

Molecular Recognition of Titanium(IV) Alkoxides by 2,6-Bis(hydroxymethyl)-*p*-cresol in the Crystal Engineering of Hybrid Organic–Inorganic Networks

Adel Rammal, Frédéric Brisach, and Marc Henry*

Laboratoire de Chimie Moléculaire de l'Etat Solide
Insitut Le Bel, UMR CNRS/ULP 7513
Université Louis Pasteur, 4, Rue Blaise Pascal
67070 Strasbourg Cedex, France

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The design of hybrid organic–inorganic networks requires a fine understanding of the interactions that control molecular recognition and self-assembly processes between inorganic and organic chemical species. Here we report our study on the reaction between titanium(IV) alkoxides, known to be tetrameric $[\text{Ti}_4(\text{OR})_{16}]$ (**1**) in the solid state,¹ and an aromatic ligand such as 2,6-bis(hydroxymethyl)-*p*-cresol (BHMPC **2**). The choice of titanium(IV) alkoxides was motivated by their widespread use as precursors in both conventional (paints, inks, plastics, cosmetics, ceramics...) and high-tech (coatings, membranes, photoanodes, capacitors...) materials. From a previous study, it was known that bridging positions were more reactive toward hydrolysis or complexation than terminal ones and that tripodal ligands were able to remove selectively all bridging OR groups.² As shown in Figure 1, starting from the same planar tetrameric structure, a perfect geometrical match between octahedral edges of (**1**) and hydroxy moieties of (**2**) could be anticipated.

Upon reaction of the ligand (**2**) with $\text{Ti}(\text{OEt})_4$, a new complex for which the tetrameric structure of (**1**) was preserved but with all edges occupied by six molecules of (**2**) was obtained (cf. Figure 2).³ The inorganic core of this tetranuclear complex (**3**) is composed of two μ_3 -oxo groups bridging the four titanium atoms. The tetranuclear titanium core is surrounded by six ligands (**2**) acting by groups of two, either as chelating, chelating–bridging, or tridentate units.⁴ As the bond valence sum around atom O3 is 1.28 against 2.05 for O2, we assume that the chelating ligand (**2**) involves a CH_2OH moiety.

The persistence of (**3**) in solution was checked by ^1H and ^{13}C NMR in CDCl_3 .⁵ (**3**) has an interesting shape which may be described as an analogue of a doubly fused calix[3]arene. Due to

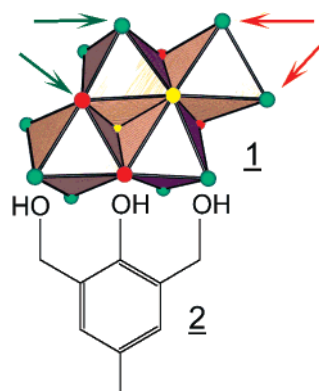


Figure 1. Molecular recognition between octahedral edges of a $[\text{Ti}_4(\text{OR})_{16}]$ tetramer (**1**) and 2,6-bis(hydroxymethyl)-*p*-cresol (**2**) molecules.

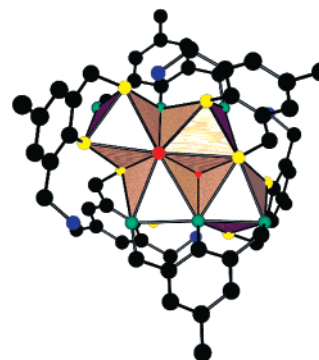


Figure 2. Molecular structure of $[\text{Ti}_4(\mu_3\text{-O})_2\{\text{Ph}(\mu_2\text{-O})(\text{CH}_2\text{OH})_2\}_2\{\text{Ph}(\mu_2\text{-O})(\text{CH}_2\text{O})(\text{CH}_2\text{OH})\}_2\{\text{Ph}(\text{O})(\text{CH}_2\text{OH})_2\}_2]$ (**3**) showing the two μ_2 -oxo groups (red), the free $-\text{CH}_2\text{OH}$ moieties (blue) and the bidentate (yellow oxygen atoms) or tridentate (green oxygen atoms) coordination mode of (**2**).

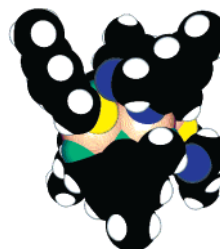


Figure 3. Divergent association of the six phenyl rings around the inorganic Ti_4O_2 core forming a doubly fused-calix[3]arene.

the presence of two divergent cavities, (**3**) may act as receptor for solvent molecules (Figure 3).

Indeed, in the X-ray crystal structure of (**3**), one dioxan molecule and one ethanol molecule are found to be trapped within each cavity. These filled double-calix type molecules form in the crystalline state a 1D-network through π -stacking of aromatic groups (Figure 4). To better characterize the crystal engineering of such inclusion networks, we assume, in the spirit of the Hohenberg–Kohn theorem,⁶ that the total molecular energy E can always be partitioned between a purely electrostatic contribution EB and a purely electronic functional $F[\rho]$ which takes care of all the exchange and electronic correlations: $E_{\text{tot}} = EB + F[\rho]$. Now, for the same molecular fragment placed into two different chemical environments (in a vacuum on one hand and inside a crystalline lattice on the other hand for example), we may safely

(1) Wright, D. A.; Williams, D. A. *Acta Crystallogr.* **1968**, B24, 1107.

(2) Schildknecht-Weymann, S.; Henry, M. *Chem. Commun.* Manuscript submitted.

(3) Orange prismatic crystals suitable for X-ray diffraction were deposited overnight from a clear red-orange solution obtained by injecting 15 mL of a solution of (**2**) (0.67 g, 4 mmol) in 1,4-dioxane into 5 mL of a solution of titanium ethoxide (0.45 g, 2 mmol) in ethanol under vigorous stirring. UV-vis: $\lambda_{\text{max}} = 343$ nm ($\epsilon = 19\,400$ $\text{cm}^{-1}\cdot\text{mol}^{-1}\cdot\text{L}$), $\lambda_{\text{max}} = 234$ nm ($\epsilon = 45\,000$ $\text{cm}^{-1}\cdot\text{mol}^{-1}\cdot\text{L}$). IR (KBr pellet): 3440 (s), 2962 (m), 2910 (m), 2853 (m), 1636 (m), 1473 (s), 1256 (s), 1219 (m), 1160 (M), 1119 (m), 1078 (m), 1046 (m), 998 (m), 871 (m), 840 (s), 673 (m), 579 (s) cm^{-1} .

(4) Crystallographic data: crystal dimensions $0.14 \times 0.11 \times 0.09$ mm^3 , formula $\text{Ti}_4\text{O}_{26}\text{C}_{66}\text{H}_{88}$, FW 1487.0, triclinic, space group $P-1$, $a = 11.1076$ (9) Å, $b = 11.871$ (2) Å, $c = 11.655$ (2) Å, $\alpha = 80.769$ (5)°, $\beta = 70.036$ (5)°, $\gamma = 77.303$ (5)°, $V = 1764.1$ (5) Å³, $Z = 1$, $R(\text{wR}) = 0.082$ (0.104) for 3131 reflections with $|F_o| \geq 3.0\sigma(F_o)$. μ_3 -oxo: Ti1–O1 = 1.953 (2) Å, Ti2–O1 = 1.948 (6) Å, Ti2–O1 = 2.011 (7) Å with Ti–O–Ti bond angles = 100.4 (2)–108.0 (2)°. Chelating: Ti1–O2 = 1.843 (7) Å (phenolic), Ti1–O3 = 2.084 (7) Å (alcoholic). Chelating–bridging: Ti2–O7 = 1.867 (9) Å (phenolic) and Ti1–O5 = 1.967 (6) Å, Ti2–O5 = 2.004 (8) Å (alcoholic). Tridentate: Ti2–O10 = 2.048 (9) Å, Ti1–O10 = 2.085 (7) Å (phenolic) and Ti1–O8 = 1.808 (7) Å, Ti2–O9 = 1.857 (9) Å (alcoholic).

(5) ^1H NMR: δ 2.16 (6H, CH₃), 2.20 (6H, CH₃), 2.22 ppm (6H, CH₃), 4.0–6.0 (24H, CH₂), 6.70 (2H, PhH), 6.79 (4H, PhH), 6.84 (2H, PhH), 6.92 (2H, PhH), 6.95 (2H, PhH) ppm. ^{13}C NMR: Tridentate δ 20.5 (CH₃), 73.5 (2 \times CH₂O), 125.2–128.0 (5 \times C_{Ph}), 152.1 ppm (OC_{Ph}). Bridging–chelating: δ 20.2 (CH₃), 74.1, 74.7 (CH₂O), 128.7–131.6 (5 \times C_{Ph}), 157.4 ppm (OC_{Ph}). Chelating δ 20.2 (CH₃), 60.6, 62.2 (CH₂O), 128.1–128.8 (5 \times C_{Ph}), 158.6 ppm (OC_{Ph}).

(6) Hohenberg, P.; Kohn, W. *Phys. Rev. B* **1964**, 136, 864.

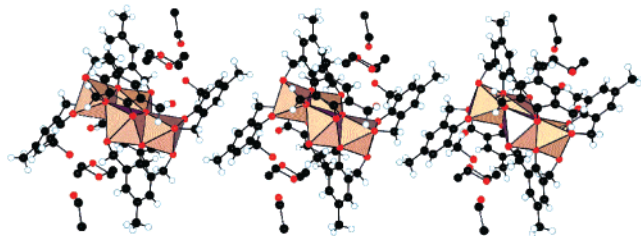


Figure 4. 1D molecular network based on compound (3) filled with dioxane and ethanol inside the two divergent cavities.

