SUPPORTING INFORMATION

Stereoisomerism of Molecular Multipropellers. 1. Static Stereochemistry of *Bis*- and *Tris*-Triaryl Systems.

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Supporting Information

(9 Tables and 8 Figures; 27 pages)

Results obtained from the analysis of the static stereochemistry of multipropeller molecules **1** and **2**, employing the procedure that uses the symmetry-adapted symbolic notation, are presented in Tables S1-S9 and in Figures S1-S8. Chlorine atoms and H substituents of the sp^3 C atoms are omitted for clarity in Figures S1-S7.

Three-dimensional structures of all the stereoisomers of the seven compounds studied are included in Figures S1-S7 along with their equivalent static representations. Symmetry relationships between all these stereoisomers are also given in the form of graphs. The following keys were adopted in the graphs:

- Green arrows represent two-fold rotations in the reference plane.
- Magenta arrows represent three-fold rotations perpendicular to the reference plane.
- Dark blue arrows relate enantiomeric forms.
- Static representations **in bold** correspond to the three-dimensional structures of the enantiomers depicted.

Table S1. Symmetry relationships between the four static representations of the three stereoisomers (1 *dl* pair and 1 *meso* diastereomeric forms) of triplet **1c**.

Symmetry relationships between the 4 static representations	Molecular symmetry
$C_{2,//}$ $\{h^+\}\{h^+\} \longleftrightarrow \sigma \longleftrightarrow \{h^-\}\{h^-\}$ $C_{2,//}$	C_2
$\{h^+\}\{h^-\} \overset{\sigma}{\longleftrightarrow} \underset{C_{2,//}}{\longleftrightarrow} \{h^-\}\{h^+\}$	C_s

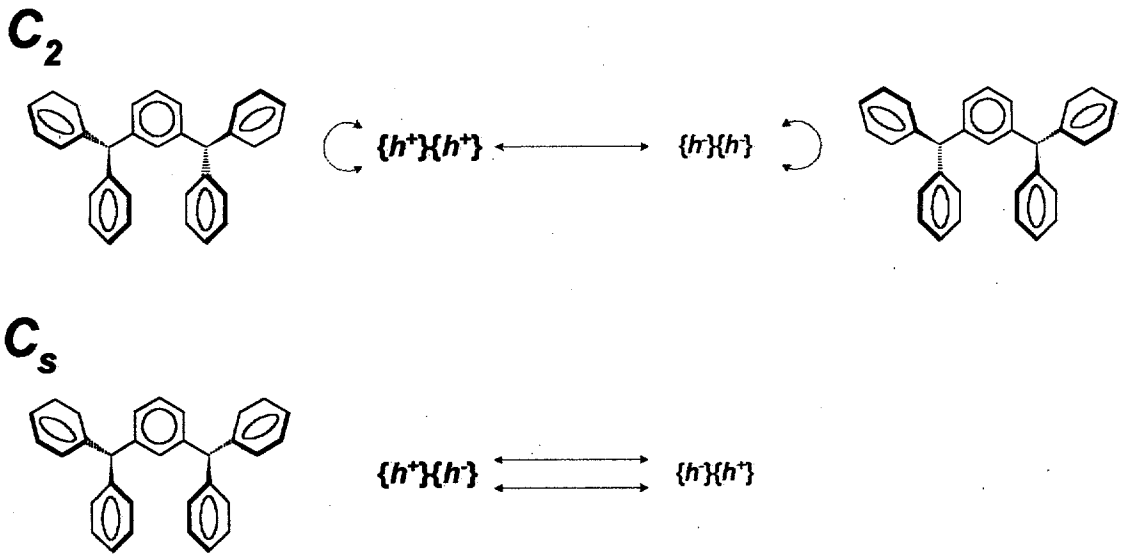


Figure S1. Stereoisomers of triplet **1c**, described with the symmetry-adapted symbolic notation, along with their symmetry relationships.

Table S2. Symmetry relationships between the 16 static representations of the eight stereoisomers (4 *dl* pairs of diastereomeric forms) of monoradical compound **1b**.

Symmetry relationships between the 16 static representations	Molecular symmetry
$\{h^+X^+\}\{h^+\} \longleftrightarrow \sigma \longleftrightarrow \{h^-X^-\}\{h^-\}$ $\uparrow C_{2,//}$ $\uparrow C_{2,//}$ $\{h^+\}\{h^+X^-\} \longleftrightarrow \sigma \longleftrightarrow \{h^-\}\{h^-X^+\}$	C_1
$\{h^+X^+\}\{h^-\} \longleftrightarrow \sigma \longleftrightarrow \{h^-X^-\}\{h^+\}$ $\uparrow C_{2,//}$ $\uparrow C_{2,//}$ $\{h^-\}\{h^+X^-\} \longleftrightarrow \sigma \longleftrightarrow \{h^+\}\{h^-X^+\}$	C_1
$\{h^+X^-\}\{h^+\} \longleftrightarrow \sigma \longleftrightarrow \{h^-X^+\}\{h^-\}$ $\uparrow C_{2,//}$ $\uparrow C_{2,//}$ $\{h^+\}\{h^+X^+\} \longleftrightarrow \sigma \longleftrightarrow \{h^-\}\{h^-X^-\}$	C_1
$\{h^+X^-\}\{h^-\} \longleftrightarrow \sigma \longleftrightarrow \{h^-X^+\}\{h^+\}$ $\uparrow C_{2,//}$ $\uparrow C_{2,//}$ $\{h^-\}\{h^+X^+\} \longleftrightarrow \sigma \longleftrightarrow \{h^+\}\{h^-X^-\}$	C_1

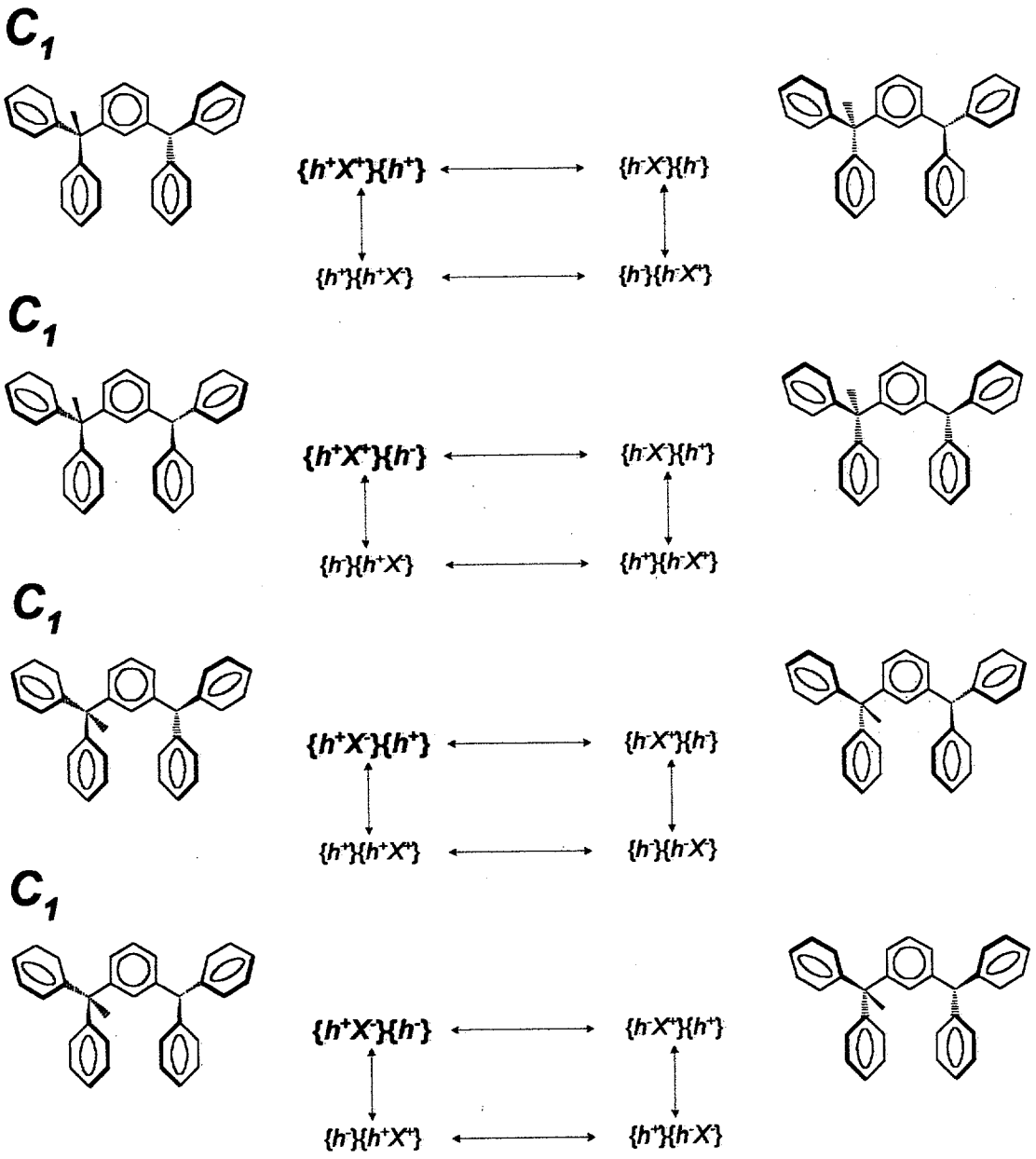


Figure S2. Stereoisomers of monoradical compound **1b**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

Table S3. Symmetry relationships between the 16 static representations of the 10 stereoisomers (4 *dl* pairs and 2 *meso* diastereomeric forms) of hydrocarbon **1a**.

