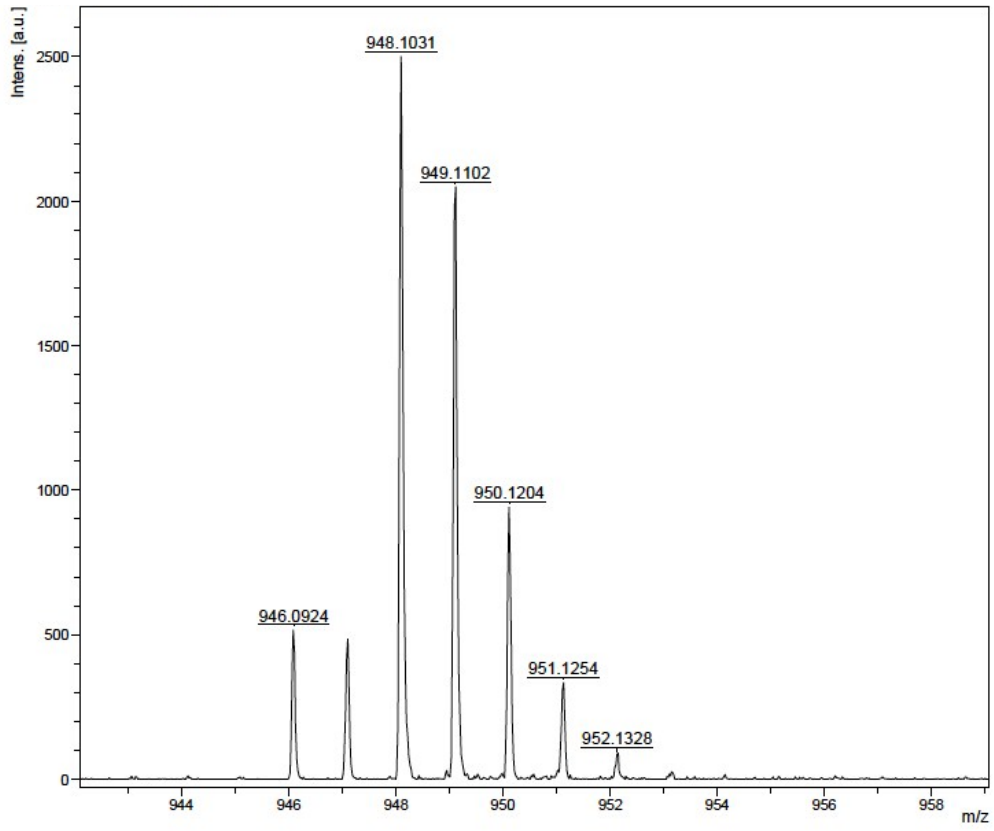


Figure S4. HRMS spectra of compound ***cis*-2b**.

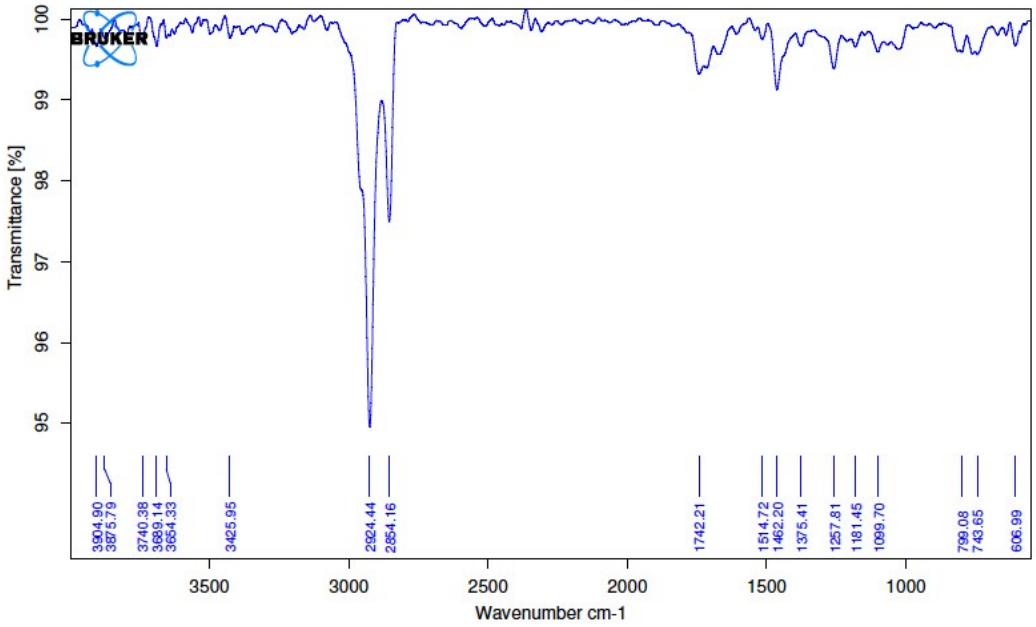


Figure S5. IR spectrum of compound ***cis*-2b** in $CHCl_3$.

Characterization of compounds *trans*-2b:

Chiral ligand/metal salt pair for the synthesis of (2*R*,5*S*)-*trans*-**2b**: *R*-DTBM-SEGPHOS / $Cu(OTf)_2$

Chiral ligand/metal salt pair for the synthesis of (2*S*,5*R*)-*trans*-**2b**: *S*-DTBM-SEGPHOS / $Cu(OTf)_2$

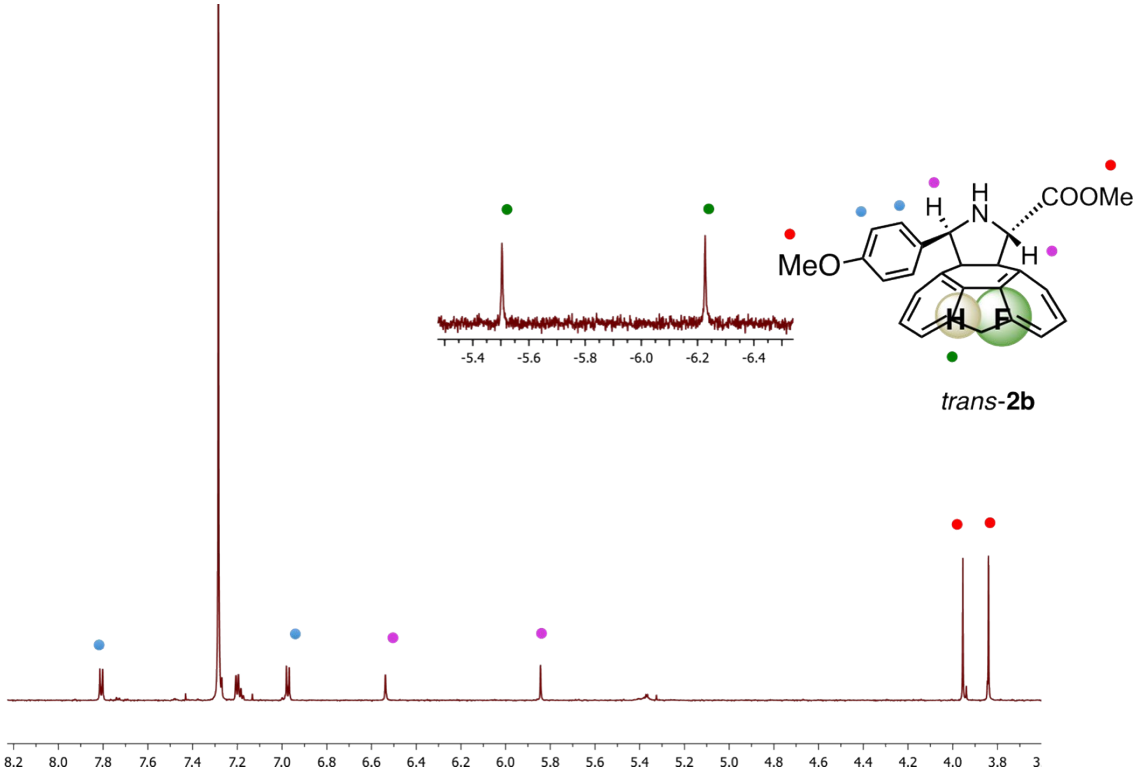


Figure S6. ^1H NMR (700 MHz, 298 K, $CDCl_3$) of compound ***trans*-2b**.

^1H NMR (700 MHz, $CDCl_3$) δ 7.80 (d, J = 8.7 Hz, 2H), 6.96 (d, J = 8.7 Hz, 2H), 6.52 (s, 1H), 5.83 (s, 1H), 3.94 (s, 3H), 3.83 (s, 3H), -5.88 (d, J = 506.0 Hz, 1H) ppm.

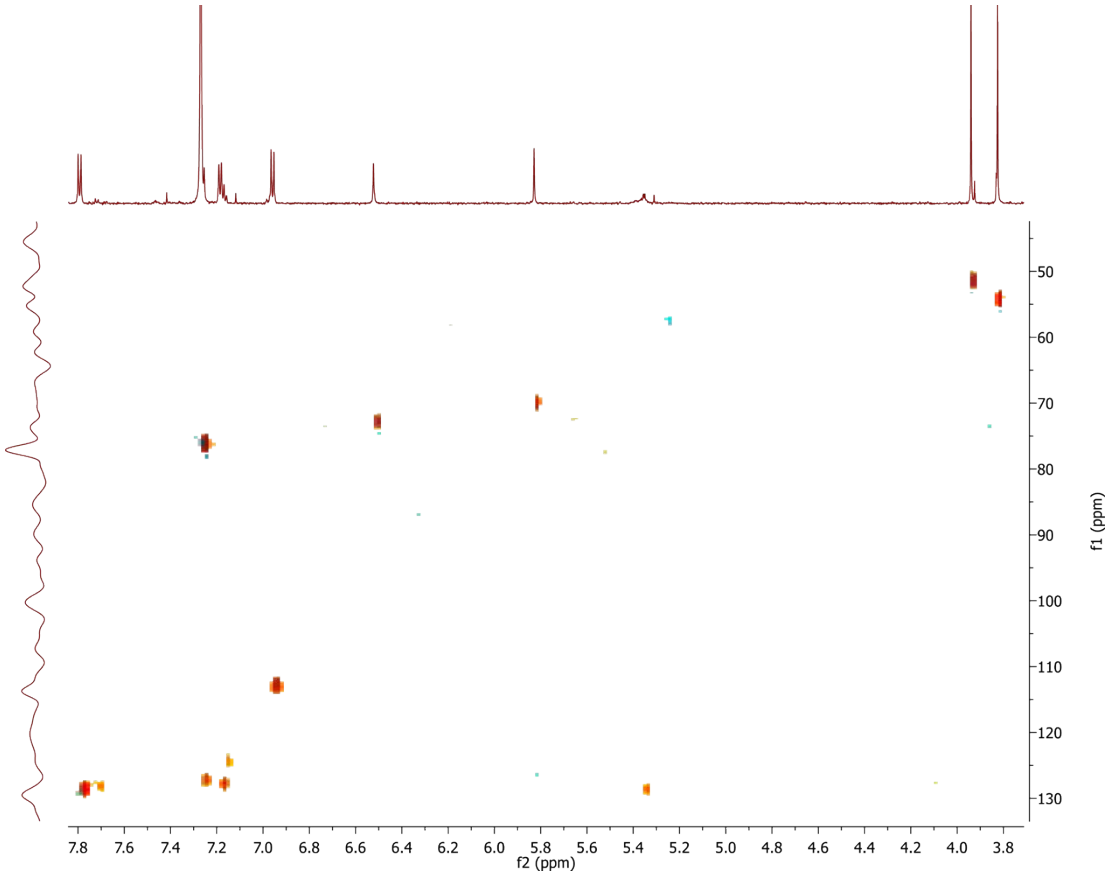


Figure S7. HSQC NMR (700 MHz, 298 K, $CDCl_3$) of compound ***trans*-2b**.

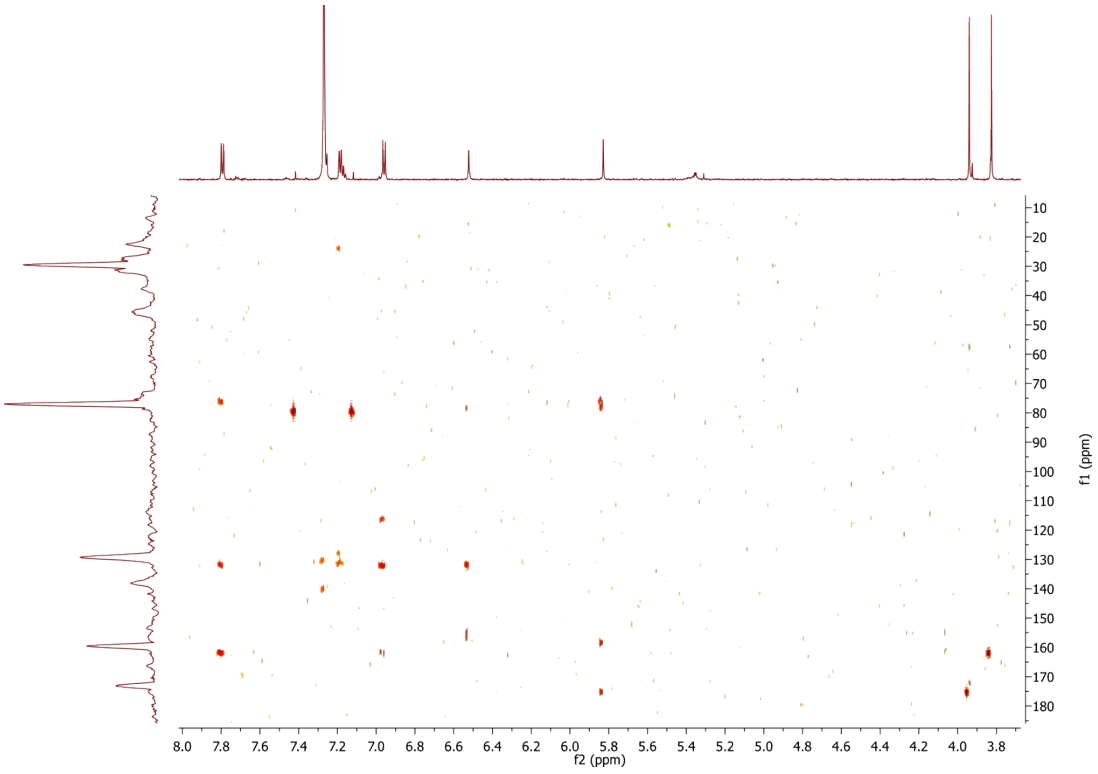


Figure S8. HMBC NMR (700 MHz, 298 K, $CDCl_3$) of compound ***trans*-2b**.