Table 1. Electrostatic Balances (EB) Computed from the Partial Charge Model⁷ for the Two Inclusion Networks Based on 3 (A) with Included 1,4-dioxan (B) and Co-solvent Molecules (S)

fragment	EB/kJ·mol ⁻¹ (S = EtOH)	EB/kJ·mol ⁻¹ (S = CHCl ₃) ¹¹
network	-14110.4	-13923.1
A ⊃ 2(B + S)	-14069.9	-13778.8
A ⊃ 2B	-13997.8	-13692.5
A ⊃ 2S	-13871.6	-13582.6
A (free)	-13794.8	-13479.4
B (free)	-88.6	-82.0
S (free)	-25.7	-8.4

assume that $F_1[\rho] \sim F_2[\rho]$. Thus a direct probing of molecular interactions E_{int} through the difference in the EB values: $E_{\text{int}} \sim \text{EB}(1) - \text{EB}(2)$ appears as possible. As, the computation of such EB values from a given charge distribution is straightforward, we may explore, with a rigorous and quantitative energetic criterion, a variety of networks. To compute a reliable charge distribution, we have used the partial charge model,⁷ which requires only the input of molecular or crystalline structures, once an electronegativity and an atomic radii scales have been selected. In the present case we have used configuration energy of elements⁸ and ab initio atomic orbital radii⁹ to approximate electronegativity values and chemical hardnesses, respectively.

The left part of Table 1 gives the results obtained for the ethanol solvate. For instance, the π -stacking energy is directly given by $\Delta E_1 = \text{EB}(N) - \text{EB}[A \supset 2(B + S)] = -40.4 \text{ kJ}\cdot\text{mol}^{-1}$ (here \supset means included), if we assume that interchain interactions are negligible. The energy associated with the inclusion of the two dioxane molecules in the two divergent cavities may be evaluated as: $\Delta E_2 = \text{EB}[A \supset 2B] - \text{EB}[A_{\text{free}}] - 2(\text{EB}[B_{\text{free}}]) = -25.8 \text{ kJ}\cdot\text{mol}^{-1}$, that is about $-13 \text{ kJ}\cdot\text{mol}^{-1}$ per molecule. Similar evaluation leads for the inclusion of ethanol to $\Delta E_3 = \text{EB}[A \supset 2S] - \text{EB}[A_{\text{free}}] - 2(\text{EB}[S_{\text{free}}]) = -25.4 \text{ kJ}\cdot\text{mol}^{-1}$, that is again $-13 \text{ kJ}\cdot\text{mol}^{-1}$ per molecule. Dioxane is thus approximately as tightly bonded as ethanol. Finally, the interaction energy between dioxane and ethanol within a cavity is evaluated as: $\Delta E_4 = \text{EB}[A \supset 2(B + S)] - \text{EB}[A \supset 2B] - 2(\text{EB}[S_{\text{free}}]) = -20.7 \text{ kJ}\cdot\text{mol}^{-1}$ or as $\Delta E_4 = \text{EB}[A \supset 2(B + S)] - \text{EB}[A \supset 2S] - 2(\text{EB}[B_{\text{free}}]) = -21.1 \text{ kJ}\cdot\text{mol}^{-1}$, that is $-10.5 \text{ kJ}\cdot\text{mol}^{-1}$ for one interaction. All of these values are typical of van der Waals interactions (energy less than $5kT$). It is worth noting that all of these values were computed on a crystal structure with no hydrogen atom on 1,4-dioxane or ethanol fragments. A careful analysis of O...O distances reveals that rather strong intramolecular hydrogen bonds should exist between O3 and O6 (252 pm) and between O4 and

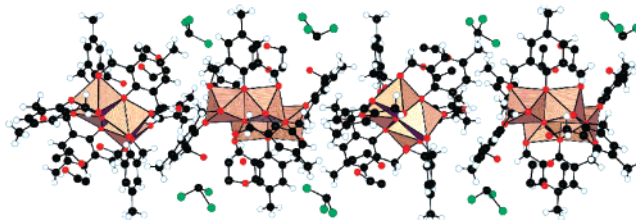


Figure 5. 1D molecular network based on compound (3) filled with dioxane and chloroform inside the two divergent cavities.

O9 (278 pm). As no intermolecular hydrogen bonds were detected, our energy values should not be significantly modified by including the missing hydrogen atoms.

To check the strength of dioxane inclusion inside the cavities, the tetranuclear complex (3) was recrystallized from chloroform.¹⁰ Crystal structure analysis showed that dioxane molecules indeed remained trapped in the cavities while EtOH molecules were replaced by CHCl₃. However, two types of inclusion complexes were present in the unit cell. The first one contained CHCl₃, forming a hydrogen bond with the neighboring dioxane ($d_{\text{O}24\cdots\text{C}61} = 308.4 \text{ pm}$). The second one contained CHCl₃, forming a hydrogen bond with the free CH₂OH arm of the chelating BHMPC ligand ($d_{\text{O}2\cdots\text{C}59} = 300.9 \text{ pm}$). These two complexes are further associated into a 1D-network through interactions between methyl groups of one complex with the phenyl rings of the other one (Figure 5). A third CHCl₃ molecule is accommodated between these chains. Table 1 (right) compares the averaged EB values of the naked fragments with the EB value of the complete network.

For this new network, the overall packing energy is found to be much lower ($\Delta E_1 = -144.3 \text{ kJ}\cdot\text{mol}^{-1}$) owing to the presence of a CHCl₃ molecule between the chains. The binding energies are found to be in this case $-25 \text{ kJ}\cdot\text{mol}^{-1}$ and $-43 \text{ kJ}\cdot\text{mol}^{-1}$ for dioxane and CHCl₃, respectively. The interaction between dioxane and CHCl₃ within the cavity is estimated as $-16.1 \text{ kJ}\cdot\text{mol}^{-1}$, a slightly lower value than that between dioxane and EtOH. These results show that changing the solvent has a rather complex effect as both the geometry and the interactions energies are deeply modified. Consequently, this work is a first step toward a better characterization of the role played by the solvent in crystal engineering. Work is currently under progress on several other molecular networks to check if a quantitative modelization of all the molecular interactions encountered in crystal engineering can be reached.

Acknowledgment. Thanks are due to A. De Cian, J. Fischer, and N. Gruber-Kyritsakas for recording crystal data and for crystal structure determination.

Supporting Information Available: Tables of crystal data, structure solution and refinement, atomic coordinates, bond lengths and angles, and anisotropic thermal parameters in CIF format. Tables of computed partial charges, frontier indexes, retrosynthetic indexes used to build Table 1 (PDF). This material is available free of charge via the Internet at <http://pubs.acs.org>.

JA0156136

(7) Henry, M. *Coord. Chem. Revs.* **1998**, 178–180, 1109.

(8) (a) Mann, J. B.; Meek, T. L.; Allen, L. C. *J. Am. Chem. Soc.* **2000**, 122, 2780. (b) Mann, J. B.; Meek, T. L.; Knight, E. T.; Capitani, J. F.; Allen, L. C. *J. Am. Chem. Soc.* **2000**, 122, 5132.

(9) Waber, J. T.; Cromer, D. T.; *J. Chem. Phys.* **1965**, 42, 4116.

(10) Crystallographic data: red-orange crystal dimensions $0.18 \times 0.10 \times 0.08 \text{ mm}^3$, formula $\text{Ti}_8\text{O}_{49}\text{C}_{131}\text{H}_{162}\text{Cl}_8$, FW 3542.1, triclinic, space group $P-1$, $a = 12.8922(4) \text{ \AA}$, $b = 14.1422(4) \text{ \AA}$, $c = 22.8758(4) \text{ \AA}$, $\alpha = 81.271(6)^\circ$, $\beta = 77.401(6)^\circ$, $\gamma = 81.550(6)^\circ$, $V = 3995.1(1) \text{ \AA}^3$, $Z = 1$, $R(\text{w}R) = 0.099$ (0.122) for 10414 reflections with $|F_0| \geq 3.0\sigma(|F_0|)$.

(11) Fractional atoms O25 and C66 have been discarded for the computation.