Symmetry relationships between the 16 static representations	Molecular symmetry
$\{h^+X^+\}\{h^+X^+\} \longleftrightarrow \sigma \longleftrightarrow \{h^-X^-\}\{h^-X^-\}$ $C_{2,//}$ $C_{2,//}$ $\{h^+X^+\}\{h^+X^-\} \longleftrightarrow \sigma \longleftrightarrow \{h^-X^+\}\{h^-X^+\}$	C_1
$\{h^+X^+\}\{h^-X^-\} \longleftrightarrow \sigma \longleftrightarrow \{h^-X^-\}\{h^+X^+\}$ $C_{2,//}$ $C_{2,//}$ $\{h^-X^+\}\{h^+X^-\} \longleftrightarrow \sigma \longleftrightarrow \{h^+X^-\}\{h^-X^+\}$	C_1
$C_{2,//}$ $\{h^+X^+\}\{h^+X^-\} \longleftrightarrow \sigma \longleftrightarrow \{h^-X^-\}\{h^-X^+\}$ $C_{2,//}$	C_2
$C_{2,//}$ $\{h^+X^-\}\{h^+X^+\} \longleftrightarrow \sigma \longleftrightarrow \{h^-X^+\}\{h^-X^-\}$ $C_{2,//}$	C_2
$\{h^+X^-\}\{h^-X^+\} \overset{\sigma}{\underset{C_{2,//}}{\longleftrightarrow}} \{h^-X^-\}\{h^+X^-\}$	C_s
$\{h^+X^-\}\{h^-X^-\} \overset{\sigma}{\underset{C_{2,//}}{\longleftrightarrow}} \{h^-X^+\}\{h^+X^+\}$	C_s

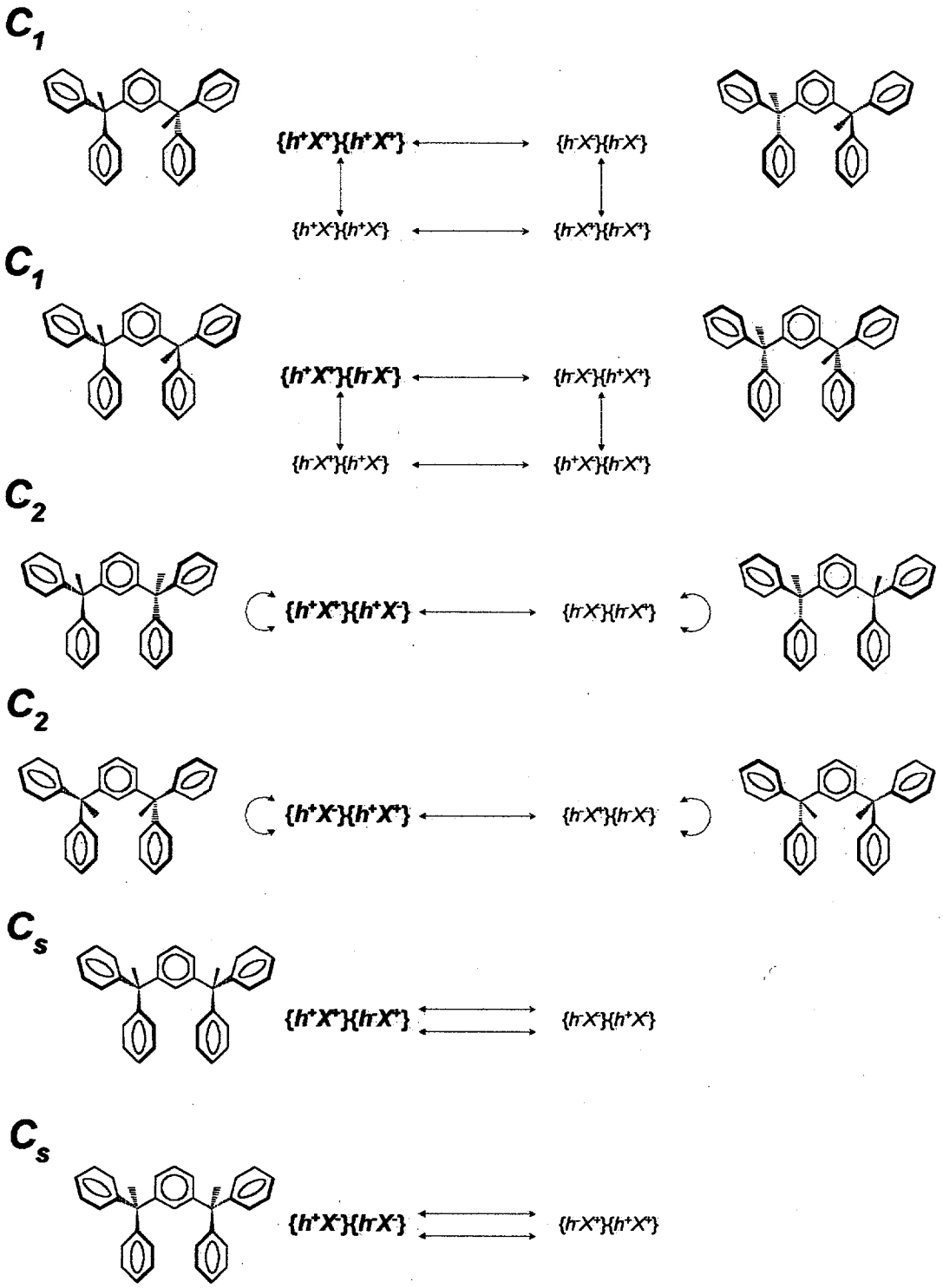
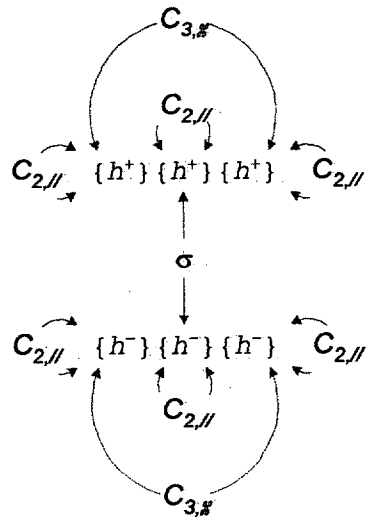


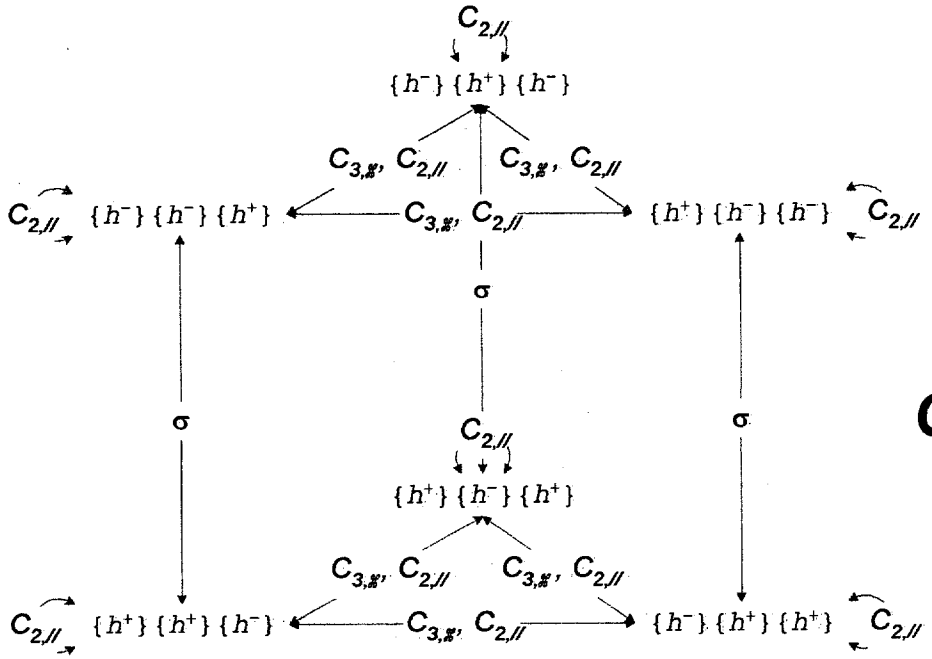
Figure S3. Stereoisomers of hydrocarbon **1a**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

Table S4. Symmetry relationships between the eight static representations of the four distinct stereoisomers (2 *dl* pairs of diastereoisomers) of quartet **2d**.