HRMS (MALDI TOF) of compound *trans*-2b: theoretical: 947.0958 m/z, found: 948.0993[M+].

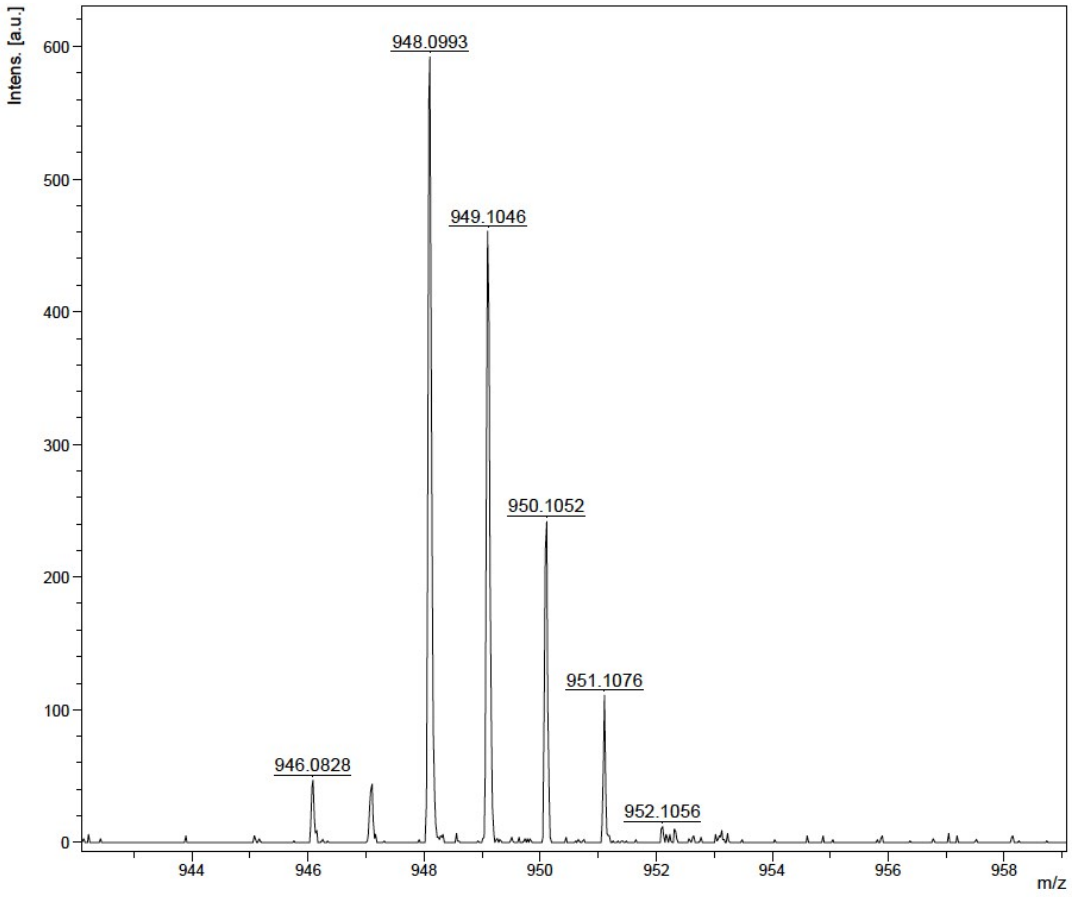


Figure S9. HRMS spectra of compound ***trans*-2b**.

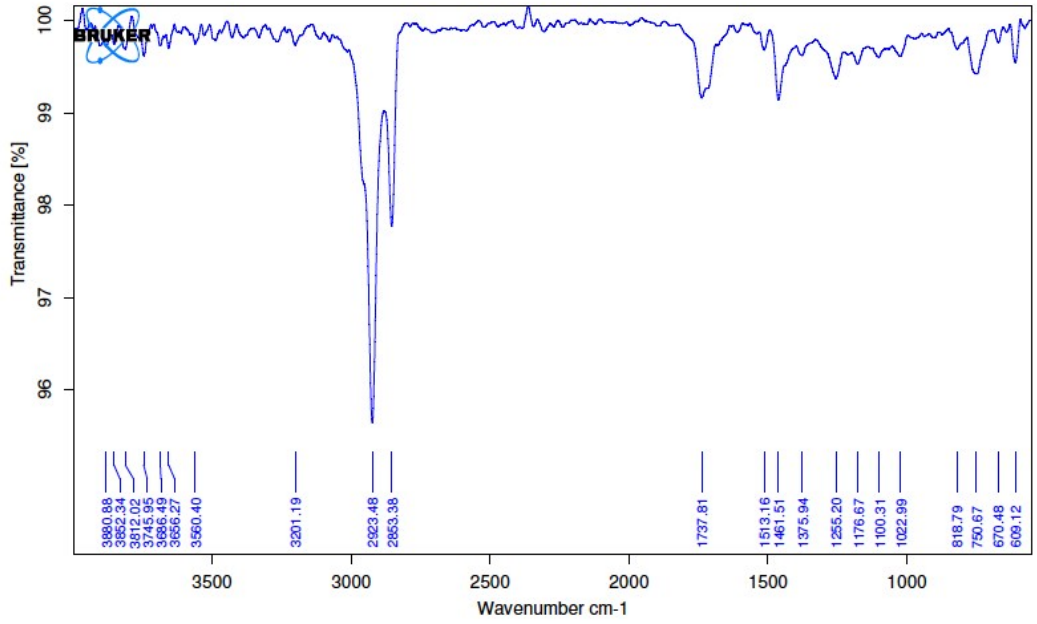


Figure S10. IR spectrum of compound ***trans*-2b** in $CHCl_3$.

The selected system used for the isomerization experiment was the enantiomer (2*S*,5*S*)-*cis*-fulleropyrrolidine for all the cases with a *cis/trans* ratio of 98/2 for **2a** and **3** and 96/4 for **2b**. The experiments were performed in chlorobenzene/acetonitrile 1:1 as solvent mixture at three different temperatures (25^{0}C, 30^{0}C, and 40^{0}C).

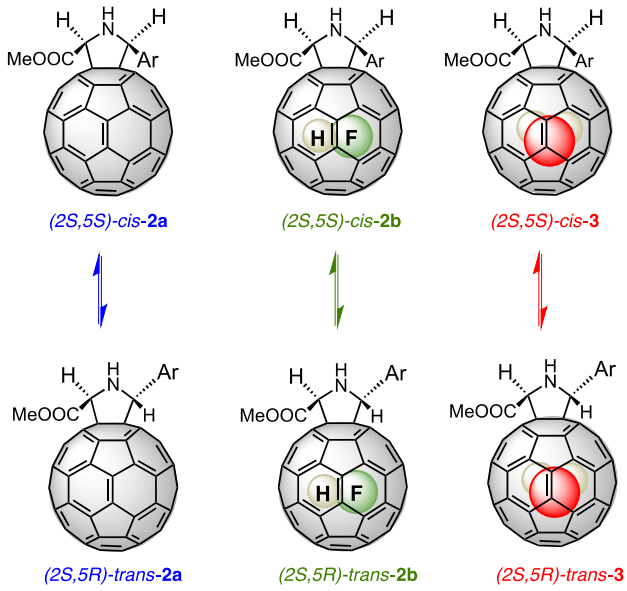


Figure S11. Isomerization process from the optically pure (2*S*,5*S*)-*cis*-pyrrolidino[60]fullerene to the (2*S*,5*R*)-*trans*-pyrrolidino[60]fullerene in C_{60}, HF@C_{60} and H_2O@C_{60} derivatives.

The reactions were monitored by HPLC until the equilibrium stages were reached (Figures S13-S20). Integration of the peak areas was used to determine the relative amount of the isomers at any time during the isomerization. These equilibrium stages and the time needed to reach them were different for each system and are summarized in Table S1. At 25^0C, the equilibrium stage was 77/23 *cis:trans* while at 30^0C and 40^0C, the equilibrium stage *cis/trans* ratio changed significantly toward 59/41 and 55/45, respectively. In all cases, the enantiomeric excesses of the *trans* derivatives remained unaltered demonstrating the enantiospecificity of the isomerization process.

HPLC profiles:

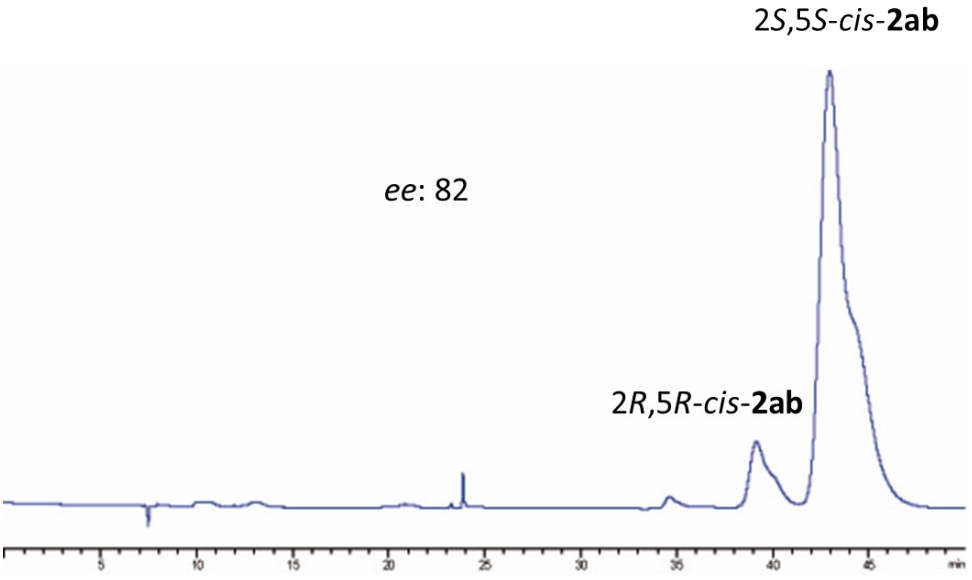


Figure S12. HPLC profile of compound *cis*-**2ab** before the isomerization reaction. Conditions: Chiral column Whelk02 (4.6 ID x 250mm; hexane/methanol (97:3); 0.5 ml/min; 320 nm; 25ºC).

HPLC profiles of compounds 2ab and 3 for monitoring the isomerization process:

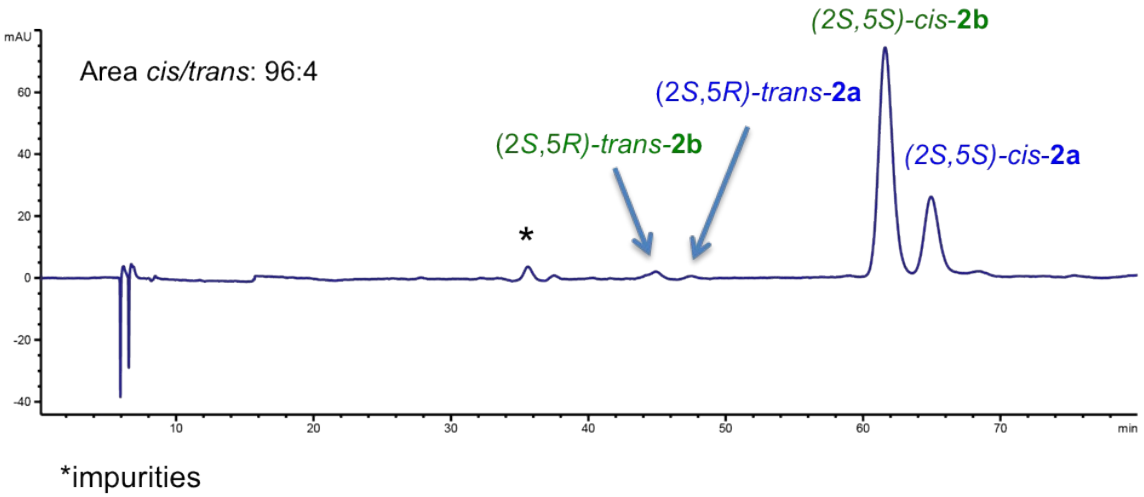


Figure S13. HPLC profile of compound **2b** (sample is composed by **2b:2a** 88:12) before the isomerization reaction at room temperature, t=0. Conditions: Buckyprep Waters (4.6 ID x 250mm; toluene/hexane/acetonitrile (20:70:10); 0.5 ml/min; 320 nm; 25ºC).