WinPacha atomic charges calculations report

Ti4_BHMPC_ETOH -> C66 H86 O26 Ti4 -> [Ti4O2 (BHMPC) 6] [1,4-dioxanne] 2 [EtOH] 2
 Molecular Recognition of Titanium(IV) Alkoxides by 2,6-bis(hydroxymethyl)-p-
 cresol in the Crystal Engineering of Hybrid Organic-Inorganic Networks

Rammal, Adel; Brisach, Frédéric; Henry, Marc
 V= 1764.15 Å³ (Z = 2) -> Rval = 8.20% T = 173K

***Atomic electronegativies (eV) and radii (pm) ***

Ti(8.170, 147.7)
 O(21.360, 45.0)
 C(15.050, 62.0)
 H(13.610, 53.0)

Madelung summation with gaussian inner-charge scaling (G = 0.15 Å⁻¹)
 Reciprocal space exploration: -2 <= (h, k, l) <= 2

Madelung constant A = 131.1617933601/2 = 65.5808966800 (dmin = 0.944 Å)
 min = -0.27341 Å⁻¹ < mean = 0.30214 Å⁻¹ < max = 2.14033 Å⁻¹
 Total electrostatic balance = -1999.76 eV = -192945.5 kJ.mol⁻¹

Mean electronegativity: <EN> = 14.09 eV
 Global hardness: <GH> = 2.49 eV (G = 0.15 Å⁻¹)

Electronic signature: #n Label(±ox) [CN] = ±q {±f}

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#16	O5(-2) [3] =	-0.667 {	-0.000 }
#39	O10(-2) [3] =	-0.630 {	0.000 }
#28	O8(-2) [2] =	-0.542 {	0.004 }
#4	O2(-2) [2] =	-0.535 {	0.004 }
#27	O7(-2) [2] =	-0.495 {	0.004 }
#38	O9(-2) [2] =	-0.486 {	0.006 }
#12	O3(-2) [2] =	-0.445 {	0.006 }
#40	O11(-2) [2] =	-0.265 {	0.012 }
#48	O13(-2) [1] =	-0.255 {	0.016 }
#43	O12(-2) [2] =	-0.249 {	0.011 }
#15	O4(-2) [1] =	-0.245 {	0.014 }
#26	O6(-2) [1] =	-0.241 {	0.013 }
#13	C8(-3) [4] =	-0.173 {	-0.003 }
#24	C17(-3) [4] =	-0.173 {	-0.003 }
#36	C26(-3) [4] =	-0.172 {	-0.003 }
#17	C10(-1) [4] =	-0.076 {	0.003 }
#11	C7(-1) [4] =	-0.062 {	0.003 }
#19	C12(-1) [3] =	-0.061 {	0.009 }
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#9	C5(-1) [3] =	-0.059 {	0.009 }
#31	C21(-1) [3] =	-0.059 {	0.009 }
#37	C27(-1) [4] =	-0.058 {	0.003 }
#29	C19(-1) [4] =	-0.056 {	0.002 }
#7	C3(-1) [3] =	-0.053 {	0.009 }
#33	C23(-1) [3] =	-0.050 {	0.009 }
#14	C9(-1) [4] =	-0.032 {	0.005 }
#30	C20(+0) [3] =	-0.031 {	0.012 }
#25	C18(-1) [4] =	-0.026 {	0.005 }
#46	C32(-2) [1] =	-0.026 {	0.031 }
#18	C11(+0) [3] =	-0.024 {	0.013 }

#6	C2(+0) [3] =	-0.017	{	0.012
#34	C24(+0) [3] =	-0.013	{	0.013
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#20	C13(+0) [3] =	-0.001	{	0.016
#10	C6(+0) [3] =	-0.000	{	0.013
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#35	C25(+1) [3] =	+0.024	{	0.011
#51	H3(+1) [1] =	+0.037	{	0.011
#67	H19(+1) [1] =	+0.040	{	0.015
#42	C29(+1) [2] =	+0.044	{	0.024
#75	H27(+1) [1] =	+0.045	{	0.012
#5	C1(+1) [3] =	+0.050	{	0.012
#23	C16(+1) [3] =	+0.054	{	0.012
#58	H10(+1) [1] =	+0.058	{	0.012
#44	C30(+1) [2] =	+0.058	{	0.023
#59	H11(+1) [1] =	+0.060	{	0.015
#41	C28(+1) [2] =	+0.065	{	0.020
#69	H21(+1) [1] =	+0.067	{	0.016
#61	H13(+1) [1] =	+0.068	{	0.014
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#66	H18(+1) [1] =	+0.076	{	0.012
#55	H7(+1) [1] =	+0.078	{	0.015
#64	H16(+1) [1] =	+0.079	{	0.018
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#73	H25(+1) [1] =	+0.081	{	0.018
#54	H6(+1) [1] =	+0.082	{	0.020
#65	H17(+1) [1] =	+0.086	{	0.012
#60	H12(+1) [1] =	+0.086	{	0.016
#53	H5(+1) [1] =	+0.086	{	0.018
#57	H9(+1) [1] =	+0.086	{	0.014
#63	H15(+1) [1] =	+0.086	{	0.020
#62	H14(+1) [1] =	+0.086	{	0.018
#71	H23(+1) [1] =	+0.087	{	0.020
#52	H4(+1) [1] =	+0.088	{	0.013
#72	H24(+1) [1] =	+0.098	{	0.019
#74	H26(+1) [1] =	+0.103	{	0.015
#2	Ti2(+4) [6] =	+2.212	{	0.063
#1	Ti1(+4) [6] =	+2.523	{	0.071

Partial electrostatic balance: <EB> = -146.24 eV = -14110.3 kJ.mol⁻¹
 Reduced electrostatic balance: <EB/2> = -73.12 eV = -7055.2 kJ.mol⁻¹
 Global ionicity: <GI> = 27.04 %

Statistical report: <Atom>[num] = mean ± 3×stdev (stdev) <avdev>
 <q(H)>[27] = 0.075 ± 0.048 (0.016) <0.012>
 <f(H)>[27] = 0.015 ± 0.008 (0.003) <0.002>
 <q(C)>[33] = -0.025 ± 0.194 (0.065) <0.048>
 <f(C)>[33] = 0.011 ± 0.024 (0.008) <0.006>
 <q(O)>[13] = -0.456 ± 0.594 (0.198) <0.159>
 <f(O)>[13] = 0.007 ± 0.019 (0.006) <0.005>
 <q(Ti)>[2] = 2.368 ± 0.659 (0.220) <0.155>

<f(Ti)>[2] = 0.067 ± 0.016 (0.005) <0.004>

WinPacha retrosynthetic report for A (2(B+S)

Current molecular fragment is: [H27C33O13Ti2]*2 = 1454.72 g.mol-1

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O1 <=>	O1 = -0.867 =>	0%
#2	O10 <=>	O1 = -0.867 =>	0%
#3	O6 <=>	O10 = -0.629 =>	0%
#4	O9 <=>	O10 = -0.629 =>	0%
#5	O7 <=>	O7 = -0.495 =>	0%
#6	O11 <=>	O7 = -0.495 =>	0%
#7	Ti2 <=>	Ti2 = +2.213 =>	0%
#8	Ti1 <=>	Ti1 = +2.524 =>	0%
#9	Ti3 <=>	Ti2 = +2.213 =>	0%
#10	Ti4 <=>	Ti1 = +2.524 =>	0%
#11	O18 <=>	O5 = -0.667 =>	0%
#12	O4 <=>	O5 = -0.667 =>	0%
#13	H22 <=>	H20 = +0.073 =>	0%
#14	H6 <=>	H20 = +0.073 =>	0%
#15	O2 <=>	O2 = -0.537 =>	0%
#16	O19 <=>	O2 = -0.537 =>	0%
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#18	O8 <=>	O9 = -0.485 =>	0%
#19	O5 <=>	O8 = -0.540 =>	0%
#20	O15 <=>	O8 = -0.540 =>	0%
#21	H17 <=>	H13 = +0.068 =>	0%
#22	H44 <=>	H13 = +0.068 =>	0%
#23	H54 <=>	H7 = +0.078 =>	0%
#24	H30 <=>	H7 = +0.078 =>	0%
#25	O12 <=>	O6 = -0.240 =>	0%
#26	O14 <=>	O6 = -0.240 =>	0%
#27	O20 <=>	O12 = -0.248 =>	0%
#28	O22 <=>	O12 = -0.248 =>	0%
#29	O17 <=>	O3 = -0.443 =>	0%
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#32	H20 <=>	H22 = +0.080 =>	1%
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#34	C2 <=>	C7 = -0.062 =>	1%
#35	C36 <=>	C8 = -0.172 =>	1%
#36	C66 <=>	C8 = -0.172 =>	1%
#37	C40 <=>	C26 = -0.171 =>	1%
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#39	C43 <=>	C1 = +0.049 =>	1%
#40	C1 <=>	C1 = +0.049 =>	1%
#41	O24 <=>	O11 = -0.261 =>	2%
#42	O26 <=>	O11 = -0.261 =>	2%
#43	C37 <=>	C17 = -0.170 =>	2%
#44	C63 <=>	C17 = -0.170 =>	2%
#45	C27 <=>	C19 = -0.055 =>	2%
#46	C4 <=>	C19 = -0.055 =>	2%
#47	H27 <=>	H18 = +0.077 =>	2%
#48	H19 <=>	H18 = +0.077 =>	2%
#49	C45 <=>	C12 = -0.060 =>	2%
#50	C15 <=>	C12 = -0.060 =>	2%