Symmetry relationships between the 8 static representations	Molecular symmetry



D_3



C_2

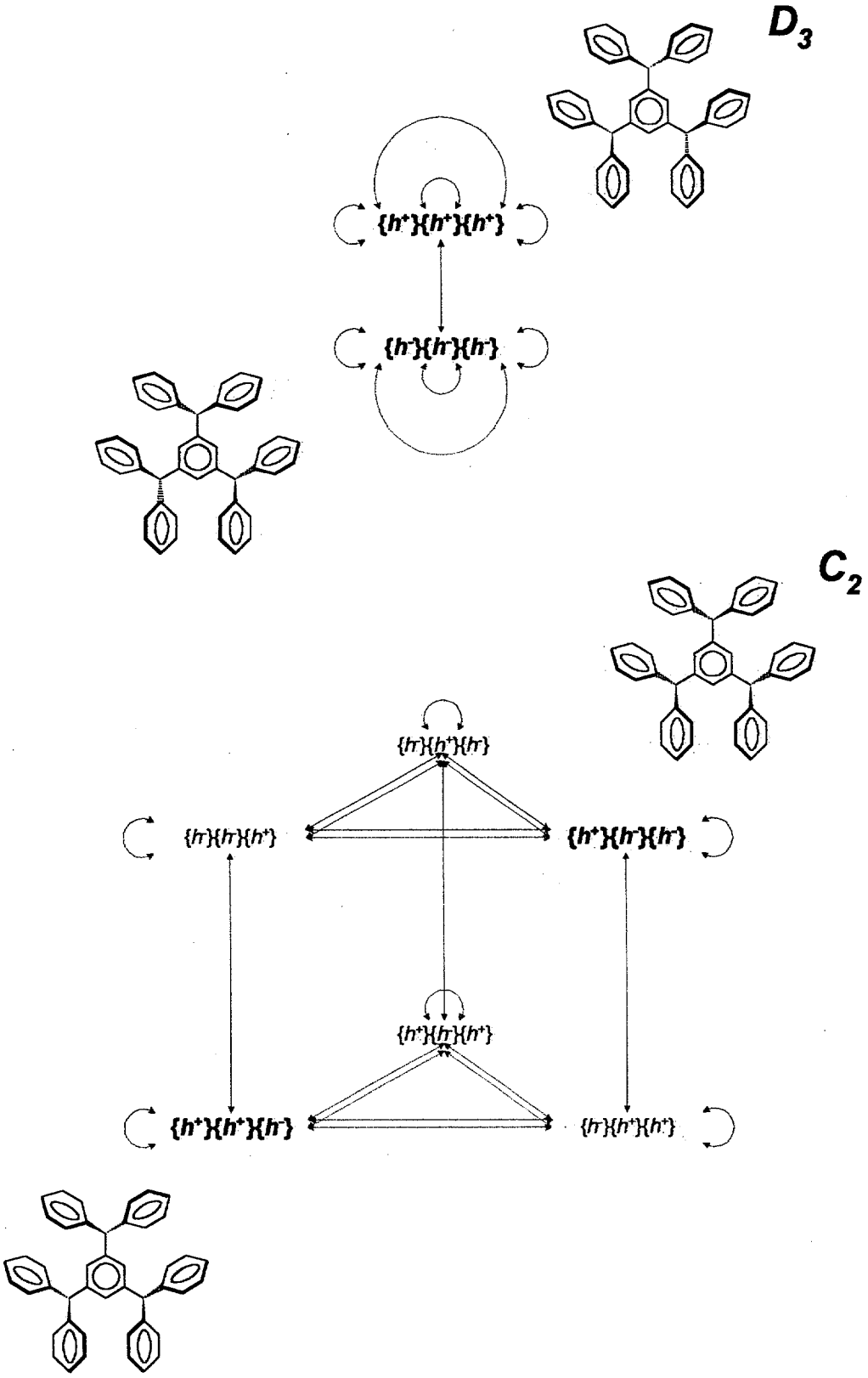
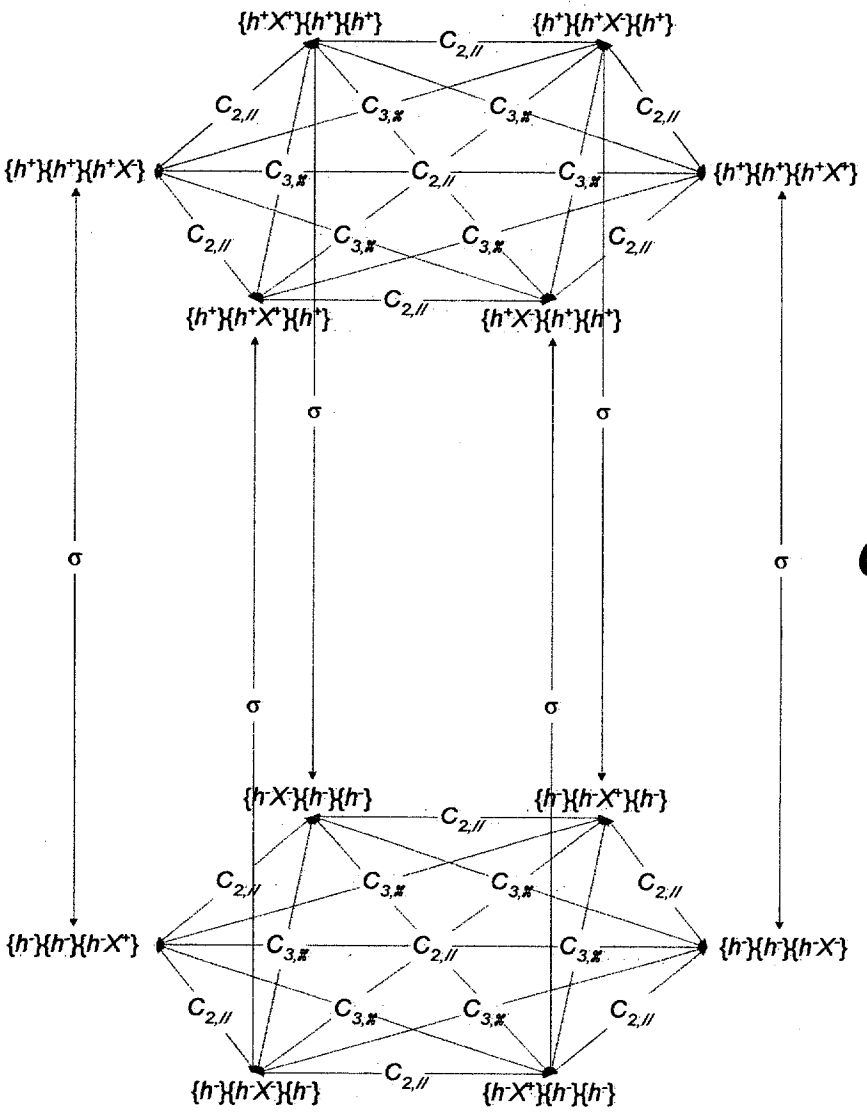


Figure S4. Stereoisomers of quartet **2d**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

Table S5. Symmetry relationships between the 12 static representations corresponding to one of the four-*dl* pairs with C1 symmetry of monoradical compound **2c**.

Symmetry relationships between the 12 static representations	Molecular symmetry



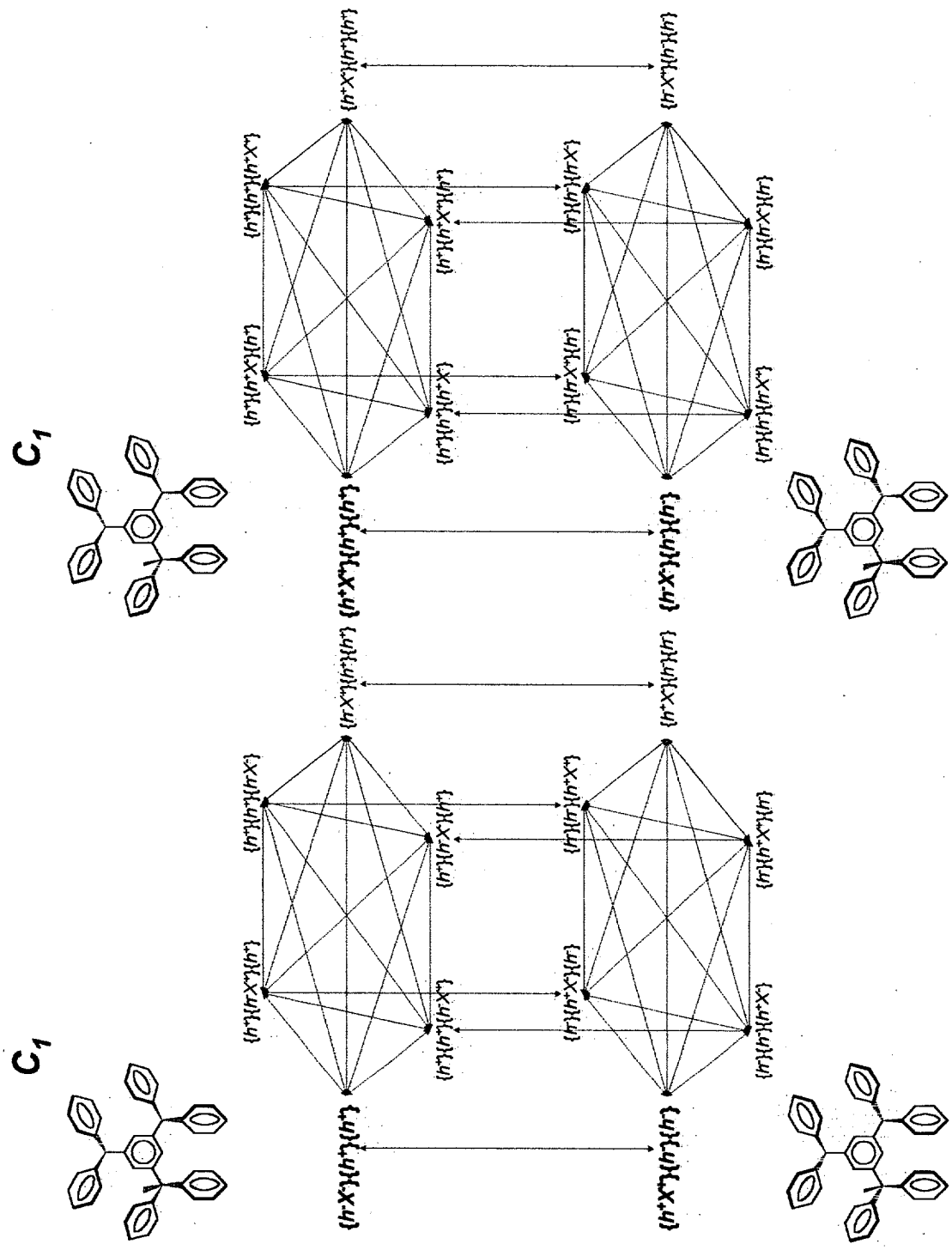


Figure S5 (a). First group of two-*dl* pairs of stereoisomers of monoradical compound **2c**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