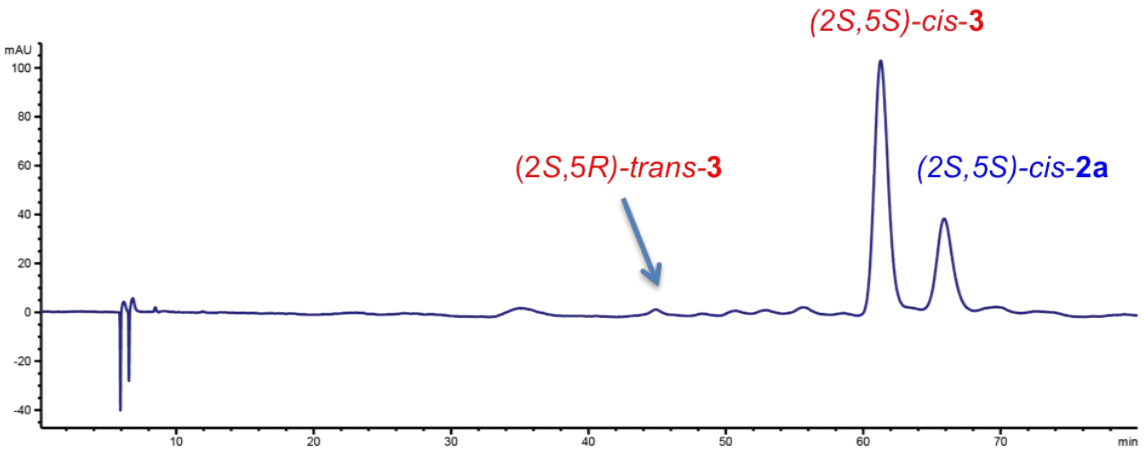


Figure S14. HPLC profile of compound **3** (sample is composed by **3:2a** 75:25) before the isomerization reaction at room temperature, t=0. Conditions: Buckyprep Waters (4.6 ID x 250mm; toluene/hexane/acetonitrile (20:70:10); 0.5 ml/min; 320 nm; 25ºC).

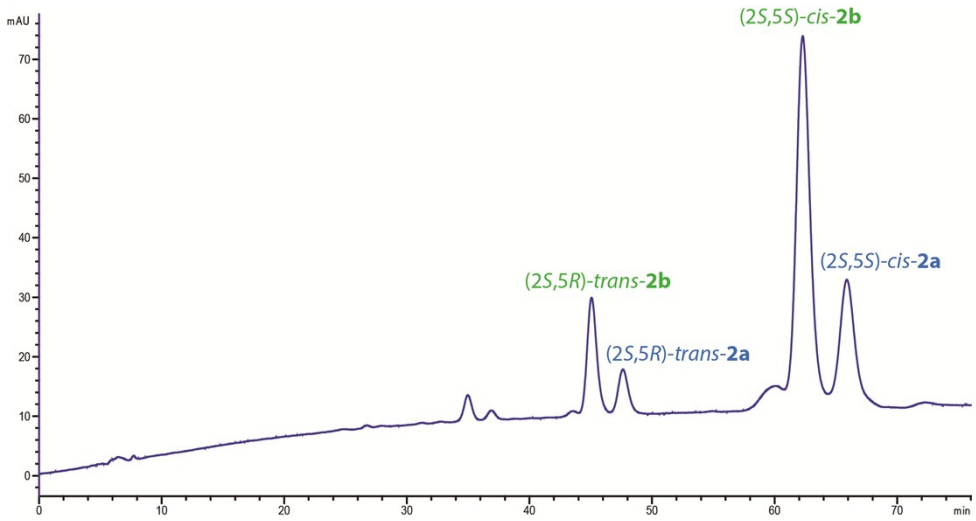


Figure S15. HPLC profile of compound **2b** (sample is composed by **2b:2a** 88:12) after the isomerization reaction at room temperature, t=final. Conditions: Buckyprep Waters (4.6 ID x 250mm; toluene/hexane/acetonitrile (20:70:10); 0.5 ml/min; 320 nm; 25ºC).

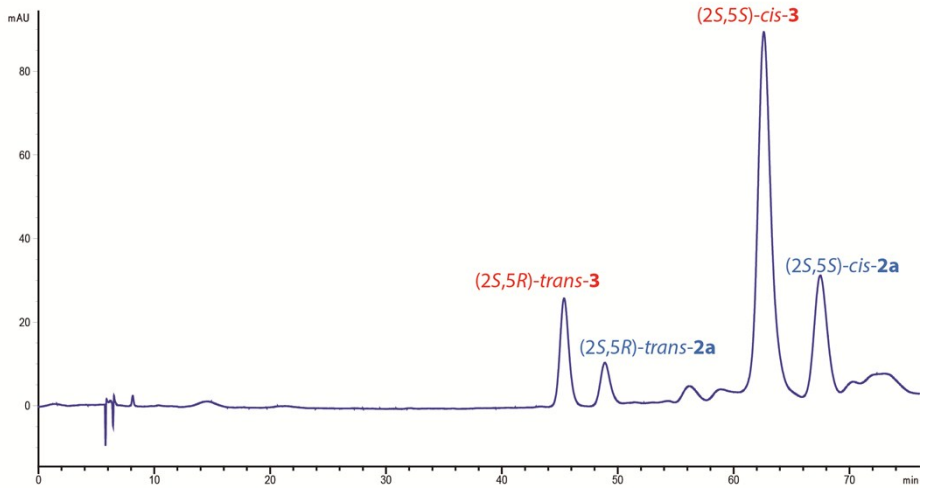


Figure S16. HPLC profile of compound **3** (sample is composed by **3:2a** 75:25) after the isomerization reaction at room temperature, t=final. Conditions: Buckyprep Waters (4.6 ID x 250 mm; toluene/hexane/acetonitrile (20:70:10); 0.5 ml/min; 320 nm; 25ºC).

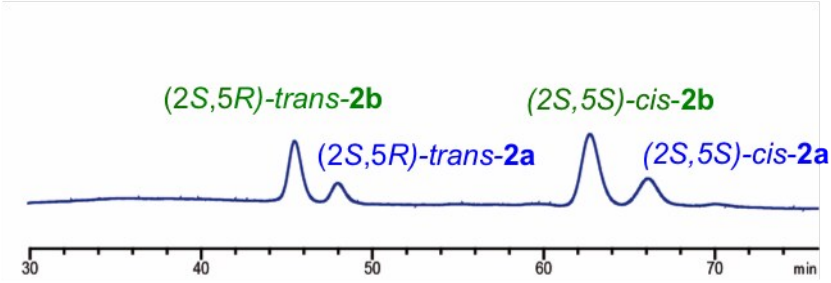


Figure S17. HPLC profile of compound **2b** (sample is composed by **2b:2a** 88:12) after the isomerization reaction at 30ºC, t=final. Conditions: Buckyprep Waters (4.6 ID x 250 mm; toluene/hexane/acetonitrile (20:70:10); 0.5 ml/min; 320 nm; 25ºC).

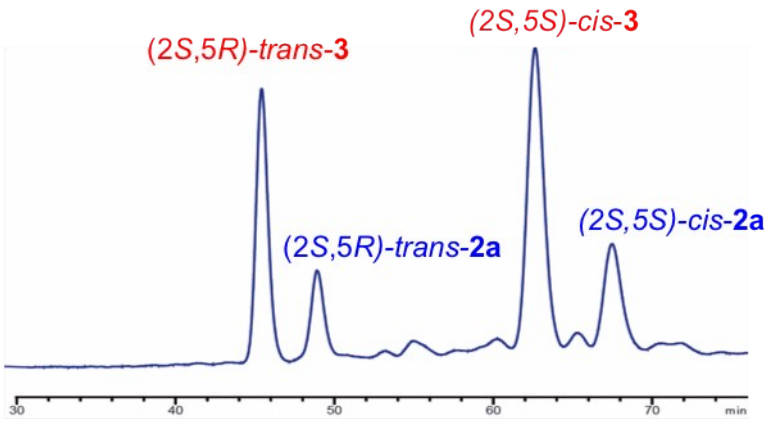


Figure S18. HPLC profile of compound **3** (sample is composed by **3:2a** 75:25) after the isomerization reaction at 30ºC, t=final. Conditions: Buckyprep Waters (4.6 ID x 250mm; toluene/hexane/acetonitrile (20:70:10); 0.5 ml/min; 320 nm; 25ºC).

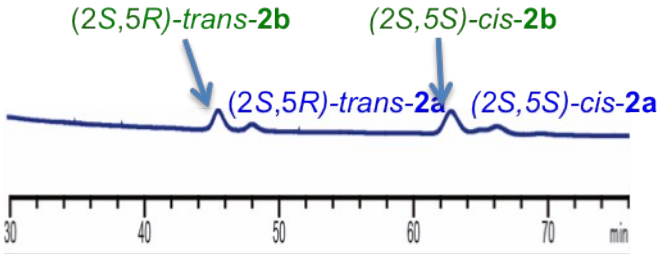


Figure S19. HPLC profile of compound **2b** (sample is composed by **2b:2a** 88:12) after the isomerization reaction at 40ºC, t=final. Conditions: Buckyprep Waters (4.6 ID x 250mm; toluene/hexane/acetonitrile (20:70:10); 0.5 ml/min; 320 nm; 25ºC).

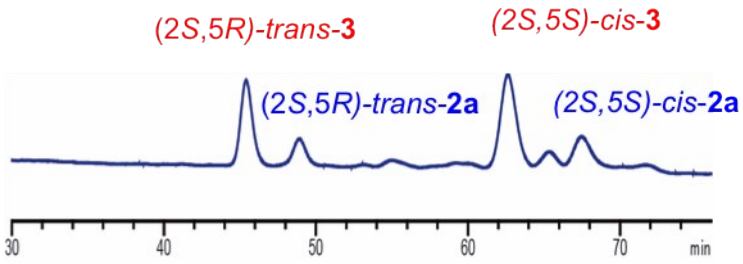


Figure S20. HPLC profile of compound **3** (sample is composed by **3:2a** 75:25) after the isomerization reaction at 40ºC, t=final. Conditions: Buckyprep Waters (4.6 ID x 250mm; toluene/hexane/acetonitrile (20:70:10); 0.5 ml/min; 320 nm; 25ºC).

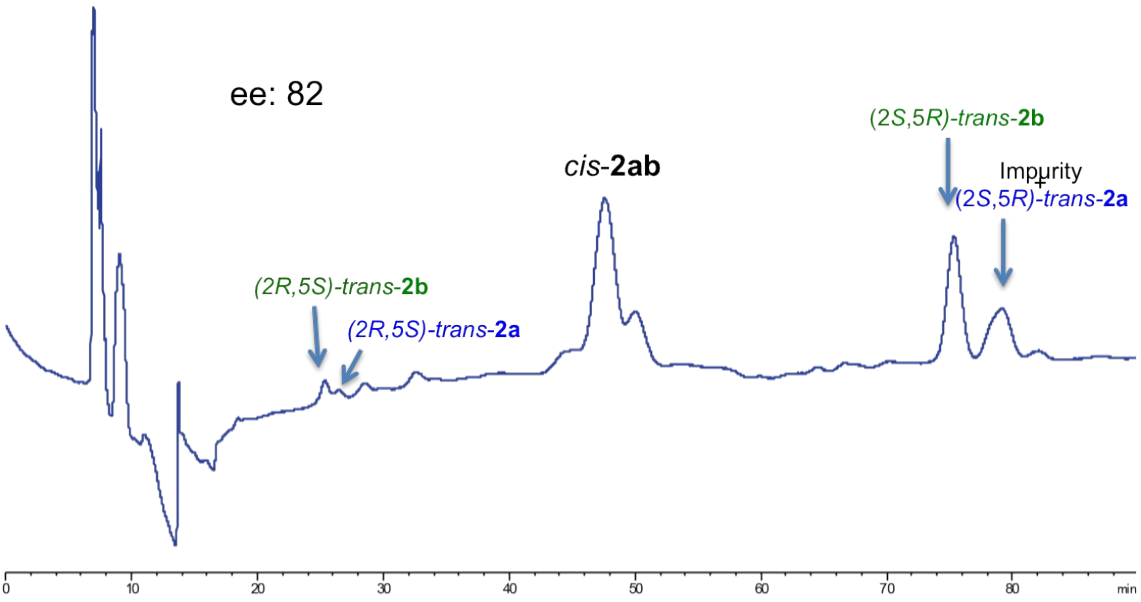


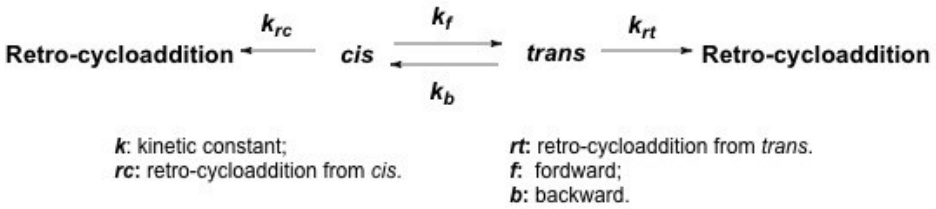
Figure S21. HPLC profile of compound *trans*-**2ab** after the isomerization reaction. Conditions: Chiral column IC (4.6 ID x 250mm; hexane/methanol (97:3); 0.5 ml/min; 320 nm; 25ºC).

The value of the *ee* is the same of that corresponding at *cis*-**2ab** before the isomerization process (Figure S12). *Note*: the conditions to observe the *ee* of compounds *trans*-**2ab** are different of those corresponding to detect the *ee* of the *cis* analogs.

Kinetic studies of the isomerization reaction.

The proposed mechanism for the isomerization (equilibrium reaction) could be outlined according to the following scheme:

Scheme S1. Representation of the reactions involved in the isomerization process.



If we ignore the retro-cycloaddition reaction contribution, the reaction rate would remain:

$$v = -\frac{d[cis]}{dt} = k_f[cis] - k_b[trans] \qquad \text{equation (1)}$$

$$\ln \frac{(x - x_e)}{(x_0 - x_e)} = -(k_f + k_b)t \qquad \text{equation (2)}$$

$$k = k_f + k_b \qquad \text{equation (3)}$$

Where x, x_e, and x_o are the concentrations of *cis* adduct at the time t, at equilibrium, and at the starting point, respectively, and k_f and k_b are the rate constants for the forward and backward *cis-trans* isomerization.