#51	O16 <=>	O4 = -0.239 =>	2%
#52	O21 <=>	O4 = -0.239 =>	2%
#53	H11 <=>	H1 = +0.070 =>	2%
#54	H47 <=>	H1 = +0.070 =>	2%
#55	C29 <=>	C21 = -0.058 =>	2%
#56	C18 <=>	C21 = -0.058 =>	2%
#57	H21 <=>	H19 = +0.041 =>	3%
#58	H5 <=>	H19 = +0.041 =>	3%
#59	C6 <=>	C25 = +0.025 =>	3%
#60	C58 <=>	C3 = -0.054 =>	3%
#61	C17 <=>	C25 = +0.025 =>	3%
#62	C11 <=>	C3 = -0.054 =>	3%
#63	C7 <=>	C27 = -0.059 =>	3%
#64	C20 <=>	C27 = -0.059 =>	3%
#65	C22 <=>	C14 = -0.058 =>	3%
#66	C47 <=>	C14 = -0.058 =>	3%
#67	H38 <=>	H3 = +0.038 =>	3%
#68	H1 <=>	H3 = +0.038 =>	3%
#69	H42 <=>	H25 = +0.083 =>	3%
#70	H37 <=>	H25 = +0.083 =>	3%
#71	C13 <=>	C5 = -0.057 =>	3%
#72	C62 <=>	C5 = -0.057 =>	3%
#73	H16 <=>	H27 = +0.047 =>	3%
#74	H8 <=>	H27 = +0.047 =>	3%
#75	C32 <=>	C16 = +0.056 =>	3%
#76	C5 <=>	C16 = +0.056 =>	4%
#77	H39 <=>	H4 = +0.092 =>	4%
#78	H2 <=>	H4 = +0.092 =>	4%
#79	H53 <=>	H6 = +0.085 =>	4%
#80	H29 <=>	H6 = +0.085 =>	4%
#81	C51 <=>	C29 = +0.046 =>	5%
#82	C55 <=>	C29 = +0.046 =>	5%
#83	H51 <=>	H16 = +0.075 =>	5%
#84	H33 <=>	H16 = +0.075 =>	5%
#85	H35 <=>	H23 = +0.083 =>	5%
#86	H40 <=>	H23 = +0.083 =>	5%
#87	C54 <=>	C28 = +0.069 =>	5%
#88	C50 <=>	C28 = +0.069 =>	5%
#89	O23 <=>	O13 = -0.241 =>	6%
#90	O25 <=>	O13 = -0.241 =>	6%
#91	C3 <=>	C10 = -0.071 =>	6%
#92	C31 <=>	C10 = -0.071 =>	6%
#93	C53 <=>	C31 = +0.074 =>	6%
#94	C57 <=>	C31 = +0.074 =>	6%
#95	H18 <=>	H17 = +0.080 =>	7%
#96	H26 <=>	H17 = +0.080 =>	7%
#97	H48 <=>	H2 = +0.075 =>	7%
#98	H12 <=>	H2 = +0.075 =>	7%
#99	C8 <=>	C2 = -0.018 =>	7%
#100	C44 <=>	C2 = -0.018 =>	7%
#101	H23 <=>	H21 = +0.062 =>	7%
#102	H14 <=>	H21 = +0.062 =>	7%
#103	H52 <=>	H5 = +0.080 =>	8%
#104	H28 <=>	H5 = +0.080 =>	8%
#105	C49 <=>	C9 = -0.029 =>	8%
#106	C10 <=>	C9 = -0.029 =>	8%
#107	H7 <=>	H26 = +0.112 =>	9%

#108	H15 <=>	H26 = +0.112 =>	9%
#109	C16 <=>	C20 = -0.028 =>	9%
#110	C28 <=>	C20 = -0.028 =>	9%
#111	C24 <=>	C18 = -0.024 =>	9%
#112	C35 <=>	C18 = -0.024 =>	9%
#113	H9 <=>	H8 = +0.082 =>	10%
#114	H45 <=>	H8 = +0.082 =>	10%
#115	C25 <=>	C23 = -0.055 =>	10%
#116	C39 <=>	C23 = -0.055 =>	10%
#117	H50 <=>	H15 = +0.078 =>	10%
#118	H32 <=>	H15 = +0.078 =>	10%
#119	H49 <=>	H14 = +0.078 =>	10%
#120	H31 <=>	H14 = +0.078 =>	10%
#121	H46 <=>	H9 = +0.077 =>	11%
#122	H10 <=>	H9 = +0.077 =>	11%
#123	C14 <=>	C11 = -0.027 =>	15%
#124	C33 <=>	C11 = -0.027 =>	15%
#125	C19 <=>	C24 = -0.015 =>	17%
#126	C26 <=>	C24 = -0.015 =>	17%
#127	C56 <=>	C30 = +0.070 =>	19%
#128	C52 <=>	C30 = +0.070 =>	19%
#129	H36 <=>	H24 = +0.077 =>	22%
#130	H41 <=>	H24 = +0.077 =>	22%
#131	C60 <=>	C33 = +0.087 =>	23%
#132	C65 <=>	C33 = +0.087 =>	23%
#133	H24 <=>	H10 = +0.042 =>	28%
#134	H3 <=>	H10 = +0.042 =>	28%
#135	H43 <=>	H12 = +0.060 =>	31%
#136	H13 <=>	H12 = +0.060 =>	31%
#137	H25 <=>	H11 = +0.041 =>	32%
#138	H4 <=>	H11 = +0.041 =>	32%
#139	C23 <=>	C15 = +0.005 =>	43%
#140	C34 <=>	C15 = +0.005 =>	44%
#141	C64 <=>	C32 = -0.007 =>	73%
#142	C59 <=>	C32 = -0.007 =>	73%
#143	C61 <=>	C4 = -0.001 =>	81%
#144	C12 <=>	C4 = -0.001 =>	81%
#145	C38 <=>	C22 = -0.001 =>	111%
#146	C30 <=>	C22 = -0.001 =>	111%
#147	C21 <=>	C13 = -0.003 =>	164%
#148	C46 <=>	C13 = -0.003 =>	164%
#149	C9 <=>	C6 = +0.001 =>	247%
#150	C48 <=>	C6 = +0.001 =>	247%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -145.826 eV = -14069.9 kJ.mol⁻¹

WinPacha retrosynthetic report for A (2B

Current molecular fragment is: [H27C31O12Ti2]*2 = 1374.68 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O10 <=>	O1 = -0.867 =>	0%
#2	O1 <=>	O1 = -0.867 =>	0%
#3	O7 <=>	O7 = -0.495 =>	0%
#4	O11 <=>	O7 = -0.495 =>	0%
#5	Ti1 <=>	Ti1 = +2.522 =>	0%

#6	Ti4 <=>	Ti1 = +2.522 =>	0%
#7	O6 <=>	O10 = -0.630 =>	0%
#8	O9 <=>	O10 = -0.630 =>	0%
#9	Ti2 <=>	Ti2 = +2.211 =>	0%
#10	Ti3 <=>	Ti2 = +2.211 =>	0%
#11	C7 <=>	C27 = -0.058 =>	0%
#12	C20 <=>	C27 = -0.058 =>	0%
#13	O4 <=>	O5 = -0.667 =>	0%
#14	O18 <=>	O5 = -0.667 =>	0%
#15	H11 <=>	H1 = +0.069 =>	0%
#16	H47 <=>	H1 = +0.069 =>	0%
#17	H53 <=>	H6 = +0.082 =>	0%
#18	H29 <=>	H6 = +0.082 =>	0%
#19	C2 <=>	C7 = -0.062 =>	0%
#20	C41 <=>	C7 = -0.062 =>	0%
#21	H5 <=>	H19 = +0.040 =>	0%
#22	H21 <=>	H19 = +0.040 =>	0%
#23	O14 <=>	O6 = -0.241 =>	0%
#24	O12 <=>	O6 = -0.241 =>	0%
#25	O8 <=>	O9 = -0.487 =>	0%
#26	O13 <=>	O9 = -0.487 =>	0%
#27	O5 <=>	O8 = -0.541 =>	0%
#28	O15 <=>	O8 = -0.541 =>	0%
#29	O20 <=>	O12 = -0.249 =>	0%
#30	O22 <=>	O12 = -0.249 =>	0%
#31	O24 <=>	O11 = -0.264 =>	0%
#32	O26 <=>	O11 = -0.264 =>	0%
#33	C17 <=>	C25 = +0.024 =>	0%
#34	O19 <=>	O2 = -0.537 =>	0%
#35	O2 <=>	O2 = -0.537 =>	0%
#36	C6 <=>	C25 = +0.024 =>	0%
#37	O3 <=>	O3 = -0.443 =>	0%
#38	O17 <=>	O3 = -0.443 =>	0%
#39	H19 <=>	H18 = +0.075 =>	0%
#40	H27 <=>	H18 = +0.075 =>	0%
#41	C55 <=>	C29 = +0.044 =>	1%
#42	C51 <=>	C29 = +0.044 =>	1%
#43	H1 <=>	H3 = +0.037 =>	1%
#44	H38 <=>	H3 = +0.037 =>	1%
#45	C18 <=>	C21 = -0.058 =>	1%
#46	C29 <=>	C21 = -0.058 =>	1%
#47	C45 <=>	C12 = -0.060 =>	1%
#48	C15 <=>	C12 = -0.060 =>	1%
#49	C53 <=>	C31 = +0.070 =>	1%
#50	C57 <=>	C31 = +0.070 =>	1%
#51	C62 <=>	C5 = -0.058 =>	2%
#52	C13 <=>	C5 = -0.058 =>	2%
#53	C66 <=>	C8 = -0.170 =>	2%
#54	C36 <=>	C8 = -0.170 =>	2%
#55	H48 <=>	H2 = +0.069 =>	2%
#56	H12 <=>	H2 = +0.069 =>	2%
#57	C22 <=>	C14 = -0.059 =>	2%
#58	C47 <=>	C14 = -0.059 =>	2%
#59	C27 <=>	C19 = -0.055 =>	2%
#60	C4 <=>	C19 = -0.055 =>	2%
#61	H6 <=>	H20 = +0.071 =>	2%
#62	H22 <=>	H20 = +0.071 =>	2%