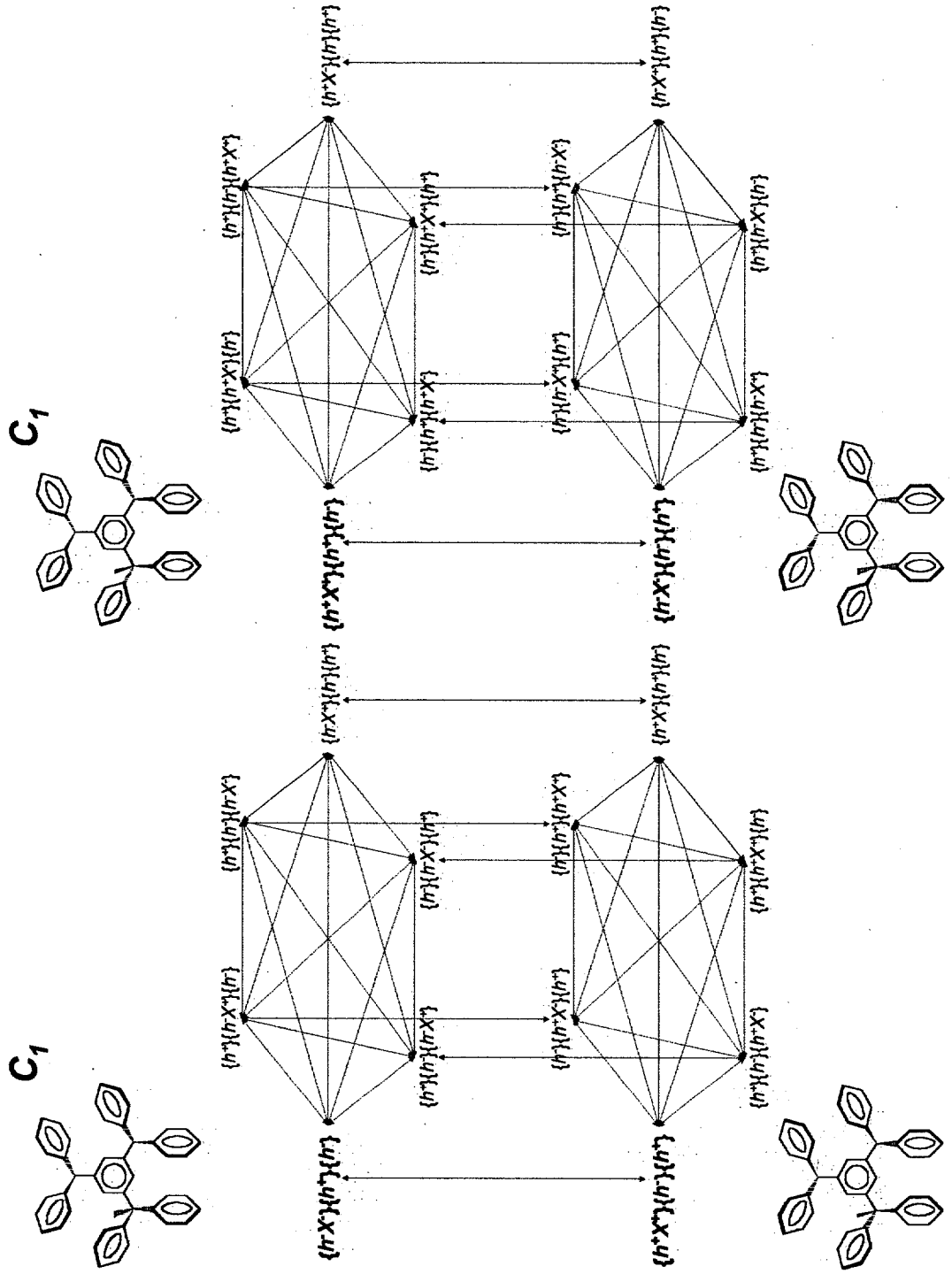
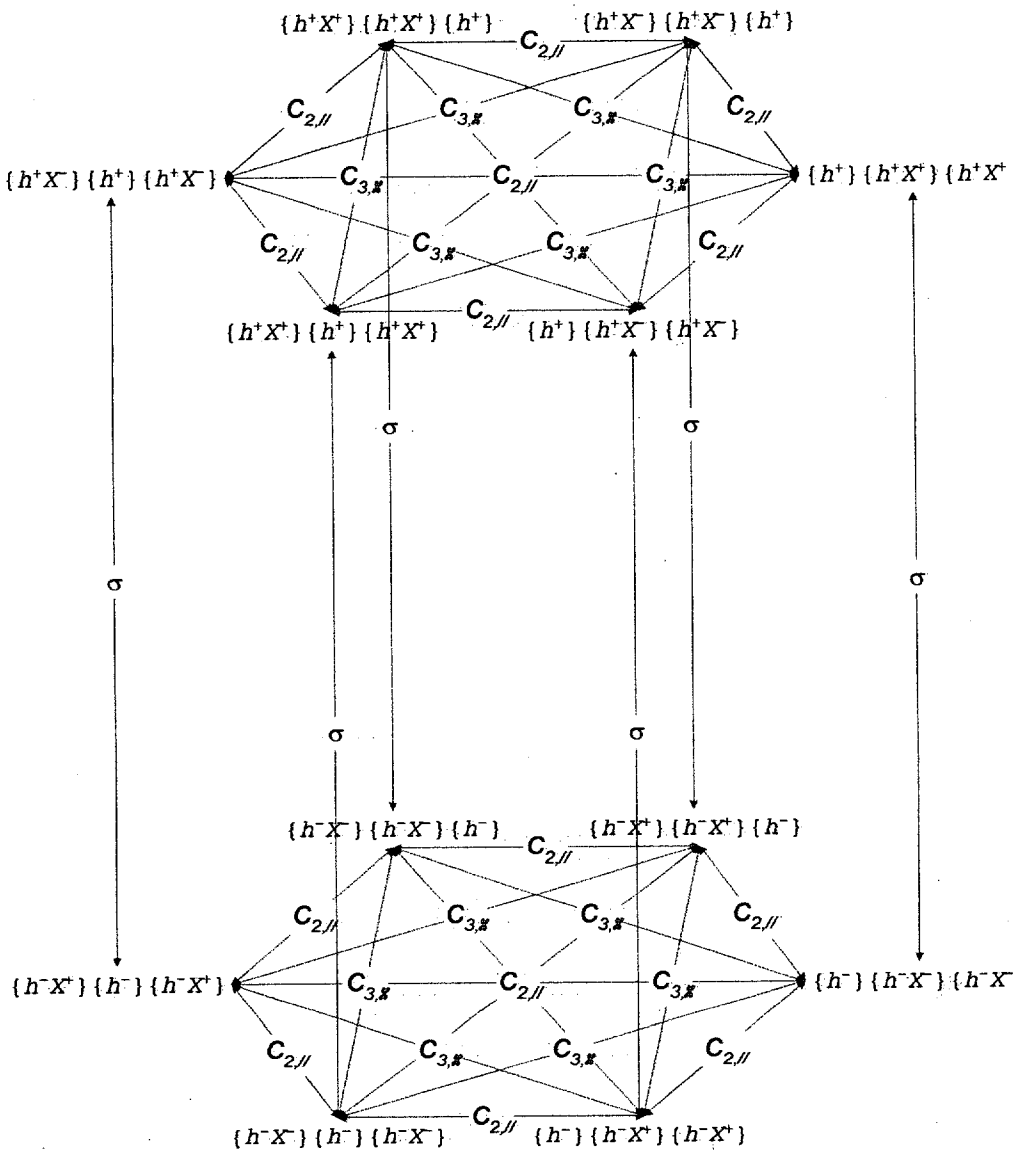


Figure S5 (b). Second group of two-*dl* pairs of stereoisomers of monoradical compound **2c**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

Table S6 (a). Symmetry relationships between the 12 static representations corresponding to one of the six-*dl* pairs of diastereomers with C_1 symmetry of monoradical compound **2b**.

Symmetry relationships between the 12 static representations with a C_1 symmetry	Molecular symmetry



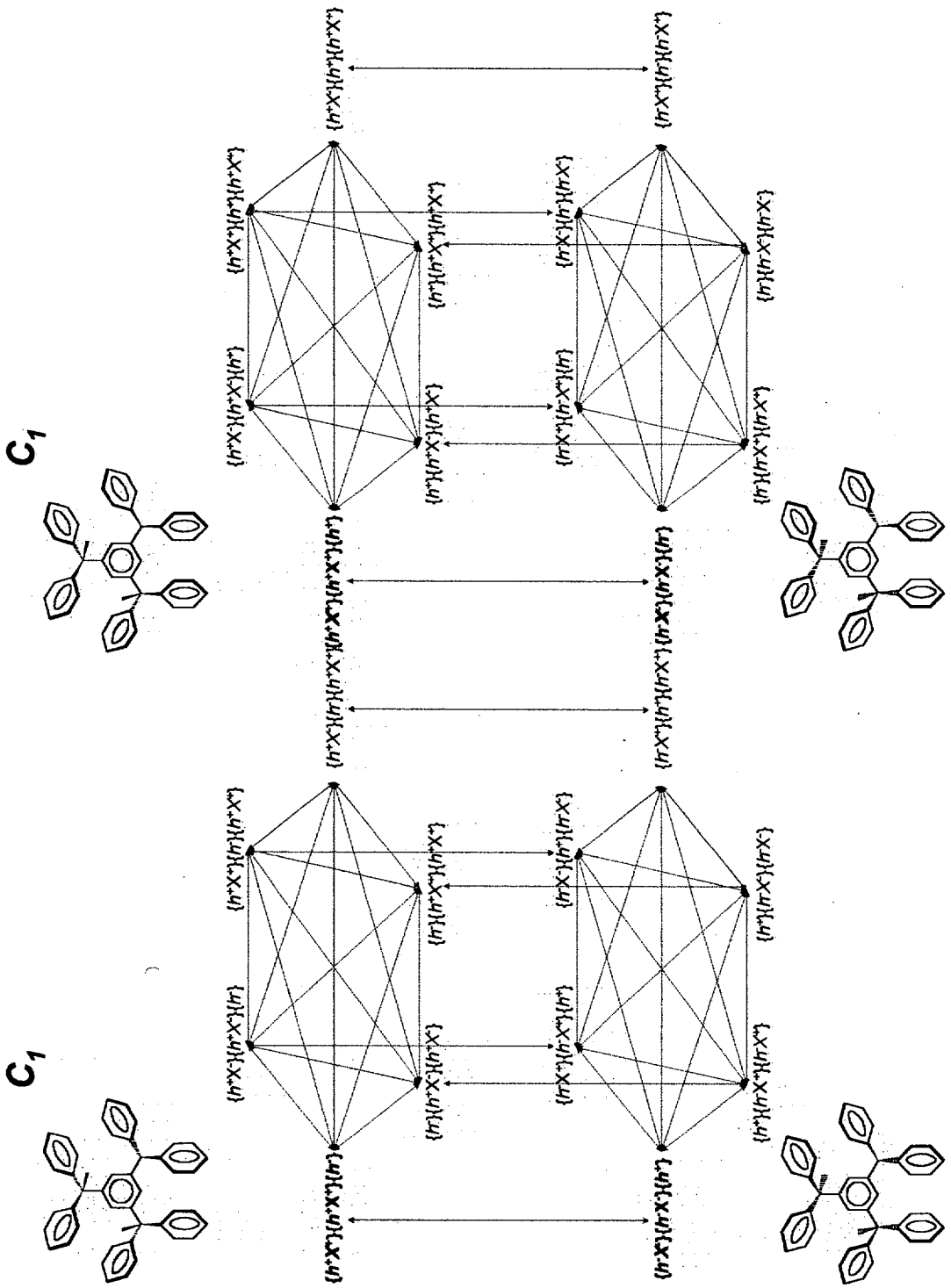


Figure S6 (a). First group of four stereoisomers with C_1 symmetry of monoradical **2b**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