In Figures S22-S30 we represent the data corresponding to compounds **2a,b** and **3** at 25ºC, 30ºC, and 40ºC following equation (2) to afford the kinetic constants for each process. It is noted that all experiments follow the same trend. To simplify the graphics A is referred to the equation 2: $A = \frac{(x - x_e)}{(x_0 - x_e)}$.

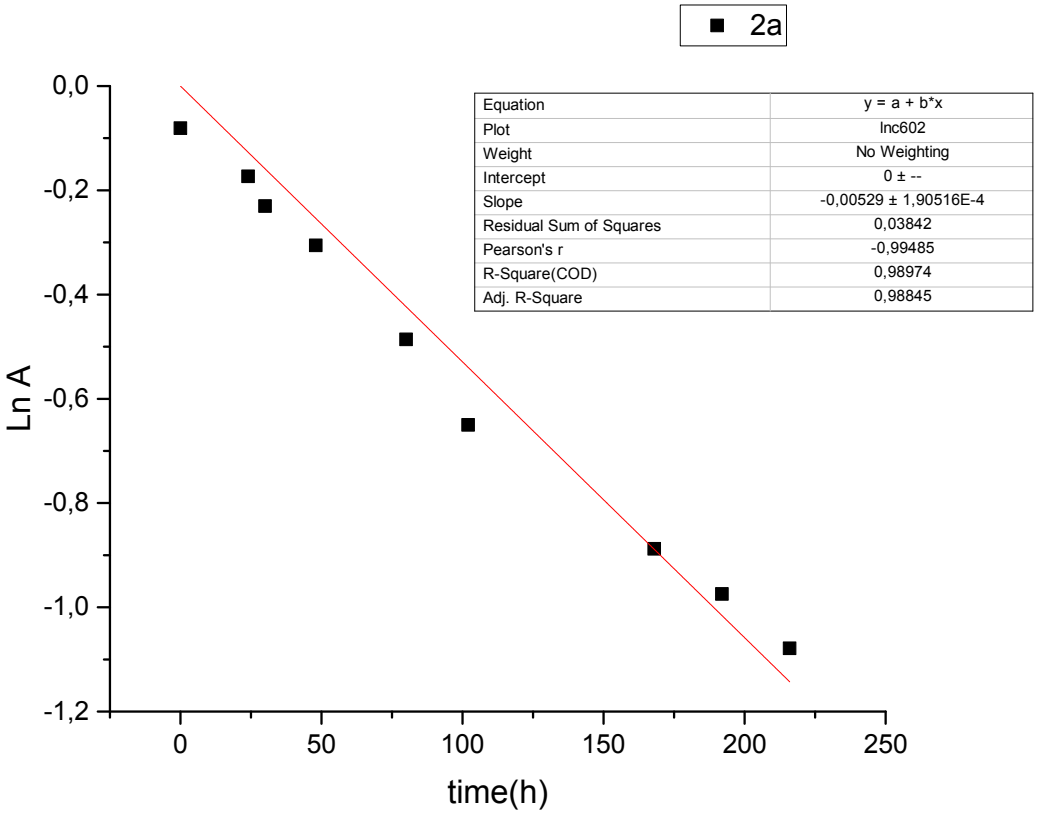


Figure S22. Plotting data of the isomerization of **2a** at room temperature.

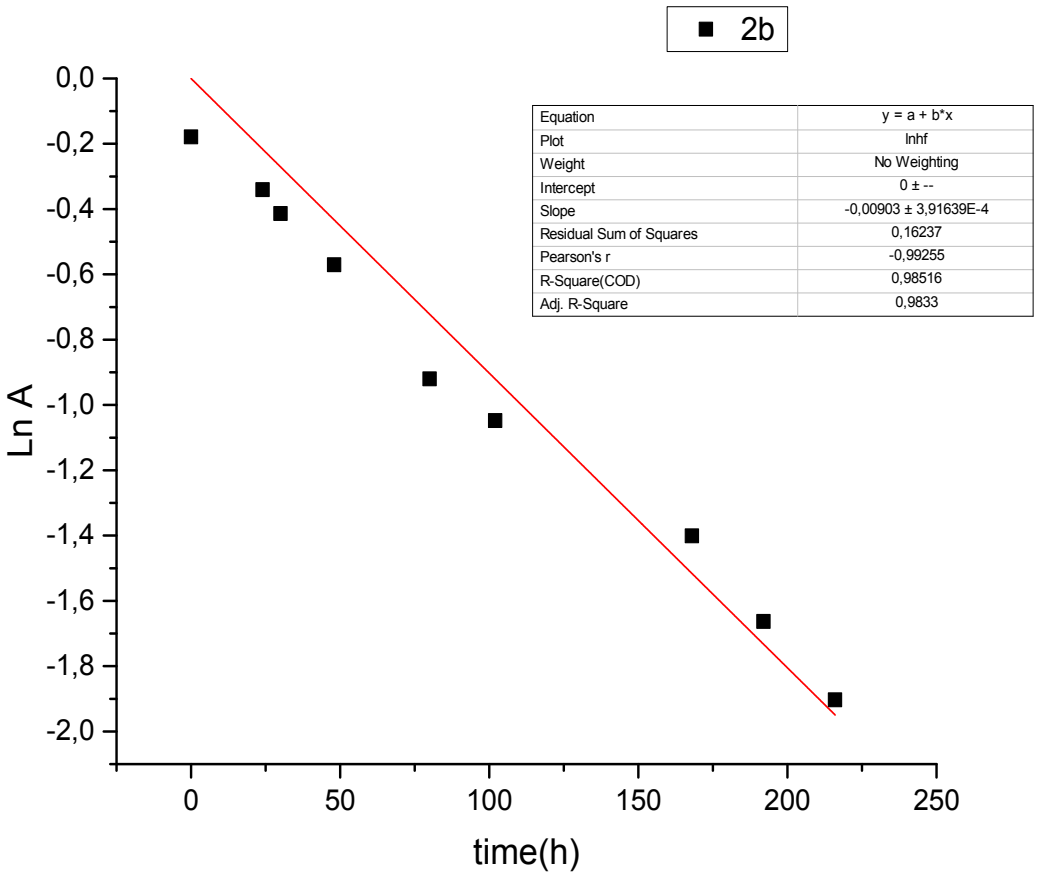


Figure S23. Plotting data of the isomerization of **2b** at room temperature.

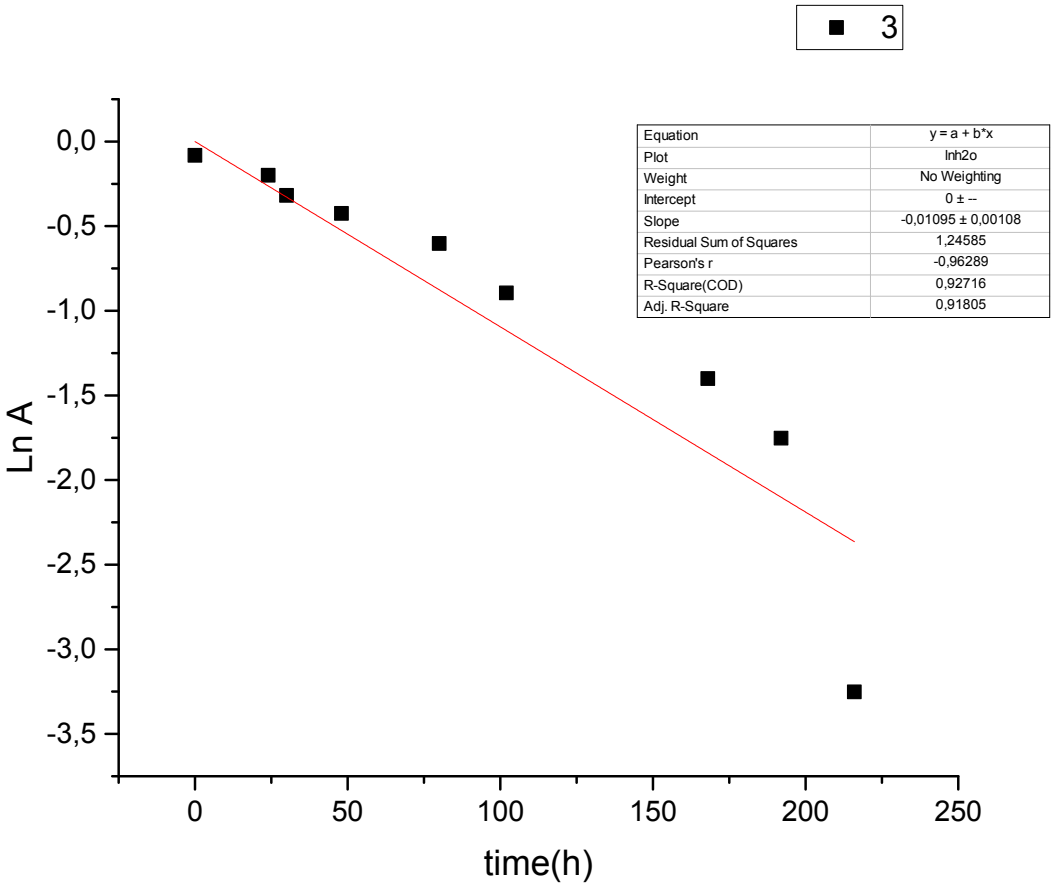


Figure S24. Plotting data of the isomerization of **3** at room temperature.

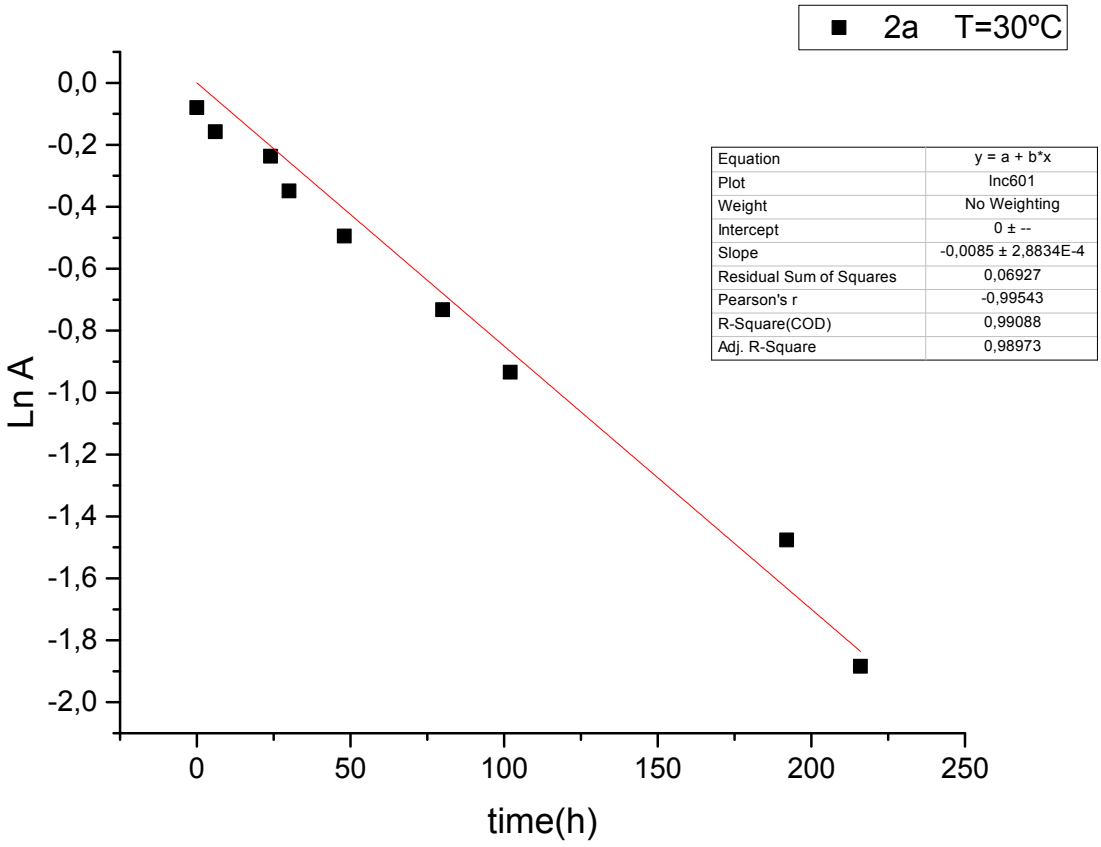


Figure S25. Plotting data of the isomerization of **2a** at 30ºC.