#63	C32 <=>	C16 = +0.056 =>	2%
#64	C5 <=>	C16 = +0.056 =>	2%
#65	C40 <=>	C26 = -0.168 =>	2%
#66	H39 <=>	H4 = +0.090 =>	2%
#67	H2 <=>	H4 = +0.090 =>	2%
#68	C42 <=>	C26 = -0.168 =>	2%
#69	C63 <=>	C17 = -0.169 =>	2%
#70	C37 <=>	C17 = -0.169 =>	2%
#71	H45 <=>	H8 = +0.072 =>	3%
#72	H9 <=>	H8 = +0.072 =>	3%
#73	C54 <=>	C28 = +0.067 =>	3%
#74	C50 <=>	C28 = +0.067 =>	3%
#75	C43 <=>	C1 = +0.049 =>	3%
#76	C1 <=>	C1 = +0.049 =>	3%
#77	H8 <=>	H27 = +0.044 =>	3%
#78	H16 <=>	H27 = +0.044 =>	3%
#79	H17 <=>	H13 = +0.066 =>	3%
#80	H44 <=>	H13 = +0.066 =>	3%
#81	O16 <=>	O4 = -0.254 =>	4%
#82	O21 <=>	O4 = -0.254 =>	4%
#83	C11 <=>	C3 = -0.055 =>	4%
#84	C58 <=>	C3 = -0.055 =>	4%
#85	H42 <=>	H25 = +0.078 =>	4%
#86	H37 <=>	H25 = +0.078 =>	4%
#87	H30 <=>	H7 = +0.075 =>	4%
#88	H54 <=>	H7 = +0.075 =>	4%
#89	C16 <=>	C20 = -0.029 =>	5%
#90	C28 <=>	C20 = -0.029 =>	5%
#91	C49 <=>	C9 = -0.030 =>	5%
#92	C10 <=>	C9 = -0.030 =>	5%
#93	C3 <=>	C10 = -0.071 =>	6%
#94	C31 <=>	C10 = -0.071 =>	6%
#95	H15 <=>	H26 = +0.096 =>	7%
#96	H7 <=>	H26 = +0.096 =>	7%
#97	H18 <=>	H17 = +0.078 =>	9%
#98	H26 <=>	H17 = +0.078 =>	9%
#99	H51 <=>	H16 = +0.072 =>	9%
#100	H33 <=>	H16 = +0.072 =>	9%
#101	C35 <=>	C18 = -0.024 =>	10%
#102	C24 <=>	C18 = -0.024 =>	10%
#103	H23 <=>	H21 = +0.060 =>	10%
#104	H14 <=>	H21 = +0.060 =>	10%
#105	H52 <=>	H5 = +0.077 =>	11%
#106	H28 <=>	H5 = +0.077 =>	11%
#107	C44 <=>	C2 = -0.019 =>	11%
#108	C8 <=>	C2 = -0.019 =>	11%
#109	H50 <=>	H15 = +0.075 =>	13%
#110	H32 <=>	H15 = +0.075 =>	13%
#111	H31 <=>	H14 = +0.075 =>	13%
#112	H49 <=>	H14 = +0.075 =>	13%
#113	C39 <=>	C23 = -0.056 =>	13%
#114	C25 <=>	C23 = -0.056 =>	13%
#115	C56 <=>	C30 = +0.067 =>	14%
#116	C52 <=>	C30 = +0.067 =>	14%
#117	H46 <=>	H9 = +0.074 =>	15%
#118	H10 <=>	H9 = +0.074 =>	15%
#119	H35 <=>	H23 = +0.074 =>	15%

#120	H40 <=>	H23 = +0.074 =>	15%
#121	C23 <=>	C15 = +0.004 =>	17%
#122	C34 <=>	C15 = +0.004 =>	18%
#123	C33 <=>	C11 = -0.028 =>	18%
#124	C14 <=>	C11 = -0.028 =>	18%
#125	H34 <=>	H22 = +0.064 =>	19%
#126	H20 <=>	H22 = +0.064 =>	19%
#127	H36 <=>	H24 = +0.073 =>	26%
#128	H41 <=>	H24 = +0.073 =>	26%
#129	C12 <=>	C4 = -0.002 =>	30%
#130	C61 <=>	C4 = -0.002 =>	30%
#131	H24 <=>	H10 = +0.040 =>	32%
#132	H3 <=>	H10 = +0.040 =>	32%
#133	H43 <=>	H12 = +0.058 =>	33%
#134	H13 <=>	H12 = +0.058 =>	33%
#135	H25 <=>	H11 = +0.040 =>	34%
#136	H4 <=>	H11 = +0.040 =>	34%
#137	C19 <=>	C24 = -0.019 =>	49%
#138	C26 <=>	C24 = -0.019 =>	49%
#139	C30 <=>	C22 = -0.004 =>	177%
#140	C38 <=>	C22 = -0.004 =>	177%
#141	C21 <=>	C13 = -0.004 =>	265%
#142	C46 <=>	C13 = -0.004 =>	266%
#143	C48 <=>	C6 = -0.002 =>	412%
#144	C9 <=>	C6 = -0.002 =>	412%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -145.078 eV = -13997.8 kJ.mol⁻¹

WinPacha retrosynthetic report for A (2S

Current molecular fragment is: [H27C29O11Ti2]*2 = 1294.64 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O3 <=>	O3 = -0.445 =>	0%
#2	O17 <=>	O3 = -0.445 =>	0%
#3	O9 <=>	O10 = -0.630 =>	0%
#4	O6 <=>	O10 = -0.630 =>	0%
#5	O4 <=>	O5 = -0.667 =>	0%
#6	O18 <=>	O5 = -0.667 =>	0%
#7	C62 <=>	C5 = -0.059 =>	0%
#8	C13 <=>	C5 = -0.059 =>	0%
#9	O7 <=>	O7 = -0.496 =>	0%
#10	O11 <=>	O7 = -0.496 =>	0%
#11	O21 <=>	O4 = -0.246 =>	0%
#12	O16 <=>	O4 = -0.246 =>	0%
#13	O10 <=>	O1 = -0.870 =>	0%
#14	O1 <=>	O1 = -0.870 =>	0%
#15	Ti1 <=>	Ti1 = +2.515 =>	0%
#16	Ti4 <=>	Ti1 = +2.515 =>	0%
#17	O15 <=>	O8 = -0.540 =>	0%
#18	O5 <=>	O8 = -0.540 =>	0%
#19	O8 <=>	O9 = -0.488 =>	0%
#20	O13 <=>	O9 = -0.488 =>	0%
#21	O19 <=>	O2 = -0.537 =>	0%
#22	O2 <=>	O2 = -0.537 =>	0%
#23	Ti3 <=>	Ti2 = +2.196 =>	1%
#24	Ti2 <=>	Ti2 = +2.196 =>	1%

#25	H39 <=>	H4 = +0.089 =>	1%
#26	H2 <=>	H4 = +0.089 =>	1%
#27	H38 <=>	H3 = +0.037 =>	1%
#28	H1 <=>	H3 = +0.037 =>	1%
#29	C45 <=>	C12 = -0.062 =>	1%
#30	C15 <=>	C12 = -0.062 =>	1%
#31	C41 <=>	C7 = -0.063 =>	2%
#32	C2 <=>	C7 = -0.063 =>	2%
#33	C40 <=>	C26 = -0.169 =>	2%
#34	C42 <=>	C26 = -0.169 =>	2%
#35	C66 <=>	C8 = -0.170 =>	2%
#36	C36 <=>	C8 = -0.170 =>	2%
#37	H48 <=>	H2 = +0.072 =>	2%
#38	H12 <=>	H2 = +0.072 =>	2%
#39	H20 <=>	H22 = +0.077 =>	2%
#40	H34 <=>	H22 = +0.077 =>	2%
#41	C37 <=>	C17 = -0.168 =>	3%
#42	C63 <=>	C17 = -0.168 =>	3%
#43	C18 <=>	C21 = -0.061 =>	3%
#44	C29 <=>	C21 = -0.061 =>	3%
#45	H53 <=>	H6 = +0.079 =>	3%
#46	H29 <=>	H6 = +0.079 =>	3%
#47	H30 <=>	H7 = +0.076 =>	3%
#48	H54 <=>	H7 = +0.076 =>	3%
#49	C4 <=>	C19 = -0.054 =>	3%
#50	C27 <=>	C19 = -0.054 =>	3%
#51	H42 <=>	H25 = +0.078 =>	3%
#52	H37 <=>	H25 = +0.078 =>	3%
#53	H16 <=>	H27 = +0.047 =>	4%
#54	H8 <=>	H27 = +0.047 =>	4%
#55	H6 <=>	H20 = +0.070 =>	4%
#56	H22 <=>	H20 = +0.070 =>	4%
#57	H11 <=>	H1 = +0.066 =>	4%
#58	H47 <=>	H1 = +0.066 =>	4%
#59	C49 <=>	C9 = -0.031 =>	4%
#60	C10 <=>	C9 = -0.031 =>	4%
#61	O23 <=>	O13 = -0.245 =>	4%
#62	O25 <=>	O13 = -0.245 =>	4%
#63	C22 <=>	C14 = -0.063 =>	4%
#64	C47 <=>	C14 = -0.063 =>	4%
#65	H7 <=>	H26 = +0.108 =>	5%
#66	H15 <=>	H26 = +0.108 =>	5%
#67	C5 <=>	C16 = +0.051 =>	5%
#68	C32 <=>	C16 = +0.051 =>	5%
#69	C7 <=>	C27 = -0.061 =>	5%
#70	C20 <=>	C27 = -0.061 =>	5%
#71	C28 <=>	C20 = -0.033 =>	6%
#72	C16 <=>	C20 = -0.033 =>	6%
#73	C60 <=>	C33 = +0.067 =>	6%
#74	C65 <=>	C33 = +0.067 =>	6%
#75	C3 <=>	C10 = -0.072 =>	6%
#76	C31 <=>	C10 = -0.072 =>	6%
#77	O14 <=>	O6 = -0.257 =>	6%
#78	O12 <=>	O6 = -0.257 =>	6%
#79	H18 <=>	H17 = +0.080 =>	7%
#80	H26 <=>	H17 = +0.080 =>	7%
#81	H19 <=>	H18 = +0.070 =>	7%