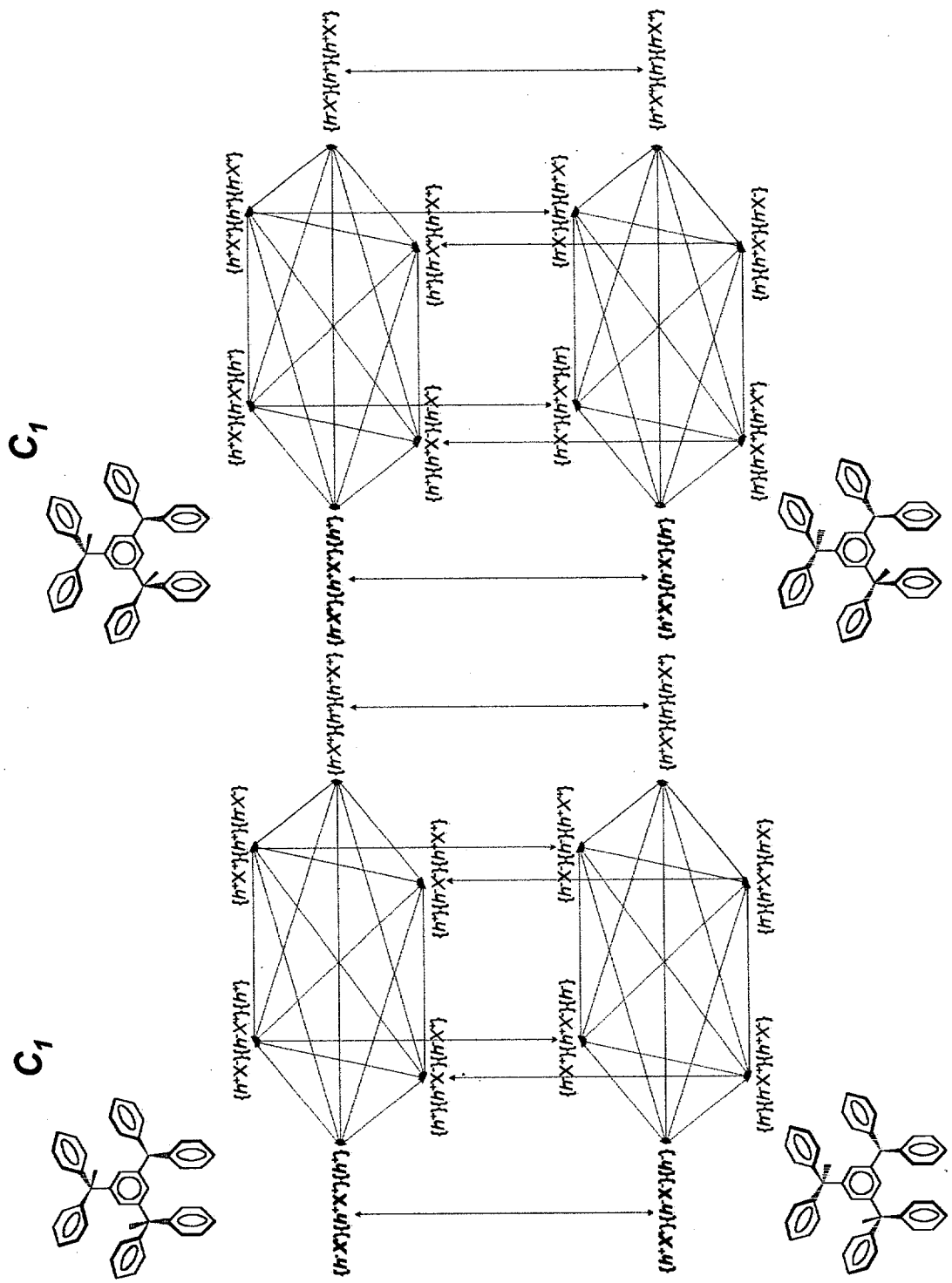


Figure S6 (b). Second group of four stereoisomers with C_1 symmetry of monoradical **2b**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

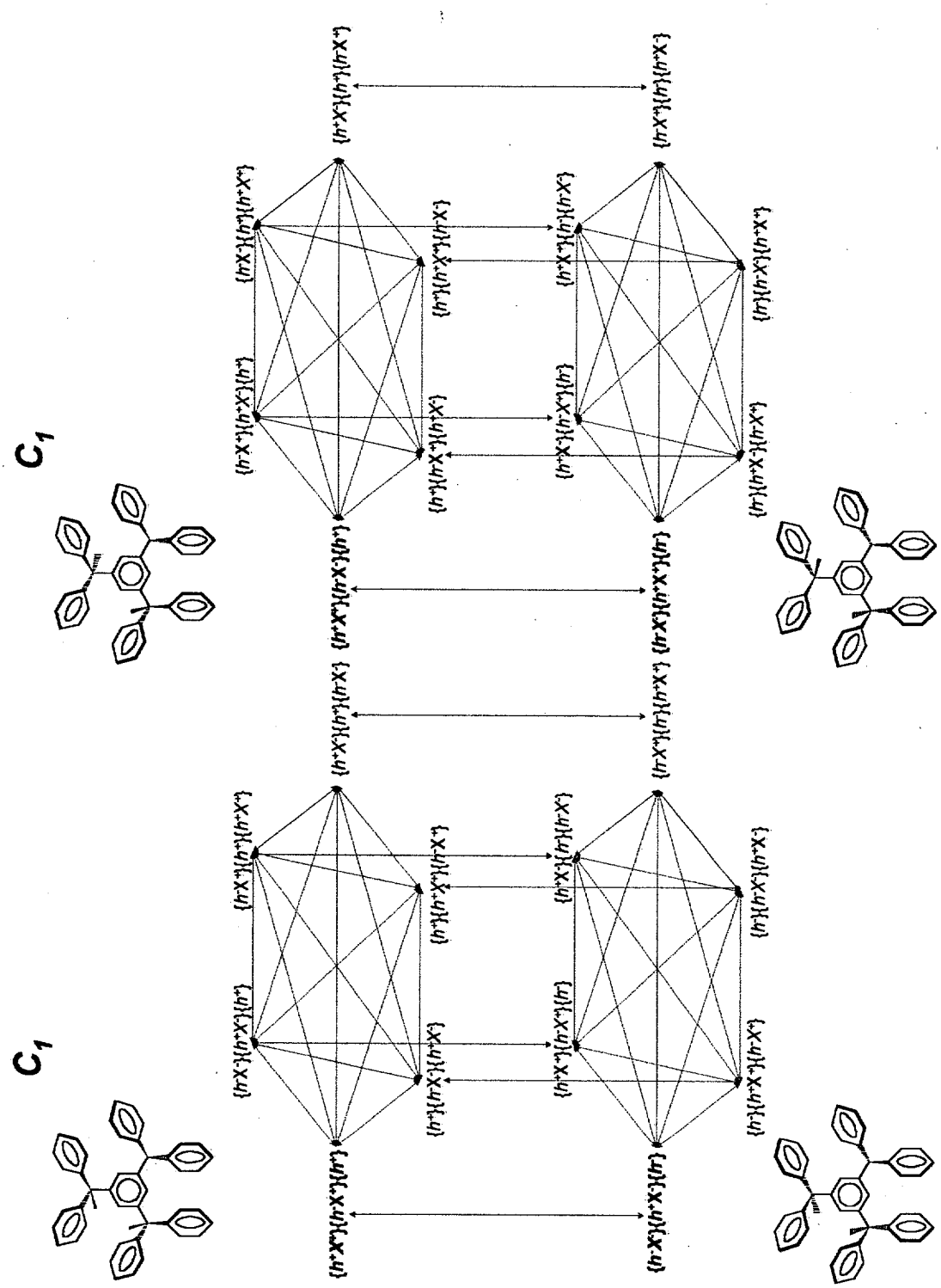
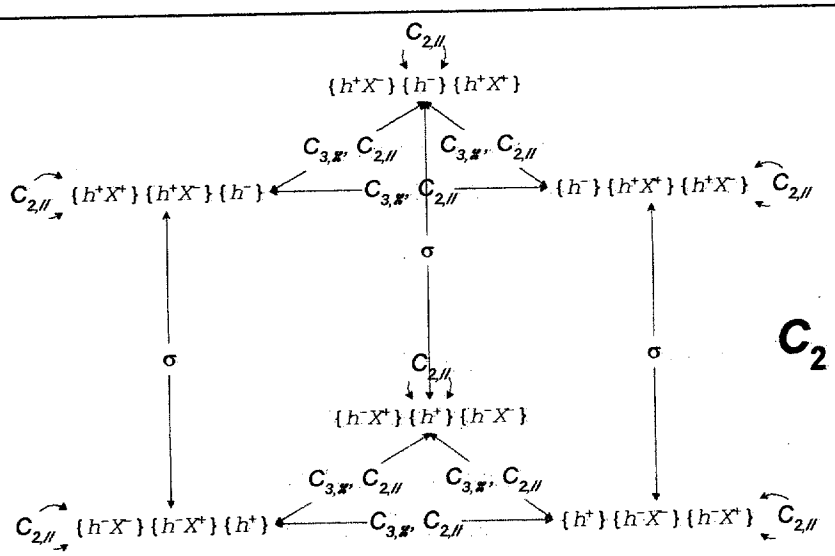


Figure S6 (c). Third group of four stereoisomers with C_1 symmetry of monoradical **2b**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

Table S6 (b). Symmetry relationships between the six static representations corresponding to one of the four *dl* pairs of diastereomers with C_2 symmetry of monoradical **2b**.