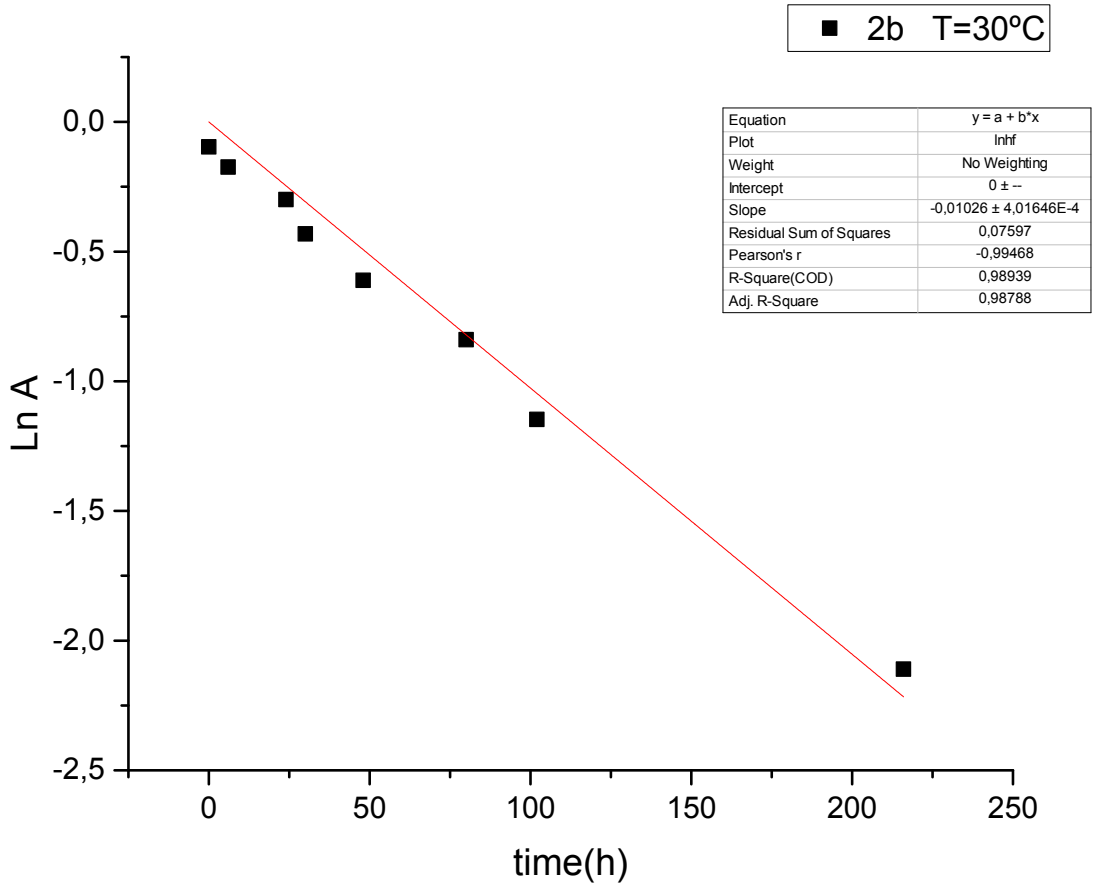


Figure S26. Plotting data of the isomerization of **2b** at 30ºC.

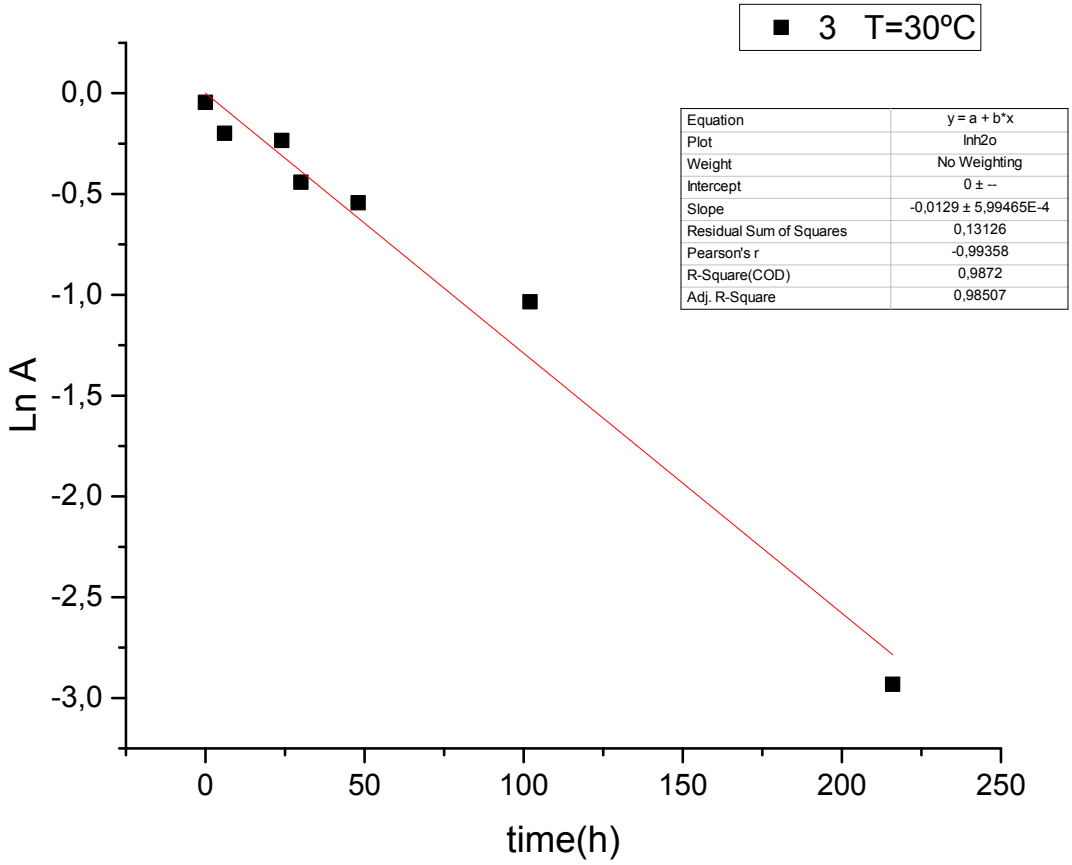


Figure S27. Plotting data of the isomerization of **3** at 30ºC.

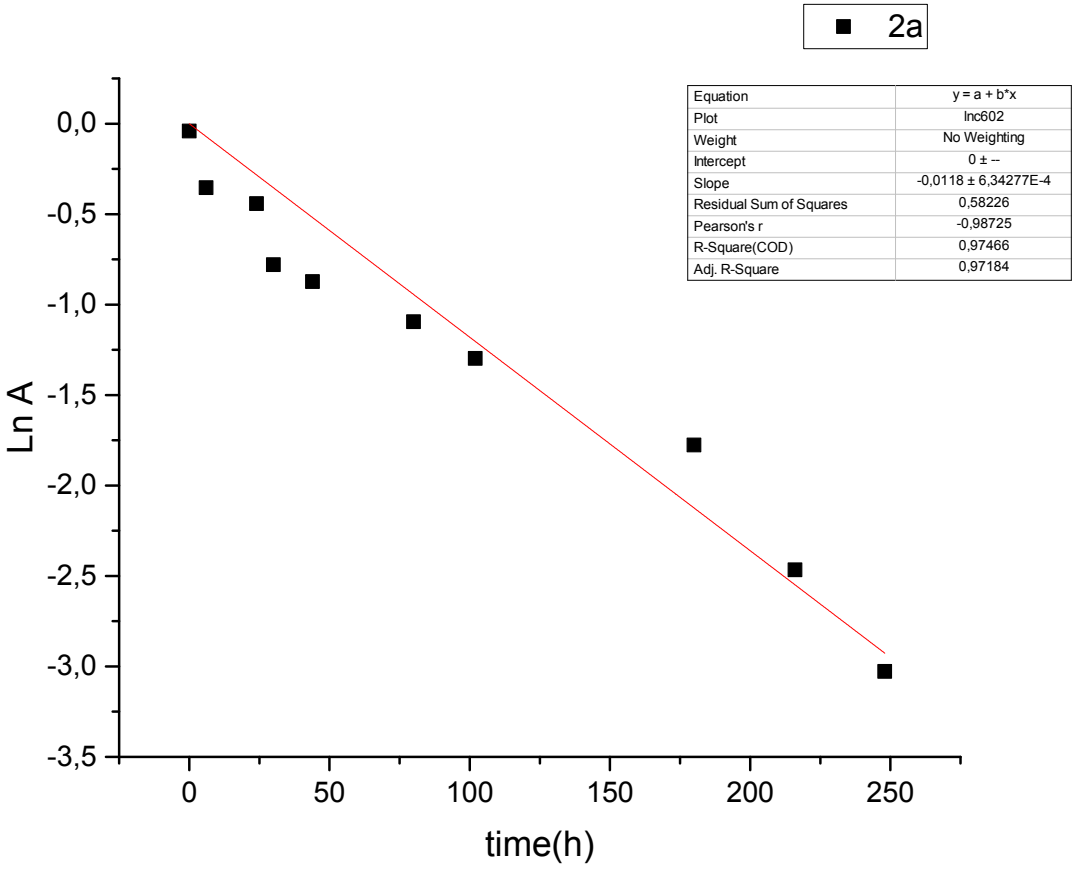


Figure S28. Plotting data of the isomerization of **2a** at 40ºC.

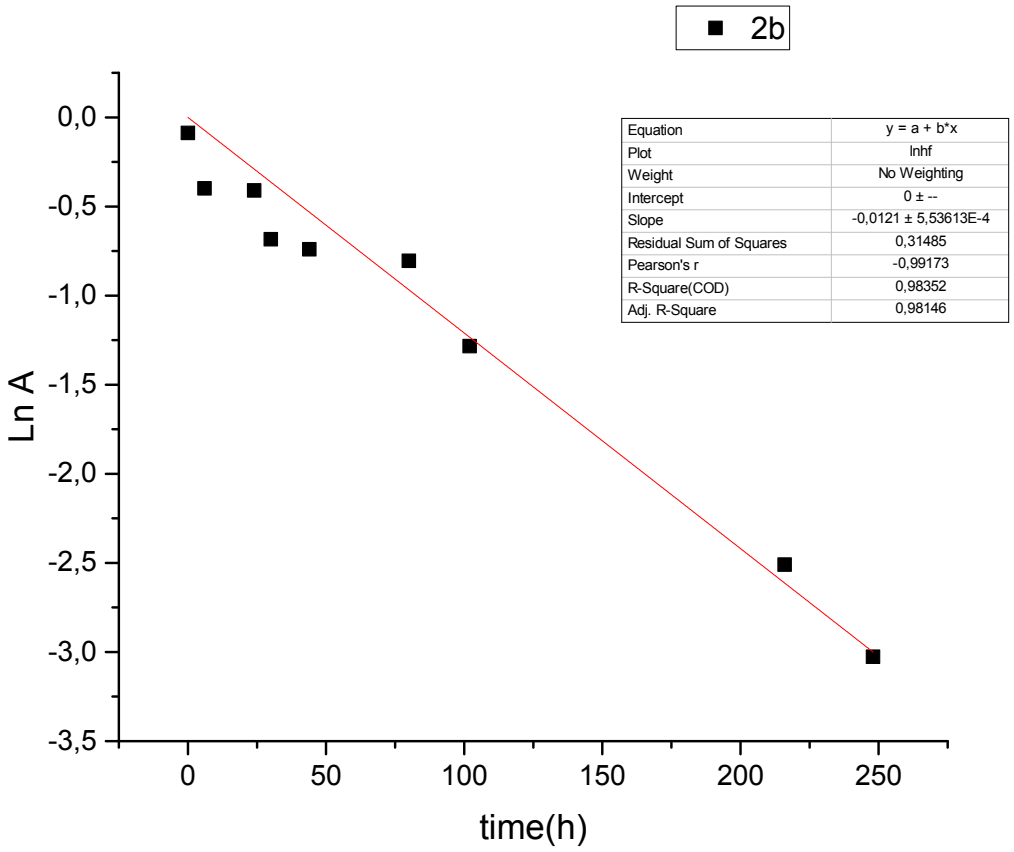


Figure S29. Plotting data of the isomerization of **2b** at 40ºC.

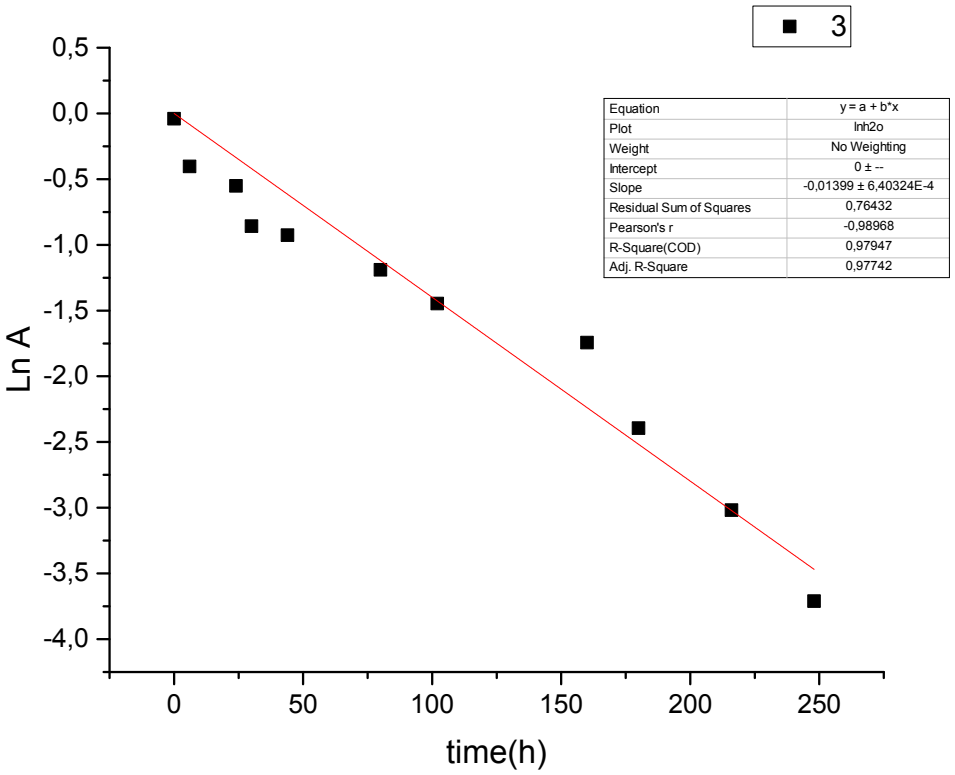


Figure S30. Plotting data of the isomerization of **3** at 40ºC.

Table S1 Comparison of isomerization reaction rates of (2*S*,5*S*)-*cis*-**2a**, (2*S*,5*S*)-*cis*-**2b** and (2*S*,5*S*)-*cis*-**3** in chlorobenzene:acetonitrile 1:1 at 25°C, 30^{0}C and 40^{0}C.