#82	H27 <=>	H18 = +0.070 =>	7%
#83	H9 <=>	H8 = +0.080 =>	7%
#84	H45 <=>	H8 = +0.080 =>	7%
#85	C43 <=>	C1 = +0.046 =>	8%
#86	C1 <=>	C1 = +0.046 =>	8%
#87	H51 <=>	H16 = +0.073 =>	8%
#88	H33 <=>	H16 = +0.073 =>	8%
#89	C58 <=>	C3 = -0.057 =>	8%
#90	C11 <=>	C3 = -0.057 =>	8%
#91	H35 <=>	H23 = +0.080 =>	8%
#92	H40 <=>	H23 = +0.080 =>	8%
#93	C35 <=>	C18 = -0.028 =>	9%
#94	C24 <=>	C18 = -0.028 =>	9%
#95	H17 <=>	H13 = +0.062 =>	9%
#96	H44 <=>	H13 = +0.062 =>	9%
#97	H46 <=>	H9 = +0.076 =>	12%
#98	H10 <=>	H9 = +0.076 =>	12%
#99	H23 <=>	H21 = +0.058 =>	12%
#100	H14 <=>	H21 = +0.058 =>	12%
#101	H21 <=>	H19 = +0.035 =>	13%
#102	H5 <=>	H19 = +0.035 =>	13%
#103	H52 <=>	H5 = +0.075 =>	13%
#104	H28 <=>	H5 = +0.075 =>	13%
#105	H49 <=>	H14 = +0.073 =>	16%
#106	H31 <=>	H14 = +0.073 =>	16%
#107	H32 <=>	H15 = +0.072 =>	16%
#108	H50 <=>	H15 = +0.072 =>	16%
#109	C25 <=>	C23 = -0.058 =>	17%
#110	C39 <=>	C23 = -0.058 =>	17%
#111	C17 <=>	C25 = +0.020 =>	18%
#112	C6 <=>	C25 = +0.020 =>	18%
#113	H36 <=>	H24 = +0.074 =>	24%
#114	H41 <=>	H24 = +0.074 =>	24%
#115	C33 <=>	C11 = -0.030 =>	26%
#116	C14 <=>	C11 = -0.030 =>	26%
#117	C8 <=>	C2 = -0.022 =>	28%
#118	C44 <=>	C2 = -0.022 =>	28%
#119	C12 <=>	C4 = -0.004 =>	29%
#120	H24 <=>	H10 = +0.041 =>	29%
#121	H3 <=>	H10 = +0.041 =>	29%
#122	C61 <=>	C4 = -0.004 =>	29%
#123	H43 <=>	H12 = +0.057 =>	33%
#124	H13 <=>	H12 = +0.057 =>	33%
#125	H25 <=>	H11 = +0.039 =>	35%
#126	H4 <=>	H11 = +0.039 =>	35%
#127	C59 <=>	C32 = -0.015 =>	40%
#128	C64 <=>	C32 = -0.015 =>	40%
#129	C26 <=>	C24 = -0.021 =>	57%
#130	C19 <=>	C24 = -0.021 =>	57%
#131	C30 <=>	C22 = -0.004 =>	186%
#132	C38 <=>	C22 = -0.004 =>	186%
#133	C23 <=>	C15 = -0.004 =>	218%
#134	C34 <=>	C15 = -0.004 =>	218%
#135	C46 <=>	C13 = -0.007 =>	491%
#136	C21 <=>	C13 = -0.007 =>	492%
#137	C9 <=>	C6 = -0.003 =>	709%
#138	C48 <=>	C6 = -0.003 =>	709%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -143.771 eV = -13871.6 kJ.mol⁻¹

WinPacha retrosynthetic report for A (free)

Current molecular fragment is: [H27C27O10Ti2]*2 = 1214.60 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O6 <=>	O10 = -0.630 =>	0%
#2	O9 <=>	O10 = -0.630 =>	0%
#3	O4 <=>	O5 = -0.667 =>	0%
#4	O18 <=>	O5 = -0.667 =>	0%
#5	O17 <=>	O3 = -0.446 =>	0%
#6	O3 <=>	O3 = -0.446 =>	0%
#7	O5 <=>	O8 = -0.541 =>	0%
#8	O15 <=>	O8 = -0.541 =>	0%
#9	O11 <=>	O7 = -0.497 =>	0%
#10	O7 <=>	O7 = -0.497 =>	0%
#11	O1 <=>	O1 = -0.870 =>	0%
#12	O10 <=>	O1 = -0.870 =>	0%
#13	Ti4 <=>	Ti1 = +2.512 =>	0%
#14	Ti1 <=>	Ti1 = +2.512 =>	0%
#15	O19 <=>	O2 = -0.538 =>	1%
#16	O2 <=>	O2 = -0.538 =>	1%
#17	C49 <=>	C9 = -0.032 =>	1%
#18	C10 <=>	C9 = -0.032 =>	1%
#19	Ti2 <=>	Ti2 = +2.192 =>	1%
#20	Ti3 <=>	Ti2 = +2.192 =>	1%
#21	O8 <=>	O9 = -0.491 =>	1%
#22	O13 <=>	O9 = -0.491 =>	1%
#23	C2 <=>	C7 = -0.063 =>	1%
#24	C41 <=>	C7 = -0.063 =>	1%
#25	H2 <=>	H4 = +0.087 =>	1%
#26	H39 <=>	H4 = +0.087 =>	1%
#27	C13 <=>	C5 = -0.061 =>	3%
#28	C62 <=>	C5 = -0.061 =>	3%
#29	C45 <=>	C12 = -0.063 =>	3%
#30	C15 <=>	C12 = -0.063 =>	3%
#31	C7 <=>	C27 = -0.059 =>	3%
#32	C20 <=>	C27 = -0.059 =>	3%
#33	C36 <=>	C8 = -0.168 =>	3%
#34	C66 <=>	C8 = -0.168 =>	3%
#35	H8 <=>	H27 = +0.044 =>	3%
#36	H16 <=>	H27 = +0.044 =>	3%
#37	C63 <=>	C17 = -0.167 =>	4%
#38	C37 <=>	C17 = -0.167 =>	4%
#39	C40 <=>	C26 = -0.166 =>	4%
#40	C42 <=>	C26 = -0.166 =>	4%
#41	C27 <=>	C19 = -0.054 =>	4%
#42	C4 <=>	C19 = -0.054 =>	4%
#43	H1 <=>	H3 = +0.036 =>	4%
#44	H38 <=>	H3 = +0.036 =>	4%
#45	C18 <=>	C21 = -0.062 =>	5%
#46	C29 <=>	C21 = -0.062 =>	5%
#47	C47 <=>	C14 = -0.064 =>	6%
#48	C22 <=>	C14 = -0.064 =>	6%

#49	C3 <=>	C10 = -0.071 =>	6%
#50	C31 <=>	C10 = -0.071 =>	6%
#51	H6 <=>	H20 = +0.068 =>	7%
#52	H22 <=>	H20 = +0.068 =>	7%
#53	O21 <=>	O4 = -0.262 =>	7%
#54	O16 <=>	O4 = -0.262 =>	7%
#55	H11 <=>	H1 = +0.064 =>	7%
#56	H47 <=>	H1 = +0.064 =>	7%
#57	O14 <=>	O6 = -0.259 =>	7%
#58	O12 <=>	O6 = -0.259 =>	7%
#59	C5 <=>	C16 = +0.050 =>	7%
#60	C32 <=>	C16 = +0.050 =>	7%
#61	H45 <=>	H8 = +0.069 =>	7%
#62	H9 <=>	H8 = +0.069 =>	7%
#63	C35 <=>	C18 = -0.028 =>	8%
#64	C24 <=>	C18 = -0.028 =>	8%
#65	H48 <=>	H2 = +0.064 =>	9%
#66	H12 <=>	H2 = +0.064 =>	9%
#67	H30 <=>	H7 = +0.071 =>	9%
#68	H54 <=>	H7 = +0.071 =>	9%
#69	H18 <=>	H17 = +0.078 =>	9%
#70	H26 <=>	H17 = +0.078 =>	9%
#71	C11 <=>	C3 = -0.058 =>	10%
#72	C58 <=>	C3 = -0.058 =>	10%
#73	H29 <=>	H6 = +0.074 =>	10%
#74	H53 <=>	H6 = +0.074 =>	10%
#75	C43 <=>	C1 = +0.045 =>	10%
#76	C1 <=>	C1 = +0.045 =>	10%
#77	H19 <=>	H18 = +0.068 =>	10%
#78	H27 <=>	H18 = +0.068 =>	10%
#79	C28 <=>	C20 = -0.034 =>	11%
#80	C16 <=>	C20 = -0.034 =>	11%
#81	H15 <=>	H26 = +0.091 =>	12%
#82	H7 <=>	H26 = +0.091 =>	12%
#83	H51 <=>	H16 = +0.069 =>	13%
#84	H33 <=>	H16 = +0.069 =>	13%
#85	H17 <=>	H13 = +0.059 =>	13%
#86	H44 <=>	H13 = +0.059 =>	13%
#87	H42 <=>	H25 = +0.070 =>	14%
#88	H37 <=>	H25 = +0.070 =>	14%
#89	H46 <=>	H9 = +0.072 =>	16%
#90	H10 <=>	H9 = +0.072 =>	16%
#91	H23 <=>	H21 = +0.055 =>	17%
#92	H14 <=>	H21 = +0.055 =>	17%
#93	H28 <=>	H5 = +0.071 =>	17%
#94	H52 <=>	H5 = +0.071 =>	17%
#95	H21 <=>	H19 = +0.033 =>	18%
#96	H5 <=>	H19 = +0.033 =>	18%
#97	H49 <=>	H14 = +0.069 =>	20%
#98	H31 <=>	H14 = +0.069 =>	20%
#99	H32 <=>	H15 = +0.069 =>	20%
#100	H50 <=>	H15 = +0.069 =>	20%
#101	H35 <=>	H23 = +0.069 =>	21%
#102	H40 <=>	H23 = +0.069 =>	21%
#103	C39 <=>	C23 = -0.061 =>	22%
#104	C25 <=>	C23 = -0.061 =>	22%
#105	C6 <=>	C25 = +0.018 =>	24%