Symmetry relationships between the 6 static representations with C_2 symmetry	Molecular symmetry
	C_2

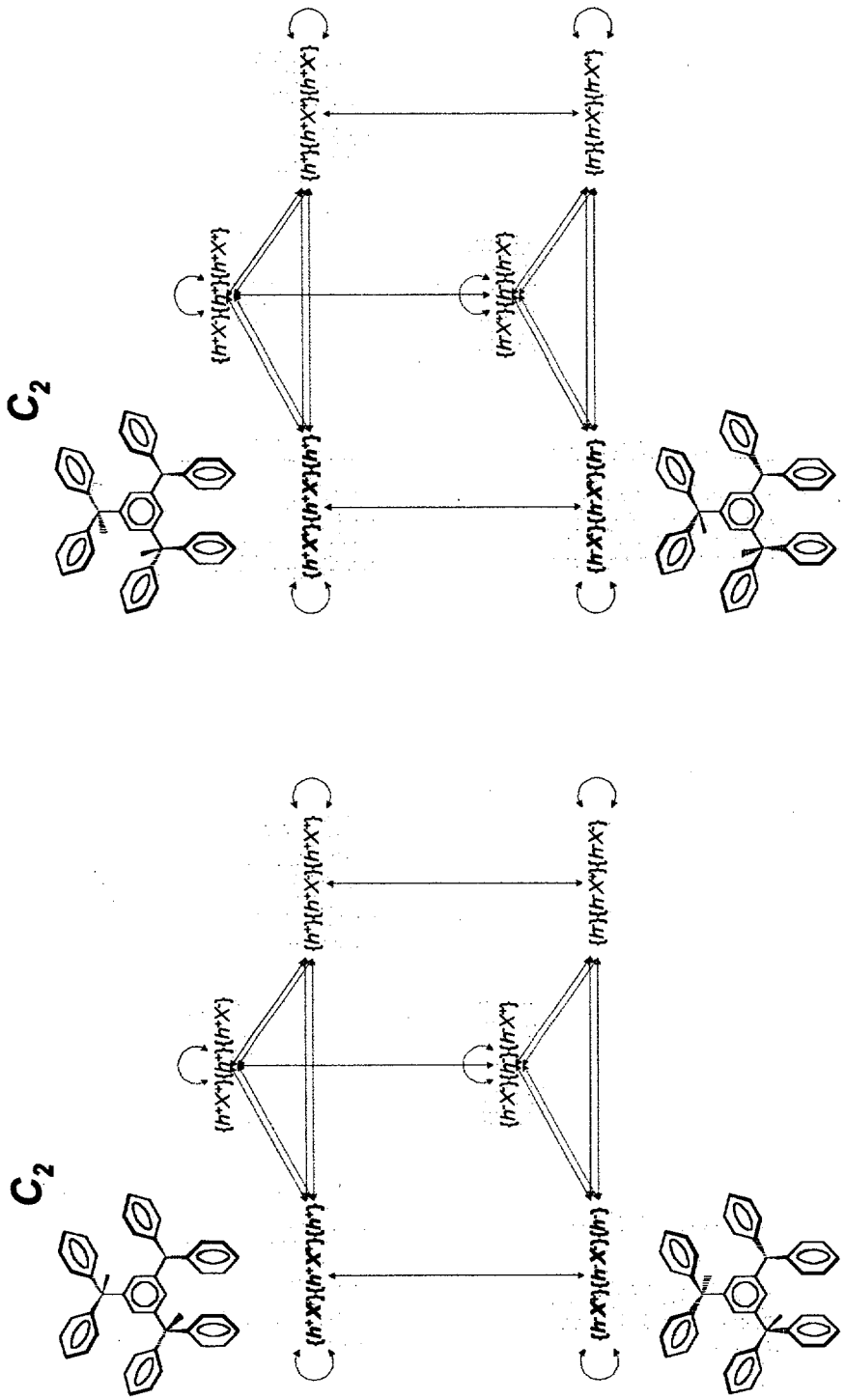


Figure S6 (d). Fourth group of four stereoisomers with C_2 symmetry of monoradical **2b**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

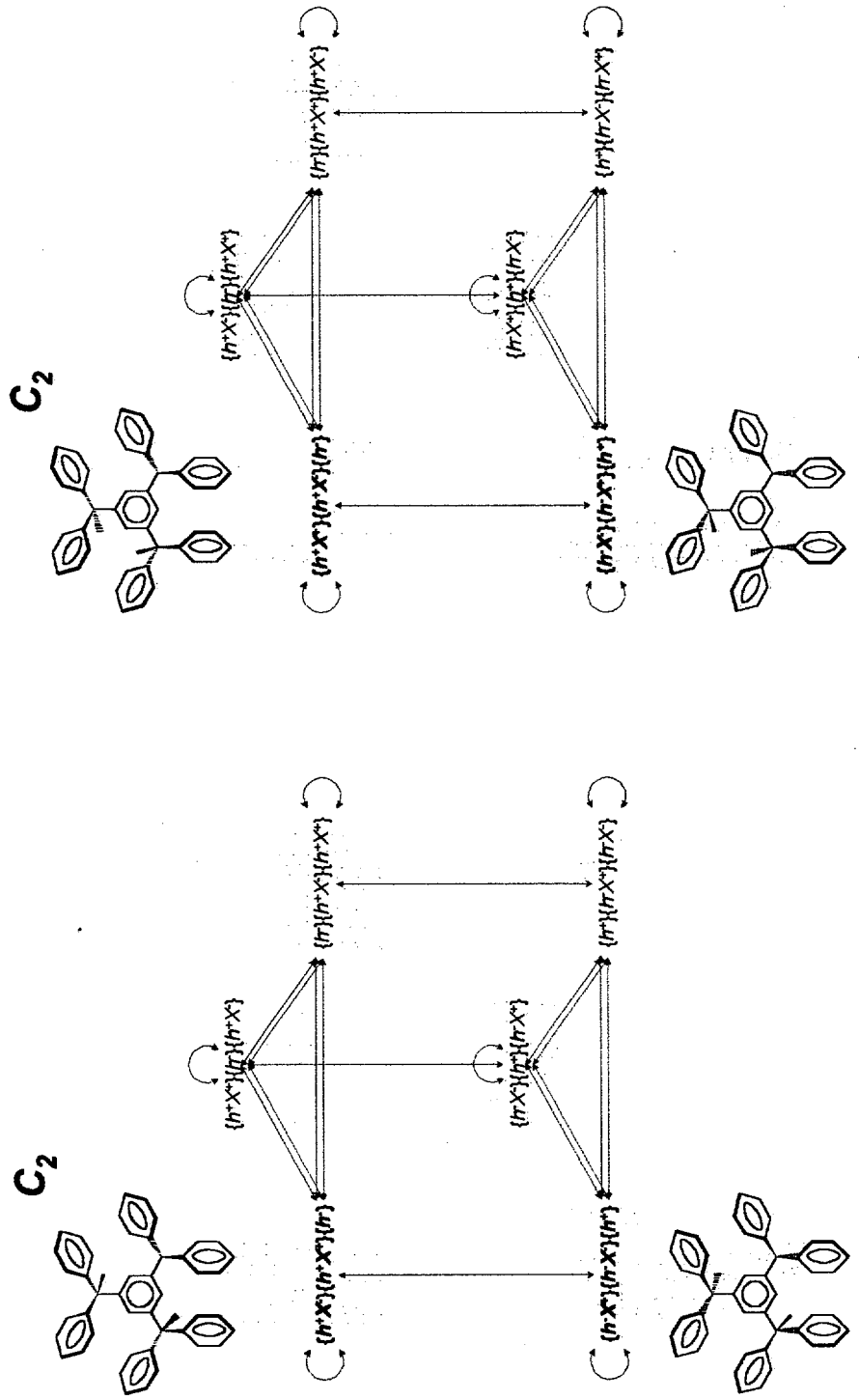


Figure S6 (e). Fifth group of four stereoisomers with C_2 symmetry of monoradical **2b**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

Table S7 (a). Symmetry relationships between the 12 static representations corresponding to one of the five *dl* pairs of diastereoisomers with C_1 symmetry of hydrocarbon **2a**.