Compound	**T (^{0}C)**	***cis/trans* eq**	**k (h^{-1})**
2a	25	77/23	$5.29x10^{-3} \pm 1.90x10^{-4}$
2b	25	77/23	$9.03x10^{-3} \pm 3.92x10^{-4}$
3	25	77/23	$10.95x10^{-3} \pm 1.08x10^{-3}$
2a	30	59/41	$8.50x10^{-3} \pm 2.88x10^{-4}$
2b	30	59/41	$10.26x10^{-3} \pm 4.01x10^{-4}$
3	30	59/41	$12.90x10^{-3} \pm 5.99x10^{-4}$
2a	40	55/45	$11.80x10^{-3} \pm 6.34x10^{-4}$
2b	40	55/45	$12.10x10^{-3} \pm 5.54x10^{-4}$
3	40	55/45	$13.99x10^{-3} \pm 6.40x10^{-4}$

Computational details

All Density Functional Theory (DFT) optimizations have been performed with the Amsterdam Density Functional (ADF) program.[1,b 2] The molecular orbitals (MOs) were expanded in an uncontracted set of Slater type orbitals (STOs) of triple-ζ (TZP) quality containing diffuse functions and one set of polarization functions. Core electrons (*1s* for 2nd period and *1s2s2p* for 3rd) were not treated explicitly during the geometry optimizations (frozen core approximation),[2] as it was shown to have a negligible effect on the obtained geometries.[3] An auxiliary set of *s*, *p*, *d*, *f*, and *g* STOs was used to fit the molecular density and to represent the Coulomb and exchange potentials accurately for each SCF cycle. The GGA functional OLYP was used to locate all stationary points.[4] OLYP has been extensively used for the study of E2 and S_N2 reaction mechanisms that involve charged species.[5,6] The zwitterionic *cis-trans* intermediates included in this study could only be located using this GGA functional. Previous studies have shown that the GGA functional OLYP is numerically robust and agrees well with available experimental and CCSD(T) geometries.[7] Acetonitrile (MeCN) solvent effects were included through the use of COSMO,[8-10] during all the optimization process.

The actual geometry optimizations were performed with the QUILD[11] (QUantum-regions Interconnected by Local Descriptions) program, which functions as a wrapper around the ADF program. The QUILD program constructs all input files for ADF, runs ADF, and collects all data; ADF is used only for the generation of the energy and gradients. Furthermore, the QUILD program uses improved geometry optimization techniques, such as adapted delocalized coordinates[12] and specially constructed model Hessians with the appropriate number of eigenvalues.[11] The latter is of particular use for TS searches. All TSs were characterized by computing the analytical[13] vibrational frequencies, to have one imaginary frequency corresponding to the approach of the two reacting carbons. Activation barriers obtained with the M06-2X/6-311++G(d,p)//OLYP/TZP method are somewhat overestimated because of the intrinsic multiconfigurational character of the diradical intermediates and transition state for the *cis*/*trans* conversion.

Single Point (SP) calculations were performed with the hybrid meta exchange-correlation DFT functional M06-2X[14,15] with the 6-311+G(d,p) basis set using the Gaussian 09 suite of programs.[16] It has been found that M06-2X provides reasonable

energetics of π–π stacking interactions and non-bonded interactions, and yields accurate reaction and activation energies for the study of fullerene and related carbon systems as compared to experiment.[14,15,17] Solvent effects were included in geometry optimizations using the Conductor-like Polarizable Continuum Model (CPCM) with acetonitrile as the solvent.[18, 19] An UltraFine integration grid was used in all cases as it was found to significantly influence energetics.[20]

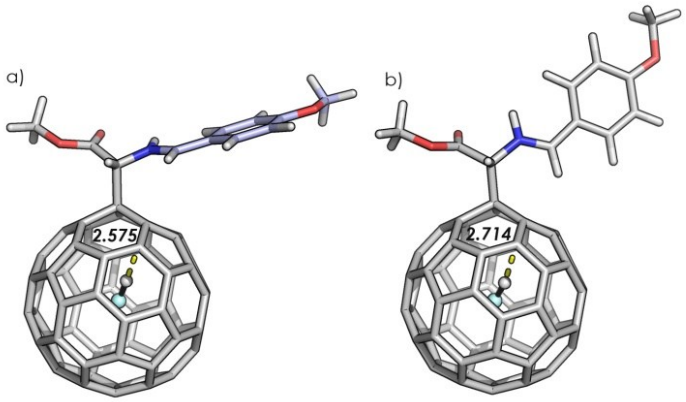
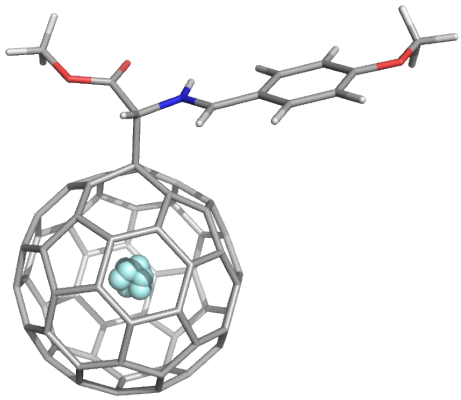


Figure S31. Optimized geometries at OLYP/TZP level of theory of a) INT-(*2S,5S*)-*cis*-**2b** and b) $TS^{cis \rightarrow trans}$ for HF@C_{60}. Distances are in Å.

Table S2. Relative stabilities of different HF orientations inside C_{60} for products, and intermediates (in kcal/mol)



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Orientation	*Prod (2S,5S)-cis*	*Int (2S,5S)-cis*	*Int (2S,5R)-trans*	*Prod (2S,5R)-trans*
i1	**0.0**	24.0	28.3	1.7
i2	0.1	24.0	28.3	1.8
i3	0.2	**23.9**	**28.3**	1.9

i4	0.2	24.0	28.3	**1.6**
i5	0.2	24.0	28.3	1.9
i6	0.4	26.4	30.8	2.1
i7	0.3	26.3	30.7	2.1
i8	0.2	24.0	28.3	1.9
i9	0.4	26.2	30.6	2.1
i10	0.2	25.3	29.8	2.0

Acidity of HF and H_2O in encapsulated species

To further discuss the acidity of encapsulated HF and H_2O, we compare here the deprotonation energies of HF and H_2O in HF/H_2O@C_{60} and in the intermediate HF/H_2O-INT(2S,5S)-cis-**2a** at the M06-2X/6-311+G(d,p)(PCM:acetonitrile)//OLYP/TZP(COSMO:acetonitrile) level of theory. The results are the following:

1) $HF + F^-@C_{60} \rightarrow F^- + HF@C_{60}$ ΔE = -8.3 kcal/mol

Eq. 1 indicates that HF is less acidic when encapsulated in C_{60}. This can be understood from the Gibbs energy of solvation of F^- and $F^-@C_{60}$. Solvation energy in the latter is lower than in the former because of the screening effect of the cage, which makes the deprotonation of HF@C_{60} in acetonitrile less favorable than that of free HF.

2) $HF@C_{60}$ + F^--INT(2*S*,5*S*)-*cis*-**2a** → $F^-@C_{60}$ + HF-INT(2*S*,5*S*)-*cis*-**2a** ΔE = -9.6 kcal/mol

Eq. 2 shows that HF is more acidic in HF@C_{60} than in the zwitterionic intermediate HF-INT(2*S*,5*S*)-*cis*-**2a**. Again the reason is found in the reduced stability of the encapsulated anionic species. In the case of F^--INT(2*S*,5*S*)-*cis*-**2a**, there is an electrostatic repulsion between the negatively charged C atom of the zwitterion and the negatively charged F- that is not present in F-@C_{60}. This repulsion makes the deprotonation in HF-INT(2*S*,5*S*)-*cis*-**2a** less favored than in HF@C_{60}.

In the case of water, we have similar results:

3) $H_2O + OH^-@C_{60} \rightarrow OH^- + H_2O@C_{60}$ ΔE = -5.5 kcal/mol
4) $H_2O@C_{60}$ + OH^--INT(2*S*,5*S*)-*cis*-**2a** → $OH^-@C_{60}$ + H_2O-INT(2S,5S)-*cis*-**2a** ΔE = -14.7 kcal/mol

In addition, we found:

5) $H_2O + F^- \rightarrow HF + OH^-$ $\Delta E = +25.5$ kcal/mol

6) $H_2O@C_{60} + F^-@C_{60} \rightarrow HF@C_{60} + OH^-@C_{60}$ $\Delta E = +22.8$ kcal/mol

7) H_2O-INT(2*S*,5*S*)-*cis*-**2a** + F^--INT(2*S*,5*S*)-*cis*-**2a** →

HF-INT(2*S*,5*S*)-*cis*-**2a** + OH^--INT(2*S*,5S)-*cis*-**2a** $\Delta E = +27.8$ kcal/mol

Reactions 5-7 show that the relative deprotonation energies of HF are lower than those of H_2O indicating that HF is more acidic than H_2O also when these molecules are encapsulated inside C_{60}. This is particularly clear in the case of INT(2*S*,5*S*)-*cis*-**2a**. The increase in the relative acidity of encapsulated HF as compared to H_2O in INT(2*S*,5*S*)-*cis*-**2a** is also in line with the fact that HF is more stabilized when going from HF@C_{60} to HF-INT(2*S*,5*S*)-*cis*-**2a** than H_2O does in the same process (by about 1 kcal/mol, see Figure 5 in the paper). The reason is the stronger hydrogen bond (H-bond) interaction of HF with the negatively charged C atom of the zwitterionic intermediate INT(2*S*,5*S*)-*cis*-**2a**.

To reach the transition state (TS) of the *cis*-to-*trans* rotation ($TS^{cis \rightarrow trans}$ in Figure 5), the H-bond between the encapsulated moiety and the C on the fullerene cage is slightly disrupted because of the less localized negative charge on the C atom and the more delocalized character of the TS. This is clearly shown by the elongation of the F-H···C distance measured for the optimized TS (2.71 Å, see Figure 6 in the paper) as compared to the F-H···C distance in the optimized HF-INT(2*S*,5*S*)-*cis*-**2a** (2.57 Å, see Figure 6 in the paper). Thus, the barrier for the *cis*-to-*trans* rotation will be higher when a stronger H-bond is occurring. This is indeed the case for HF that exhibits a stronger H-bond as compared to H_2O-INT(2*S*,5*S*)-*cis*-**2a**, which translates into a *ca.* 0.4 kcal/mol increase in the activation barrier for the *cis*-to-*trans* rotation. Our calculations are in total agreement with the experimental kinetic measures (see Figure 5 in the paper).

As a whole, we find a pK_a reduction when going from free HF/H_2O to encapsulated HF/H_2O-INT(2*S*,5*S*)-*cis*-**2a**. The reason is basically twofold: 1) the screening effect of the cage and 2) the electrostatic repulsion between the negatively charged C atom of the zwitterion and the negatively charged F^-/OH^-. We also find that free and encapsulated HF molecule has a lower pK_a than H_2O (HF is more acidic) and that HF-INT(2*S*,5*S*)-*cis*-**2a** is better stabilized because of the stronger H-bond (23.9 *vs*. 24.9 kcal/mol for

HF/H_2O, see Figure 5). Nevertheless, due to the more delocalized negative charge on the fullerene carbon atoms in the TS for the *cis*-to-*trans* rotation, the H-bond is slightly broken in the TS, and thus the barrier becomes larger in the HF system with a stronger H-bond as compared to H_2O (0.4 kcal/mol higher, see Figure 5).

Cartesian coordinates of optimized structures:

HF@C_{60}

C	3.10740017	-1.41766469	-0.96968023
C	2.43232693	-2.55761806	-0.37847887
C	2.65517695	-0.88893180	-2.18193475
C	3.51110490	-0.52896959	0.10368109
C	1.32904762	-3.12616641	-1.02091847
C	2.41785693	-2.37342323	1.06056415
C	1.50963485	-1.47942320	-2.84808435
C	2.58815969	0.54822090	-2.36630776
C	3.08455443	-1.11990769	1.35844172
C	3.44628834	0.85610616	-0.07419543
C	0.85953645	-2.57749755	-2.27867192
C	0.17049615	-3.53275094	-0.24889231
C	1.30112980	-2.76542447	1.80416219
C	0.73538023	-0.40778977	-3.44524154
C	1.40190400	0.84551743	-3.14722529
C	2.97690995	1.40484086	-1.33255660
C	2.60996258	-0.30411701	2.38951845
C	2.95324024	1.70260857	0.99559715
C	-0.58976787	-2.64576963	-2.28480032
C	-1.01554258	-3.23666591	-1.02984582
C	0.15647987	-3.35623333	1.13718370
C	0.80822189	-1.91878505	2.87361828
C	-0.66070664	-0.47414767	-3.45282735
C	0.64805280	1.98829790	-2.86620289
C	2.19301352	2.59037142	-1.04023252
C	2.54289354	1.13310432	2.20426474
C	1.45044232	-0.71111512	3.16093239
C	2.17844479	2.77422012	0.39876664
C	-1.33588174	-1.61429177	-2.86192713
C	-2.17343083	-2.77653092	-0.39619793
C	-1.04431101	-2.87632214	1.79546184
C	-0.64119919	-1.98699765	2.86863315
C	-1.44367227	0.71218174	-3.16150730
C	1.05111743	2.87727007	-1.79332525
C	-0.80141070	1.92017294	-2.87226924
C	1.34207484	1.61412849	2.86112176
C	0.66696709	0.47443961	3.45217411
C	1.02254058	3.23805532	1.03258741
C	-2.53725981	-1.13372301	-2.20439282
C	-2.94796692	-1.70456351	-0.99463250
C	-2.18832059	-2.59275556	1.04355180
C	-1.39538209	-0.84462691	3.15149510
C	-2.60367972	0.30516748	-2.38963280