#106	C17 <=>	C25 = +0.018 =>	24%
#107	H20 <=>	H22 = +0.060 =>	25%
#108	H34 <=>	H22 = +0.060 =>	25%
#109	H36 <=>	H24 = +0.070 =>	29%
#110	H41 <=>	H24 = +0.070 =>	29%
#111	C33 <=>	C11 = -0.031 =>	32%
#112	C14 <=>	C11 = -0.031 =>	32%
#113	H24 <=>	H10 = +0.039 =>	33%
#114	H3 <=>	H10 = +0.039 =>	33%
#115	C44 <=>	C2 = -0.023 =>	35%
#116	C8 <=>	C2 = -0.023 =>	35%
#117	H43 <=>	H12 = +0.055 =>	36%
#118	H13 <=>	H12 = +0.055 =>	36%
#119	H25 <=>	H11 = +0.037 =>	37%
#120	H4 <=>	H11 = +0.037 =>	37%
#121	C26 <=>	C24 = -0.026 =>	97%
#122	C19 <=>	C24 = -0.026 =>	97%
#123	C61 <=>	C4 = -0.007 =>	110%
#124	C12 <=>	C4 = -0.007 =>	110%
#125	C23 <=>	C15 = -0.005 =>	261%
#126	C34 <=>	C15 = -0.005 =>	261%
#127	C30 <=>	C22 = -0.009 =>	278%
#128	C38 <=>	C22 = -0.009 =>	278%
#129	C46 <=>	C13 = -0.009 =>	642%
#130	C21 <=>	C13 = -0.009 =>	642%
#131	C9 <=>	C6 = -0.006 =>	1627%
#132	C48 <=>	C6 = -0.006 =>	1627%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -142.974 eV = -13794.8 kJ.mol⁻¹

WinPacha retrosynthetic report for S (free)

Current molecular fragment is: [C2O]*1 = 40.02 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O1 <=>	O13 = -0.201 =>	21%
#2	C1 <=>	C33 = +0.129 =>	82%
#3	C2 <=>	C32 = +0.072 =>	379%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -0.266 eV = -25.7 kJ.mol⁻¹

WinPacha retrosynthetic report for B (free)

Current molecular fragment is: [C2O]*2 = 80.04 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O1 <=>	O12 = -0.231 =>	7%
#2	O2 <=>	O11 = -0.236 =>	11%
#3	C3 <=>	C31 = +0.113 =>	64%
#4	C2 <=>	C30 = +0.115 =>	97%
#5	C4 <=>	C28 = +0.139 =>	113%
#6	C1 <=>	C29 = +0.100 =>	127%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -0.919 eV = -88.6 kJ.mol⁻¹

WinPacha atomic charges calculations report

Ti4_BHMPC_CHCL3 -> C131 H162 Cl18 O49 Ti8 -> {[Ti4O2(BHMPC)6][1,4-dioxanne]2[CHCl3]2.CHCl3}2.(CO)

Molecular Recognition of Titanium(IV) Alkoxides by 2,6-bis(hydroxymethyl)-p-cresol in the Crystal Engineering of Hybrid Organic-Inorganic Networks

Rammal, Adel; Brisach, Frédéric; Henry, Marc

V= 3995.12 Å³ (Z = 2) -> Rval = 9.90% T = 173K

***Atomic electronegativies (eV) and radii (pm) ***

Ti(8.170, 147.7)
O(21.360, 45.0)
C(15.050, 62.0)
Cl(16.970, 72.4)
H(13.610, 53.0)

Madelung summation with gaussian inner-charge scaling (G = 0.12 Å⁻¹)

Reciprocal space exploration: -2 <= (h, k, l) <= 2

Madelung constant A = 268.81788885/2 = 134.40894443 (dmin = 0.945 Å)

min = -0.23620 Å⁻¹ < mean = 0.21454 Å⁻¹ < max = 2.37021 Å⁻¹

Total electrostatic balance = -4095.02 eV = -395105.5 kJ.mol⁻¹

Mean electronegativity: <EN> = 14.39 eV

Global hardness: <GH> = 1.67 eV (G = 0.12 Å⁻¹)

Electronic signature: #n Label(±ox) [CN] = ±q {±f}

	Atom	Charge	Fukui
#78	O20(-2) [3] =	-0.857 {	-0.002 }
#39	O10(-2) [3] =	-0.855 {	-0.002 }
#27	O7(-2) [3] =	-0.663 {	-0.000 }
#53	O13(-2) [3] =	-0.660 {	-0.000 }
#65	O16(-2) [3] =	-0.627 {	0.000 }
#26	O6(-2) [3] =	-0.627 {	0.000 }
#77	O19(-2) [2] =	-0.531 {	0.002 }
#15	O4(-2) [2] =	-0.528 {	0.002 }
#64	O15(-2) [2] =	-0.528 {	0.002 }
#3	O1(-2) [2] =	-0.523 {	0.002 }
#54	O14(-2) [2] =	-0.490 {	0.002 }
#42	O11(-2) [2] =	-0.488 {	0.002 }
#25	O5(-2) [2] =	-0.487 {	0.003 }
#38	O9(-2) [2] =	-0.487 {	0.002 }
#14	O3(-2) [2] =	-0.438 {	0.003 }
#66	O17(-2) [2] =	-0.434 {	0.003 }
#100	O24(-2) [2] =	-0.269 {	0.005 }
#76	O18(-2) [1] =	-0.263 {	0.006 }
#79	O21(-2) [2] =	-0.257 {	0.005 }
#82	O22(-2) [2] =	-0.256 {	0.006 }
#11	O2(-2) [1] =	-0.248 {	0.007 }
#97	O23(-2) [1] =	-0.246 {	0.006 }
#50	O12(-2) [1] =	-0.243 {	0.006 }
#37	O8(-2) [1] =	-0.239 {	0.006 }
#35	C26(-3) [4] =	-0.183 {	-0.001 }
#51	C35(-3) [4] =	-0.182 {	-0.002 }
#12	C8(-3) [4] =	-0.179 {	-0.001 }
#74	C53(-3) [4] =	-0.177 {	-0.002 }

#62	C44 (-3) [4] =	-0.173	{	-0.001
#23	C17 (-3) [4] =	-0.172	{	-0.001
#92	C16 (+0) [2] =	-0.148	{	0.015
#88	C13 (+0) [2] =	-0.146	{	0.014
#94	C17 (-1) [1] =	-0.141	{	0.016
#90	C14 (-1) [1] =	-0.137	{	0.015
#91	C15 (+0) [2] =	-0.134	{	0.015
#96	C19 (-1) [1] =	-0.132	{	0.016
#86	C11 (+0) [2] =	-0.123	{	0.015
#95	C18 (-1) [1] =	-0.116	{	0.017
#87	C12 (+1) [3] =	-0.099	{	0.018
#28	C19 (-1) [4] =	-0.074	{	0.001
#52	C36 (-1) [4] =	-0.069	{	0.001
#13	C9 (-1) [4] =	-0.067	{	0.001
#16	C10 (-1) [4] =	-0.063	{	0.001
#63	C45 (-1) [4] =	-0.062	{	0.001
#67	C46 (-1) [4] =	-0.062	{	0.001
#6	C3 (-1) [3] =	-0.061	{	0.004
#24	C18 (-1) [5] =	-0.060	{	0.002
#71	C50 (-1) [3] =	-0.060	{	0.004
#32	C23 (-1) [3] =	-0.060	{	0.005
#30	C21 (-1) [3] =	-0.059	{	0.004
#45	C30 (-1) [3] =	-0.059	{	0.004
#55	C37 (-1) [5] =	-0.059	{	0.002
#47	C32 (-1) [3] =	-0.059	{	0.004
#8	C5 (-1) [3] =	-0.056	{	0.004
#59	C41 (-1) [3] =	-0.054	{	0.004
#69	C48 (-1) [3] =	-0.054	{	0.004
#18	C12 (-1) [3] =	-0.052	{	0.005
#57	C39 (-1) [3] =	-0.052	{	0.004
#20	C14 (-1) [3] =	-0.051	{	0.004
#49	C34 (-1) [4] =	-0.034	{	0.002
#36	C27 (-1) [4] =	-0.032	{	0.002
#10	C7 (-1) [4] =	-0.032	{	0.002
#75	C54 (-1) [4] =	-0.029	{	0.002
#48	C33 (+0) [3] =	-0.023	{	0.006
#29	C20 (+0) [3] =	-0.022	{	0.005
#60	C42 (+0) [3] =	-0.022	{	0.006
#17	C11 (+0) [3] =	-0.020	{	0.006
#68	C47 (+0) [3] =	-0.020	{	0.006
#9	C6 (+0) [3] =	-0.017	{	0.006
#56	C38 (+0) [3] =	-0.014	{	0.006
#21	C15 (+0) [3] =	-0.009	{	0.006
#72	C51 (+0) [3] =	-0.003	{	0.006
#70	C49 (+0) [3] =	-0.001	{	0.007
#7	C4 (+0) [3] =	-0.000	{	0.006
#5	C2 (+0) [3] =	+0.000	{	0.006
#46	C31 (+0) [3] =	+0.005	{	0.007
#31	C22 (+0) [3] =	+0.006	{	0.007
#33	C24 (+0) [3] =	+0.006	{	0.006
#19	C13 (+0) [3] =	+0.007	{	0.007
#44	C29 (+0) [3] =	+0.007	{	0.006
#58	C40 (+0) [3] =	+0.008	{	0.007
#61	C43 (+1) [3] =	+0.024	{	0.005
#102	C65 (-2) [1] =	+0.026	{	0.010
#22	C16 (+1) [3] =	+0.028	{	0.005
#138	H36 (+1) [1] =	+0.041	{	0.006