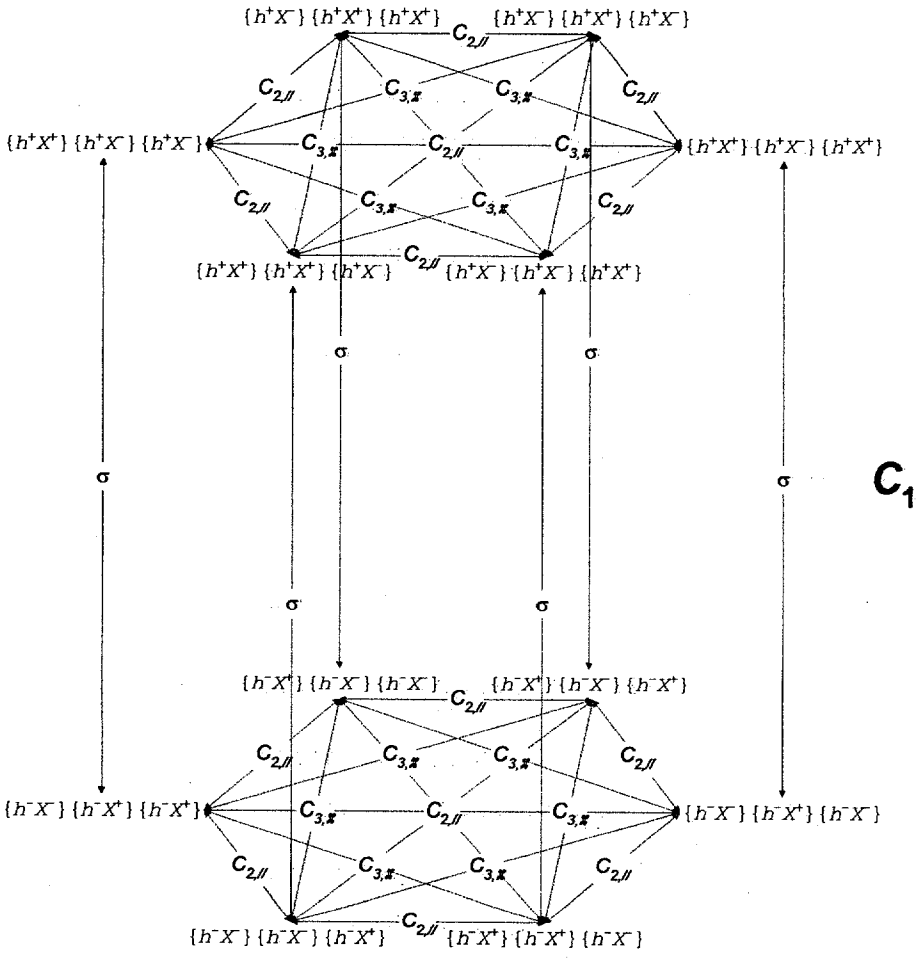
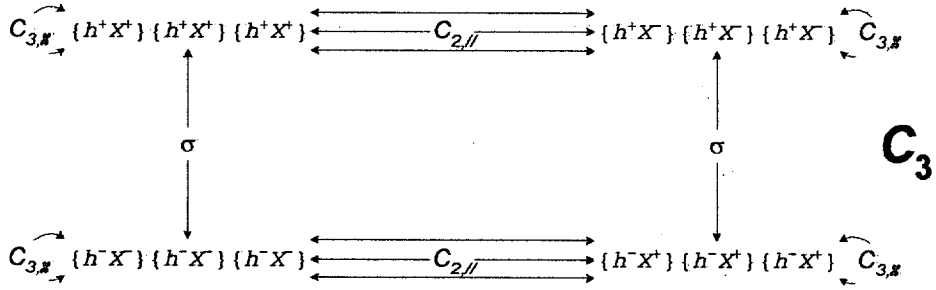
Symmetry relationships between the 12 static representations with C_1 symmetry	Molecular symmetry
	C_1

Table S7 (b). Symmetry relationships between the four static representations corresponding to the unique *dl* pair of diastereomers with C_3 symmetry of hydrocarbon **2a**.

Symmetry relationships between the 4 static representations with C_3 symmetry	Molecular symmetry
	C_3

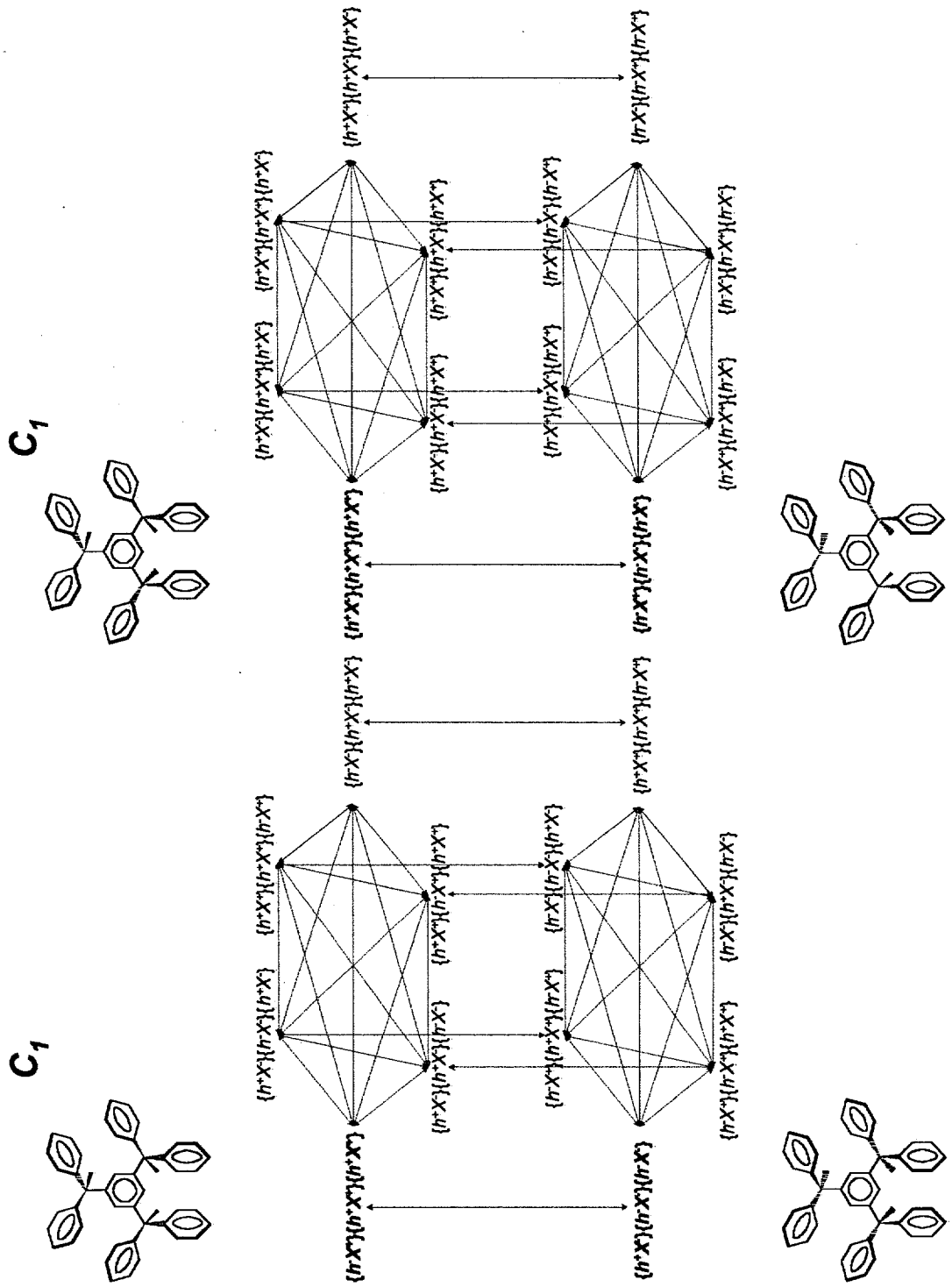


Figure S7 (a). First group of four stereoisomers with C_1 symmetry of hydrocarbon **2a**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

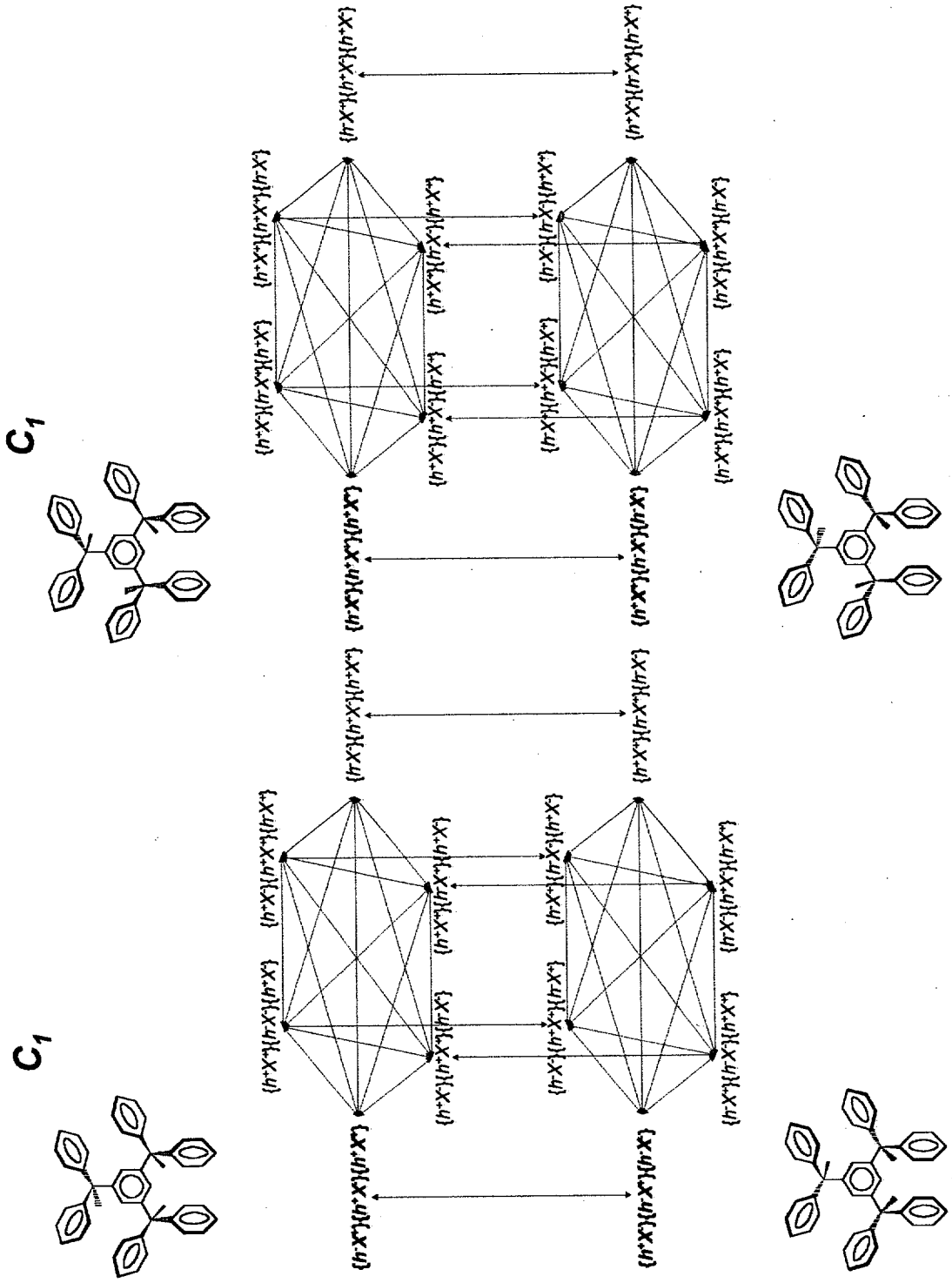


Figure S7 (b). Second group of four stereoisomers with C_1 symmetry of hydrocarbon **2a**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