C	-0.14922765	3.35837339	-1.13511175
C	-1.29422331	2.76748912	-1.80224452
C	0.59661884	2.64723245	2.28685177
C	-0.72900465	0.40879359	3.44903433
C	-0.16322788	3.53490265	0.25130128
C	-3.43960731	-0.85662828	0.07680287
C	-2.97137275	-1.40617635	1.33672261
C	-2.58247111	-0.54800551	2.37086330
C	-3.07877143	1.12304205	-1.35788619
C	-2.41367316	2.37894310	-1.05933448
C	-0.85279959	2.57920563	2.28160037
C	-1.50288965	1.48111222	2.85221750
C	-1.32244205	3.12876580	1.02355221
C	-3.50426442	0.53082381	-0.10120726
C	-2.64878368	0.89064903	2.18601271
C	-2.42854360	2.56340785	0.38124152
C	-3.10245690	1.42160916	0.97360098
F	-0.06681545	0.00520014	-0.00832458
H	-0.98521490	0.10249920	-0.11098565

PROD (2S,5S)-cis

C	4.40860437	-0.23418026	1.81792703
C	4.30312134	1.15527322	1.41933762
C	3.52718702	-0.75795629	2.76931719
C	4.75472920	-1.01234844	0.64410089
C	3.31867731	1.97114821	1.98493761
C	4.58483274	1.23639649	-0.00299759
C	2.50604516	0.08509582	3.35288564
C	2.96254663	-2.08461506	2.58176328
C	4.86404399	-0.10346987	-0.48081389
C	4.21263228	-2.28810790	0.46454057
C	2.40177165	1.42672238	2.97030474
C	2.57829314	2.89501490	1.14864539
C	3.87158191	2.13044541	-0.80740785
C	1.30692965	-0.71590177	3.52070338
C	1.59348774	-2.05949430	3.05043068
C	3.30164453	-2.83512445	1.45127205
C	4.41757714	-0.50158069	-1.74523563
C	3.75667225	-2.70524290	-0.84753692
C	1.09898361	2.01627492	2.74152263
C	1.20556391	2.91448237	1.61982477
C	2.84916637	2.97306238	-0.21912739
C	3.40826002	1.71656681	-2.11998287
C	0.05116708	-0.14713930	3.28820751
C	0.60861114	-2.79277811	2.37867642
C	2.28341302	-3.59188208	0.74973953
C	3.85299888	-1.82739202	-1.93182278
C	3.67722613	0.42241690	-2.57731255
C	2.56428751	-3.51065527	-0.67226495
C	-0.05918568	1.24210932	2.88949514
C	0.15189190	2.99144130	0.69967820
C	1.75819507	3.07438722	-1.17078140

C	2.10285220	2.30508120	-2.33958307
C	-0.96953146	-0.90123093	2.58772641
C	0.96104511	-3.57391796	1.20474612
C	-0.69594684	-2.20495773	2.14907947
C	2.76407601	-1.72184365	-2.87888659
C	2.64819351	-0.32957824	-3.27264201
C	1.51323964	-3.41289565	-1.58966122
C	-1.14617916	1.36008171	1.94369531
C	-1.05392484	2.23042365	0.87567958
C	0.43326552	3.07306808	-0.71721386
C	1.10376907	1.57556746	-2.99747139
C	-1.71575947	0.01506093	1.75176736
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C	-1.14616282	-2.61490958	0.84065085
C	1.61416278	-2.50095451	-2.71528918
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C	0.14258247	-3.38820761	-1.11721659
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C	-1.84386074	-1.70149944	0.03688467
C	0.30757303	-1.91575082	-2.93618401
C	0.19216862	-0.56705911	-3.29992537
C	-0.59633650	-2.45837777	-1.95353332
C	-2.36968328	0.56081508	-0.67800364
C	-0.83611173	0.26787085	-2.71891665
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H	-3.96004130	0.99194599	-2.09372471
C	-3.04311918	4.25370811	0.12247864
O	-3.55874087	4.34730802	1.22413912
O	-2.41585712	5.25069506	-0.52145964
C	-2.34103473	6.52629318	0.17889689
H	-1.78268520	6.41339285	1.11103004
H	-1.81678304	7.19287460	-0.50495565
H	-3.34634081	6.89926158	0.38554578
C	-4.93343116	-0.19927854	-0.63630873
C	-5.39198937	-0.39485606	0.67188345
C	-5.43441326	-1.05132957	-1.63405767
C	-6.30229759	-1.40441754	0.99019655
H	-5.04611979	0.23659474	1.48579529
C	-6.33508216	-2.06749171	-1.33746721
H	-5.11636949	-0.92090926	-2.66637219
C	-6.77293649	-2.25868252	-0.01651279
H	-6.62694425	-1.51309368	2.01895822
H	-6.71054724	-2.72006784	-2.12236544
O	-7.64960379	-3.29260036	0.17700416
C	-8.11638249	-3.55273539	1.51327268
H	-8.67914710	-2.70037147	1.90937081
H	-8.77632952	-4.41702969	1.42575372

H	-7.28328401	-3.79460285	2.18255524
H	-4.36065824	2.12814829	0.57160621
F	1.29163948	-0.27452276	0.02775328
H	0.46782333	-0.65762265	0.22272226

INT (2S,5S)-cis

C	4.27274847	0.47213506	-2.29974460
C	4.01274692	-0.95430339	-2.28824054
C	3.34762602	1.34726005	-2.88114963
C	4.91841176	0.81968908	-1.04921420
C	2.83684409	-1.45529887	-2.85635783
C	4.49300566	-1.48705346	-1.02664900
C	2.12831085	0.82850953	-3.46311294
C	3.02746285	2.60484323	-2.22722086
C	5.04939507	-0.38949425	-0.25986730
C	4.60457771	2.02974103	-0.41872520
C	1.87695541	-0.54776765	-3.45921281
C	2.09709613	-2.50264212	-2.18159295
C	3.77928879	-2.50129686	-0.38014364
C	1.05695501	1.76671233	-3.17244480
C	1.61581968	2.87160798	-2.41971444
C	3.65033431	2.93988310	-1.02098007
C	4.87348463	-0.34589836	1.12832858
C	4.42624592	2.07787473	1.01934044
C	0.54743223	-1.03631842	-3.15501839
C	0.67958523	-2.23671021	-2.36841298
C	2.55886193	-3.01473580	-0.96909959
C	3.59647949	-2.45623666	1.05990589
C	-0.22438751	1.29018395	-2.87589665
C	0.86682560	3.45207654	-1.38626091
C	2.87755305	3.54917085	0.04551158
C	4.55253708	0.91214821	1.78066689
C	4.12951097	-1.39273279	1.79609411
C	3.35716639	3.01566697	1.30738348
C	-0.48184831	-0.13155938	-2.86261143
C	-0.22062114	-2.47128986	-1.31894955
C	1.62398616	-3.28234212	0.11170590
C	2.26416290	-2.94055991	1.35693394
C	-1.00989518	1.90113599	-1.81187826
C	1.51603442	3.80394137	-0.13377370
C	-0.46537232	2.97992017	-1.08615626
C	3.62483468	0.64105508	2.86062082
C	3.35322291	-0.78242023	2.86249114
C	2.45934962	2.75690003	2.34563371
C	-1.42016380	-0.40697799	-1.79203883
C	-1.31573124	-1.57883797	-1.05378195
C	0.26080256	-3.00262144	-0.05761146
C	1.51204156	-2.34451365	2.37818722
C	-1.76908917	0.86836881	-1.15860659
C	0.58381615	3.53681570	0.94444628
C	-0.63519250	3.01842563	0.35138182
C	2.58726275	1.54252273	3.13472633
C	2.06611542	-1.25208267	3.14409637
C	1.04587928	3.02297797	2.16060863

C	-1.73226423	-1.68279283	0.42704571
C	-0.52608173	-2.44447827	1.00563422
C	0.09627919	-2.09018520	2.19529275
C	-1.88924397	0.88182373	0.24305742
C	-1.33708834	1.99931859	1.00256574
C	1.25878357	1.06512190	3.44593014
C	0.98894454	-0.31793142	3.44316730
C	0.30828831	1.97005505	2.83478676
C	-1.81865175	-0.30401476	1.04112420
C	-0.23104385	-0.83947112	2.88578577
C	-0.86224316	1.47055779	2.25568199
C	-1.13261234	0.03501846	2.25189213
C	-4.82152679	-0.80410767	1.02135556
C	-3.12576480	-2.51300904	0.68129414
N	-4.26942377	-1.73902047	0.27639560
H	-3.17295913	-2.68607866	1.75669221
H	-4.49417848	-0.77164346	2.05579911
C	-3.18749135	-3.84330443	-0.06508658
O	-3.64034078	-3.95212245	-1.19410554
O	-2.67300005	-4.83730231	0.66655998
C	-2.64557944	-6.15388312	0.03786047
H	-2.03964623	-6.12451434	-0.87003136
H	-2.19529018	-6.80951798	0.78199756
H	-3.66251538	-6.47478023	-0.19623898
C	-5.84342683	0.10307885	0.60864005
C	-6.31084621	0.21925919	-0.72117859
C	-6.42660346	0.93589637	1.59823249
C	-7.31649299	1.10929806	-1.05333191
H	-5.88568285	-0.38433888	-1.51825385
C	-7.43102563	1.82452343	1.27849828
H	-6.08220403	0.86744497	2.62739389
C	-7.89256620	1.92052548	-0.05249033
H	-7.64702337	1.17404502	-2.08305141
H	-7.87869746	2.45724987	2.04015203
O	-8.87942688	2.81657241	-0.26343106
C	-9.40713360	2.98791027	-1.59919813
H	-9.85084422	2.05642466	-1.96309201
H	-10.17804084	3.75237098	-1.50227149
H	-8.62561748	3.33244123	-2.28285730
H	-4.56234227	-1.87042912	-0.68759408
F	1.48654494	0.24945722	0.01181549
H	0.59866743	0.11905603	0.26004243

PROD *(2S,5R)-trans*

C	4.83275645	0.20124116	0.72254333
C	4.58973518	1.28988440	-0.20325208
C	4.27808093	0.23841698	2.00610361
C	4.83231177	-1.03734269	-0.03204466
C	3.80150825	2.37636299	0.18722076
C	4.43805147	0.72335021	-1.53188371
C	3.45910123	1.36139180	2.40993621
C	3.70691339	-0.96591489	2.58535175
C	4.58712301	-0.71434676	-1.42467722
C	4.28175499	-2.19536653	0.52491546

C	3.22533068	2.41405431	1.51925799
C	2.83207365	2.93498203	-0.73483817
C	3.50561712	1.26615889	-2.42148002
C	2.37741193	0.85197306	3.23320922
C	2.53610683	-0.58610989	3.34664167
C	3.71184548	-2.16080164	1.85831413
C	3.79759988	-1.56077607	-2.21005236
C	3.46661214	-3.07658570	-0.28888244
C	1.90254806	2.99424896	1.41712620
C	1.65929828	3.31262216	0.03270826
C	2.68721815	2.39142920	-2.01313398
C	2.68457047	0.38739635	-3.23578129
C	1.09875379	1.40507115	3.12257606
C	1.40922581	-1.41466454	3.36066164
C	2.54497124	-3.02068887	1.86916110
C	3.22637943	-2.76507042	-1.63094193
C	2.82858385	-1.00071584	-3.12772201
C	2.39305226	-3.58726004	0.54091158
C	0.85359389	2.49371784	2.19900134
C	0.37990780	3.11275478	-0.50073660
C	1.36183862	2.20260342	-2.57498716
C	1.36184801	0.97304559	-3.32910355
C	-0.07093555	0.54967435	3.13540616
C	1.41480631	-2.65596064	2.60724565
C	0.08421607	-0.83731780	3.26091744
C	1.90442916	-2.94916107	-2.19142221
C	1.65394018	-1.85508893	-3.11246742
C	1.11665452	-3.76792309	-0.00019927
C	-0.46609339	2.31967366	1.63343949
C	-0.70607443	2.64229129	0.31279929
C	0.22859380	2.54906911	-1.82548116
C	0.22559507	0.15098484	-3.29932011
C	-1.04704247	1.10112557	2.22231396
C	0.09205579	-2.84082872	2.04257875
C	-0.72385428	-1.71149636	2.44889353
C	0.86642004	-3.44286848	-1.39343762
C	0.37753962	-1.28774774	-3.19134387
C	-0.05403984	-3.38555102	0.76493142
C	-1.76449248	1.96130763	-0.55476457
C	-0.94842268	1.72518267	-1.82693163
C	-0.94413976	0.54136770	-2.53972857
C	-1.82971231	0.26385615	1.45159403
C	-1.64360042	-1.15561557	1.54987345
C	-0.45727086	-2.86222647	-1.48536387
C	-0.69975944	-1.79686074	-2.36366201
C	-1.02135096	-2.82171578	-0.15904718
C	-2.39407128	0.63420179	0.08394042
C	-1.52502966	-0.68033064	-1.95303537
C	-1.79437691	-1.71828490	0.22516921
C	-2.07692302	-0.64429506	-0.68694140
C	-3.97447145	0.99094259	0.16684371
C	-3.05878956	2.86857466	-0.90258965
N	-4.21298763	1.99913994	-0.85969668
H	-2.94585124	3.28106072	-1.90545824
C	-3.21918935	4.05595008	0.06222815

O	-3.79776764	4.01933052	1.13384077
O	-2.63246851	5.15655563	-0.44894892
C	-2.67455563	6.35153378	0.38188124
H	-3.70987032	6.63839441	0.57759645
H	-2.16698866	7.11981567	-0.20038395
H	-2.15170186	6.17535775	1.32486882
H	-4.08355127	1.49100473	1.13119043
C	-4.95617804	-0.15773894	0.13278577
C	-5.56592876	-0.57968137	1.32576962
C	-5.31574163	-0.82223977	-1.04605135
C	-6.48533493	-1.62188571	1.34483970
H	-5.32456446	-0.07984181	2.26166868
C	-6.24354001	-1.86573727	-1.05094454
H	-4.88094208	-0.54096948	-2.00171882
C	-6.83443936	-2.27668629	0.15193571
H	-6.94894437	-1.93332067	2.27819686
H	-6.49132444	-2.34381786	-1.99190847
O	-7.75294630	-3.28494018	0.27228372
C	-8.16528613	-3.98305246	-0.91679237
H	-8.89217653	-4.72319660	-0.57917730
H	-7.31891329	-4.49128621	-1.39216065
H	-8.64077791	-3.30160377	-1.63091633
H	-4.33580702	1.56877552	-1.77202363
F	1.34445860	-0.21395524	-0.04899164
H	0.84725056	-0.13376285	-0.83008084

INT (2S,5R)-trans

N	-4.28969554	-1.38150412	0.86461404
C	3.83189422	1.04928458	-2.68265208
C	3.37284677	-0.26778692	-3.07892011
C	2.94747665	2.13445388	-2.70376808
C	4.76181281	0.88751769	-1.58249641
C	2.04545469	-0.45482100	-3.47887709
C	4.01477954	-1.24350928	-2.21781219
C	1.57297972	1.93831915	-3.11159335
C	2.95304833	3.09712638	-1.61497124
C	4.86934745	-0.52799765	-1.29016634
C	4.76034323	1.81393292	-0.53159711
C	1.12813341	0.66993606	-3.50075500
C	1.31189867	-1.62088098	-3.02947909
C	3.30555867	-2.37040726	-1.78925604
C	0.73220829	2.78435136	-2.28097011
C	1.58730968	3.51224742	-1.36564837
C	3.84906063	2.94081115	-0.55296654
C	4.98571023	-0.96672222	0.03480682
C	4.88634701	1.36348802	0.84018095
C	-0.16906551	0.19678050	-3.06262699
C	-0.05958426	-1.21099332	-2.77134720
C	1.92935989	-2.55867491	-2.20220229
C	3.42551530	-2.82512084	-0.41509811
C	-0.51858401	2.32046402	-1.85889002
C	1.15512385	3.73656352	-0.04974661

C	3.40601581	3.18557547	0.80742231
C	4.99011822	-0.00213461	1.12185233
C	4.24555914	-2.12822938	0.47923504
C	4.04736593	2.20941912	1.66904126
C	-0.97302638	1.00808697	-2.25149535
C	-0.75580389	-1.74050976	-1.67515432
C	1.20271403	-3.12756171	-1.07880142
C	2.12386620	-3.29080432	0.01660950
C	-0.97531687	2.56610483	-0.49670196
C	2.08845890	3.57870146	1.05403446
C	-0.14329744	3.28155532	0.38931052
C	4.27255844	-0.57476158	2.24312458
C	3.79972437	-1.88317704	1.84112843
C	3.34863299	1.66116203	2.74711099
C	-1.70523194	0.43602566	-1.13680518
C	-1.63567719	-0.92913899	-0.87728320
C	-0.11176763	-2.71479145	-0.81354513
C	1.69018277	-3.04356668	1.32658747
C	-1.73202068	1.42616228	-0.05817005
C	1.36385732	3.01215523	2.17516409
C	-0.01244331	2.82053931	1.75654553
C	3.45294912	0.24002948	3.03798081
C	2.54052410	-2.33377354	2.25218501
C	1.98216129	2.07122488	3.00556424
C	-1.75898815	-1.52371301	0.54215771
C	-0.57572312	-2.51811492	0.53028297
C	0.32040563	-2.64437957	1.58317986
C	-1.56565133	0.94848173	1.25835147
C	-0.71043214	1.68835527	2.18676792
C	2.16075886	-0.22431615	3.48627986
C	1.69324174	-1.49513775	3.09133215
C	1.24944452	0.90067274	3.45217997
C	-1.50445751	-0.43965477	1.57753427
C	0.32384318	-1.70428891	2.70756228
C	-0.07465385	0.72038228	3.04133982
C	-0.54930760	-0.60003185	2.62670762
C	-3.14428048	-2.29003390	0.84723637
H	-3.05228367	-2.65810158	1.86814842
C	-4.92370188	-0.86859777	-0.16440877
C	-3.40537715	-3.49725378	-0.06392278
O	-3.83794516	-3.42884699	-1.20137801
O	-3.06522064	-4.63158442	0.56635691
C	-3.20328894	-5.86359120	-0.20174929
C	-6.01887974	0.04085821	-0.10598527
C	-6.56594420	0.48083380	-1.34014380
C	-6.59130490	0.52945709	1.09308246
C	-7.62487471	1.36078794	-1.37498306
C	-7.65303081	1.41235725	1.06958488
C	-8.18399314	1.83819756	-0.16917137
O	-9.21429149	2.69297596	-0.30668825
C	-9.85329295	3.23726717	0.87285230
H	-4.25062510	-6.02113256	-0.46745883
H	-2.85243047	-6.64972449	0.46531672
H	-2.58793668	-5.81690108	-1.10277666
H	-4.57744530	-1.18957492	-1.13990003

H	-6.14313990	0.11725316	-2.27352498
H	-6.21217594	0.21996265	2.06332104
H	-8.04226303	1.69611584	-2.32043263
H	-8.06824622	1.76736396	2.00515472
H	-10.64165505	3.88548658	0.49100065
H	-9.14109831	3.82246393	1.46138647
H	-10.28841233	2.43814940	1.47958737
H	-4.58336907	-1.10638591	1.79480074
F	1.57035043	0.20869546	0.02750945
H	0.77285091	0.04662271	0.48037670

TS CIS → TRANS

N	-4.490155	1.410257	-0.438695
C	4.105835	-0.725511	2.554492
C	3.622291	0.602369	2.877695
C	3.274106	-1.836706	2.737485
C	4.936974	-0.623695	1.370828
C	2.323614	0.773818	3.369485
C	4.151318	1.523777	1.889271
C	1.929022	-1.657264	3.239756
C	3.236409	-2.888997	1.735644
C	4.960031	0.764493	0.955645
C	4.894432	-1.636316	0.404326
C	1.460575	-0.378239	3.558717
C	1.505915	1.868177	2.886987
C	3.361727	2.582815	1.430220
C	1.062577	-2.600883	2.553253
C	1.873689	-3.372720	1.634227
C	4.037391	-2.790195	0.593725
C	4.952701	1.092488	-0.405978
C	4.891591	-1.299821	-1.005632
C	0.113339	0.008041	3.192309
C	0.137324	1.386723	2.777331
C	2.015559	2.753924	1.938660
C	3.352238	2.921312	0.017765
C	-0.236537	-2.219572	2.198680
C	1.349634	-3.724267	0.381384
C	3.499746	-3.165949	-0.700894
C	4.914591	0.039374	-1.406958
C	4.129596	2.183195	-0.881454
C	4.028095	-2.244256	-1.690289
C	-0.717045	-0.896548	2.518528
C	-0.667755	1.792718	1.703108
C	1.178219	3.192392	0.835120
C	2.001233	3.297336	-0.340917
C	-0.787946	-2.598018	0.904900
C	2.185275	-3.626644	-0.804902
C	0.002681	-3.354388	0.015678
C	4.086280	0.487276	-2.509310
C	3.588740	1.806582	-2.177519
C	3.223786	-1.816153	-2.749184
C	-1.562199	-0.447638	1.427929
C	-1.583108	0.892017	1.054924
C	-0.131320	2.706253	0.713340

C	1.476455	2.922376	-1.584810
C	-1.627184	-1.527460	0.438837
C	1.351156	-3.184868	-1.905331
C	0.006293	-3.006352	-1.390450
C	3.243208	-0.422422	-3.164587
C	2.281688	2.171638	-2.517584
C	1.859801	-2.296021	-2.858603
C	-1.852506	1.363527	-0.399996
C	-0.690630	2.381683	-0.565277
C	0.110302	2.453542	-1.694297
C	-1.575470	-1.153477	-0.920245
C	-0.769037	-1.939578	-1.851255
C	1.899788	-0.046029	-3.540068
C	1.408363	1.234529	-3.213273
C	1.043896	-1.195412	-3.337642
C	-1.620533	0.199882	-1.362112
C	0.064846	1.424701	-2.736800
C	-0.249687	-1.027079	-2.833446
C	-0.751831	0.303651	-2.492945
C	-4.740555	0.133902	-0.314586
C	-3.224642	2.134012	-0.663664
C	-3.357387	3.449307	0.136455
C	-2.978464	5.796917	0.055718
C	-6.037324	-0.452804	-0.192962
C	-7.250069	0.275719	-0.154783
C	-6.103515	-1.867895	-0.112091
C	-8.467577	-0.366991	-0.039367
C	-7.312576	-2.519860	-0.005631
C	-8.512723	-1.777902	0.034404
C	-10.918924	-1.825435	0.223553
O	-3.811604	3.515469	1.266166
O	-2.931106	4.489755	-0.591147
O	-9.641731	-2.504391	0.144095
H	-3.212140	2.397317	-1.725889
H	-3.890669	-0.535124	-0.312249
H	-2.349630	5.797408	0.948534
H	-2.592999	6.490915	-0.689790
H	-4.008792	6.045362	0.319126
H	-7.258455	1.361019	-0.209029
H	-5.187136	-2.451136	-0.136448
H	-9.376240	0.222114	-0.007588
H	-7.359042	-3.603584	0.053098
H	-11.103803	-1.241845	-0.682540
H	-11.656029	-2.623522	0.308795
H	-10.958093	-1.184464	1.108909
H	-5.294170	2.028760	-0.463693
F	1.708832	-0.212130	0.021097
H	0.883770	-0.230513	-0.407738

TS RETRO PRATO

C	4.620161	-0.067316	1.922074
C	4.344786	1.335467	1.678258
C	3.794744	-0.804604	2.777966
C	5.088964	-0.653462	0.681160

C	3.252107	1.950220	2.297129
C	4.640593	1.615283	0.285347
C	2.661312	-0.167814	3.416346
C	3.404436	-2.157524	2.422368
C	5.098560	0.385316	-0.330921
C	4.710087	-1.955599	0.338678
C	2.395177	1.185370	3.184799
C	2.414998	2.864487	1.545692
C	3.834362	2.500604	-0.436911
C	1.571655	-1.127272	3.456906
C	2.033867	-2.359977	2.848967
C	3.856692	-2.721664	1.225964
C	4.734404	0.084634	-1.647806
C	4.335409	-2.269190	-1.026674
C	1.030521	1.628022	2.980305
C	1.040284	2.659818	1.969884
C	2.700559	3.134690	0.206381
C	3.456407	2.188298	-1.803398
C	0.255820	-0.697576	3.258107
C	1.159427	-3.115688	2.058510
C	2.952667	-3.508750	0.408870
C	4.344543	-1.268588	-2.002701
C	3.896346	0.999780	-2.394309
C	3.248854	-3.229062	-0.984223
C	-0.019444	0.702433	3.012866
C	0.002418	2.718265	1.031234
C	1.623238	3.210390	-0.765623
C	2.090715	2.630307	-2.002783
C	-0.655877	-1.485833	2.444124
C	1.631248	-3.704410	0.817156
C	-0.207026	-2.681509	1.858962
C	3.271981	-1.189713	-2.974973
C	2.989660	0.212723	-3.211587
C	2.212917	-3.153664	-1.918322
C	-1.097009	0.785141	2.046182
C	-1.099885	1.788109	1.079870
C	0.300518	2.996358	-0.359921
C	1.213918	1.867280	-2.783467
C	-1.501551	-0.576998	1.707743
C	0.555539	-3.626939	-0.152811
C	-0.576378	-2.988189	0.492553
C	2.220409	-2.112681	-2.931618
C	1.671874	0.640233	-3.400175
C	0.840779	-3.356188	-1.494408
C	-1.625689	1.565800	-0.303953
C	-0.613393	2.239215	-1.175990
C	-0.158422	1.670740	-2.361457
C	-1.832817	-0.859210	0.375060
C	-1.376041	-2.099017	-0.233539
C	0.855628	-1.676511	-3.137481
C	0.579148	-0.318391	-3.364161
C	0.005715	-2.437443	-2.245938
C	-1.866987	0.170170	-0.634151
C	-0.556140	0.316898	-2.739033
C	-1.082012	-1.820140	-1.619960

C	-1.361324	-0.412018	-1.854250
N	-4.459762	1.745918	-0.305405
C	-4.874100	0.715853	-1.025779
C	-3.407712	2.599373	-0.616939
C	-3.426629	3.816530	0.214488
C	-2.662425	6.065077	0.389929
C	-5.945892	-0.171125	-0.677568
C	-6.700507	-0.089552	0.515027
C	-6.293659	-1.183800	-1.607692
C	-7.751216	-0.958716	0.768300
C	-7.333213	-2.059127	-1.362129
C	-8.080159	-1.955478	-0.171103
C	-9.924410	-2.788205	1.146124
O	-3.979974	3.889579	1.312172
O	-2.732334	4.822318	-0.360518
O	-9.087816	-2.852407	-0.030253
H	-3.251423	2.741730	-1.679901
H	-4.411415	0.606998	-2.000401
H	-2.172786	5.904993	1.353495
H	-2.071620	6.736926	-0.232287
H	-3.665273	6.470616	0.543547
H	-6.486324	0.668871	1.263783
H	-5.737262	-1.270452	-2.538106
H	-8.311841	-0.853679	1.689988
H	-7.593538	-2.829020	-2.084139
H	-10.447055	-1.827961	1.199449
H	-10.647386	-3.595186	1.024871
H	-9.336193	-2.951335	2.054336
H	-4.865536	1.912118	0.613472
F	1.645769	-0.244766	0.025484
H	0.727118	-0.111198	0.081098

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