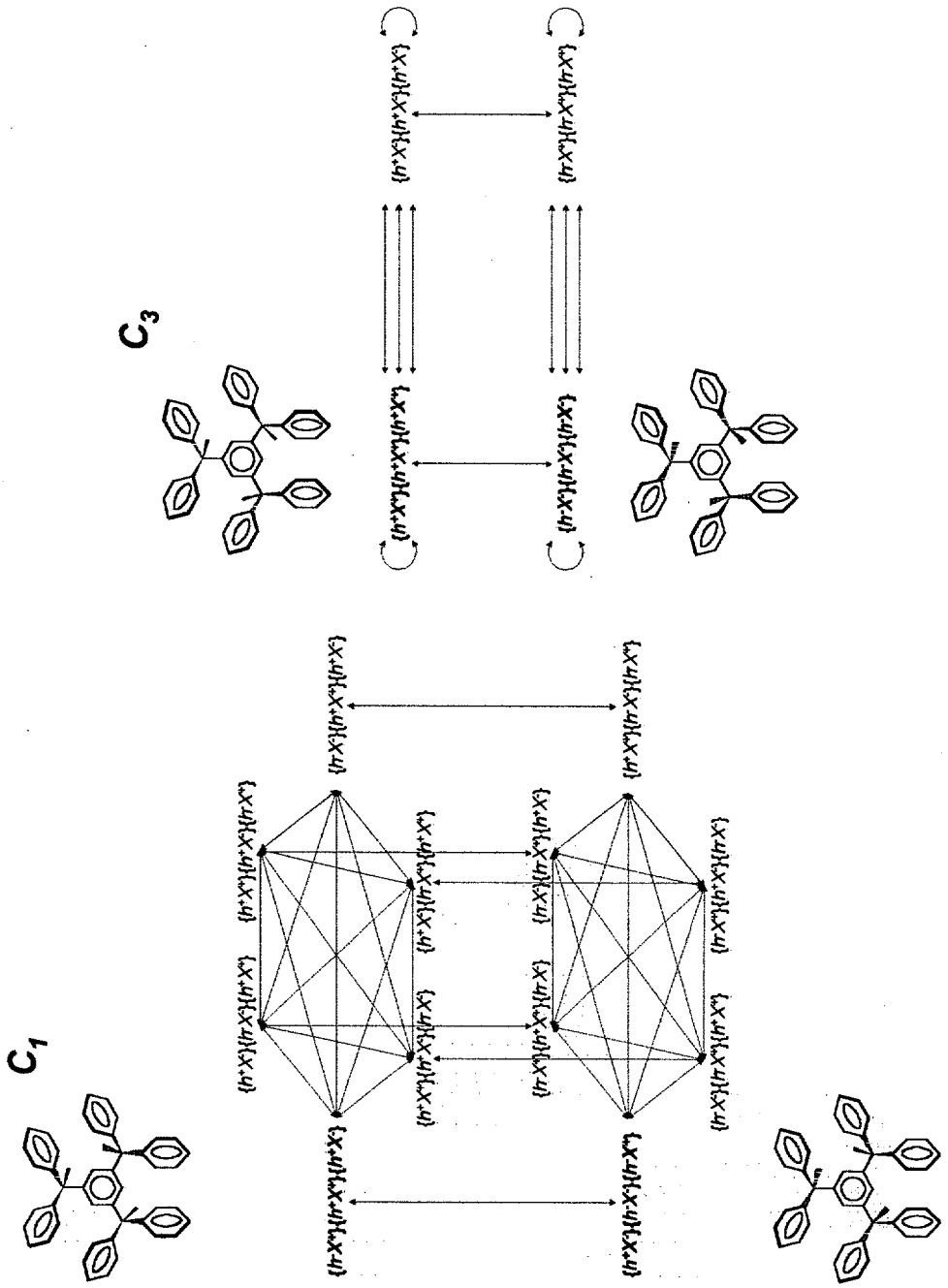


Figure S7 (c). Another pair of stereoisomers with C_1 symmetry and the unique pair of enantiomers with C_3 symmetry of chlorocarbon **2a**, described with a symmetry-adapted symbolic notation, along with their symmetry relationships.

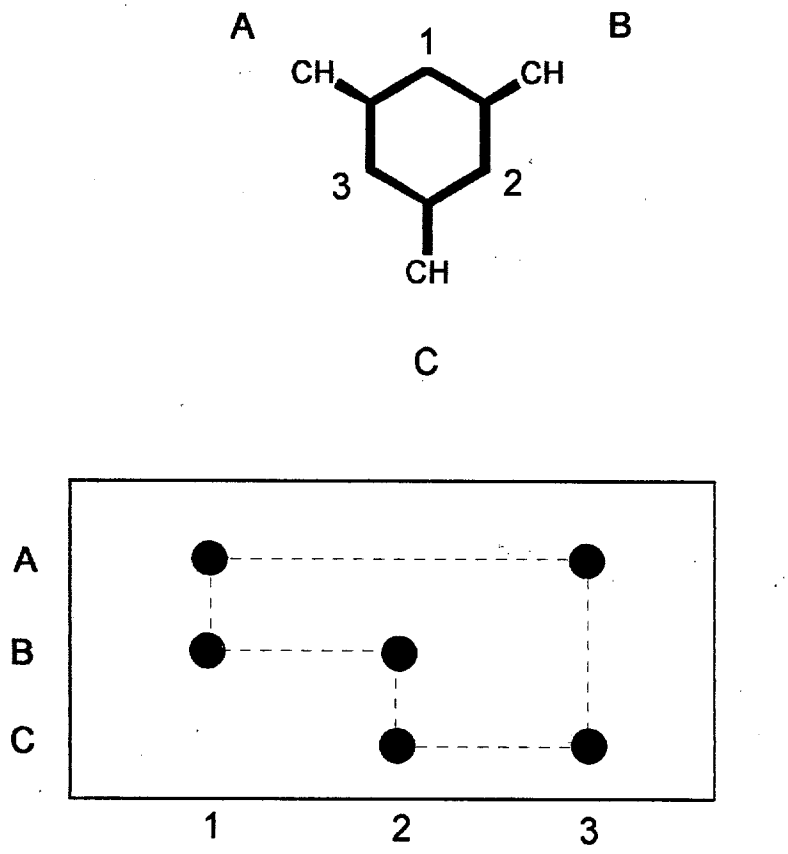


Figure S8. Coupling pattern between the hydrogen atoms (A, B, C) and the *ortho* carbon atoms (1, 2, 3) of the inner aromatic ring expected for an HMBC-NMR experiment on hydrocarbon **2a**.

Table S8. Assignment of chromatographic peaks to ^{1}H-NMR signal sets for hydrocarbon **1a**.[§]

Group of signals of ^{1}H-NMR spectra[¶]	Population (p) at 298 K (in %) in ^{1}H-NMR	HPLC	Number of HPLC peak[†]
B	4.2	4.8	1
G	9.3	21.9[‡]	4
H	13.8		
C	19.4	19.8	3
D, E	20.8	20.9	2
A, F	32.4	32.7	5

[¶] For NMR signal labeling, see Figure 10 *top*.
[†] Numbers of HPLC peaks are given by reading the chromatogram of Figure 8 (*bottom*) from left to right.
[‡] Comprises the contributions of two peaks (numbers 4a and 4b) with areas corresponding to percentage populations of 8.9% and 13.0%, respectively, as inferred by peak deconvolution.
[§] Results provided by a linear regression analysis of the HPLC and NMR populations are as follows: p(HPLC) = 1.01 p(NMR) – 0.13; with r^2 = 0.997.

Table S9. Assignment of chromatographic peaks to ^{1}H-NMR signal sets for hydrocarbon **2a**.[§]

Group of signals of ^{1}H-NMR spectra[¶]	Population (p) at 318 K (in %) in ^{1}H-NMR	HPLC	Number of HPLC peak[†]
L, M, O	9.4	22.0[‡]	2
A, H, P	12.1		
C, F, G	14.3	15.4	1
E	16.0	15.5	5
B, I, N	20.2	20.1	3
D, J, K	27.9	26.9	4

[¶] For NMR signal labeling, see Figure 10 *bottom*.
[†] Numbers of HPLC peaks are given by reading the chromatogram of Figure 9(*bottom*) from left to right.
[‡] Comprises the contributions of two peaks (numbers 2a and 2b) with areas corresponding to percentage populations of 9.6% and 12.4%, respectively, as inferred by peak deconvolution.
[§] Results provided by a linear regression analysis of the HPLC and NMR populations are as follows: p(HPLC) = 0.92·p(NMR) + 1.27; with r^2 = 0.993.