#120	H18 (+1) [1] =	+0.045	{	0.005
#84	C58 (+1) [2] =	+0.045	{	0.008
#4	C1 (+1) [3] =	+0.050	{	0.005
#137	H35 (+1) [1] =	+0.051	{	0.006
#146	H44 (+1) [1] =	+0.052	{	0.006
#34	C25 (+1) [3] =	+0.052	{	0.005
#121	H19 (+1) [1] =	+0.052	{	0.005
#149	H47 (+1) [1] =	+0.053	{	0.006
#73	C52 (+1) [3] =	+0.053	{	0.006
#140	H38 (+1) [1] =	+0.053	{	0.005
#80	C55 (+1) [2] =	+0.053	{	0.008
#43	C28 (+1) [3] =	+0.055	{	0.005
#112	H10 (+1) [1] =	+0.055	{	0.006
#98	C62 (+1) [2] =	+0.058	{	0.008
#110	H8 (+1) [1] =	+0.062	{	0.006
#122	H20 (+1) [1] =	+0.063	{	0.006
#99	C63 (+1) [2] =	+0.063	{	0.009
#151	H49 (+1) [1] =	+0.065	{	0.006
#155	H53 (+1) [1] =	+0.067	{	0.006
#150	H48 (+1) [1] =	+0.069	{	0.006
#83	C57 (+1) [2] =	+0.070	{	0.012
#103	H1 (+1) [1] =	+0.072	{	0.006
#114	H12 (+1) [1] =	+0.073	{	0.008
#89	C60 (+3) [3] =	+0.074	{	0.006
#141	H39 (+1) [1] =	+0.074	{	0.006
#142	H40 (+1) [1] =	+0.075	{	0.006
#156	H54 (+1) [1] =	+0.076	{	0.007
#117	H15 (+1) [1] =	+0.078	{	0.007
#81	C56 (+1) [2] =	+0.079	{	0.011
#115	H13 (+1) [1] =	+0.080	{	0.006
#105	H3 (+1) [1] =	+0.080	{	0.007
#106	H4 (+1) [1] =	+0.082	{	0.006
#130	H28 (+1) [1] =	+0.083	{	0.006
#145	H43 (+1) [1] =	+0.084	{	0.008
#153	H51 (+1) [1] =	+0.084	{	0.007
#127	H25 (+1) [1] =	+0.085	{	0.007
#116	H14 (+1) [1] =	+0.086	{	0.007
#113	H11 (+1) [1] =	+0.087	{	0.007
#139	H37 (+1) [1] =	+0.088	{	0.006
#147	H45 (+1) [1] =	+0.088	{	0.006
#104	H2 (+1) [1] =	+0.089	{	0.007
#123	H21 (+1) [1] =	+0.089	{	0.006
#108	H6 (+1) [1] =	+0.089	{	0.006
#143	H41 (+1) [1] =	+0.089	{	0.007
#85	C59 (+3) [3] =	+0.090	{	0.008
#133	H31 (+1) [1] =	+0.090	{	0.006
#131	H29 (+1) [1] =	+0.091	{	0.007
#118	H16 (+1) [1] =	+0.092	{	0.010
#144	H42 (+1) [1] =	+0.093	{	0.008
#124	H22 (+1) [1] =	+0.093	{	0.008
#134	H32 (+1) [1] =	+0.094	{	0.008
#93	C61 (+3) [3] =	+0.095	{	0.007
#129	H27 (+1) [1] =	+0.096	{	0.009
#152	H50 (+1) [1] =	+0.097	{	0.008
#109	H7 (+1) [1] =	+0.098	{	0.007
#132	H30 (+1) [1] =	+0.098	{	0.006
#128	H26 (+1) [1] =	+0.100	{	0.008

#148	H46(+1) [1] =	+0.100 {	0.007}
#154	H52(+1) [1] =	+0.104 {	0.010}
#119	H17(+1) [1] =	+0.106 {	0.007}
#101	C64(+1) [2] =	+0.107 {	0.008}
#136	H34(+1) [1] =	+0.109 {	0.008}
#135	H33(+1) [1] =	+0.109 {	0.010}
#107	H5(+1) [1] =	+0.110 {	0.008}
#126	H24(+1) [1] =	+0.113 {	0.008}
#125	H23(+1) [1] =	+0.116 {	0.007}
#111	H9(+1) [1] =	+0.120 {	0.007}
#40	Ti3(+4) [7] =	+2.197 {	0.028}
#2	Ti2(+4) [7] =	+2.204 {	0.027}
#41	Ti4(+4) [6] =	+2.498 {	0.032}
#1	Ti1(+4) [6] =	+2.509 {	0.031}

Partial electrostatic balance: <EB> = -288.61 eV = -27846.1 kJ.mol⁻¹
 Reduced electrostatic balance: <EB/2> = -144.30 eV = -13923.1 kJ.mol⁻¹
 Global ionicity: <GI> = 26.55 %

Statistical report: <Atom>[num] = mean ± 3×stdev (stdev) <avdev>
 <q(H)>[54] = 0.083 ± 0.057 (0.019) <0.015>
 <f(H)>[54] = 0.007 ± 0.003 (0.001) <0.001>
 <q(C)>[65] = -0.023 ± 0.207 (0.069) <0.053>
 <f(C)>[65] = 0.005 ± 0.009 (0.003) <0.002>
 <q(O)>[24] = -0.469 ± 0.565 (0.188) <0.149>
 <f(O)>[24] = 0.003 ± 0.008 (0.003) <0.002>
 <q(Cl)>[9] = -0.131 ± 0.047 (0.016) <0.012>
 <f(Cl)>[9] = 0.016 ± 0.004 (0.001) <0.001>
 <q(Ti)>[4] = 2.352 ± 0.525 (0.175) <0.152>
 <f(Ti)>[4] = 0.030 ± 0.007 (0.002) <0.002>

WinPacha retrosynthetic report for A (2(B+S) [#1]
 Current molecular fragment is: [H27C32O12Cl3Ti2]*2 = 1611.40 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O16 <=>	O7 = -0.663 =>	0%
#2	O5 <=>	O7 = -0.663 =>	0%
#3	Ti3 <=>	Ti2 = +2.203 =>	0%
#4	Ti2 <=>	Ti2 = +2.203 =>	0%
#5	O13 <=>	O9 = -0.487 =>	0%
#6	O8 <=>	O9 = -0.487 =>	0%
#7	O6 <=>	O10 = -0.855 =>	0%
#8	O10 <=>	O10 = -0.855 =>	0%
#9	O24 <=>	O22 = -0.256 =>	0%
#10	O23 <=>	O22 = -0.256 =>	0%
#11	O18 <=>	O4 = -0.529 =>	0%
#12	O3 <=>	O4 = -0.529 =>	0%
#13	O19 <=>	O1 = -0.522 =>	0%
#14	O1 <=>	O1 = -0.522 =>	0%
#15	O12 <=>	O5 = -0.486 =>	0%
#16	O7 <=>	O5 = -0.486 =>	0%
#17	O9 <=>	O6 = -0.629 =>	0%
#18	O4 <=>	O6 = -0.629 =>	0%
#19	O11 <=>	O8 = -0.240 =>	0%
#20	O15 <=>	O8 = -0.240 =>	0%
#21	Ti4 <=>	Ti1 = +2.500 =>	0%

#22	Ti1 <=>	Ti1 = +2.500 =>	0%
#23	C44 <=>	C21 = -0.060 =>	0%
#24	C19 <=>	C21 = -0.060 =>	0%
#25	H44 <=>	H16 = +0.091 =>	1%
#26	H33 <=>	H16 = +0.091 =>	1%
#27	H53 <=>	H6 = +0.088 =>	1%
#28	H26 <=>	H6 = +0.088 =>	1%
#29	C36 <=>	C17 = -0.174 =>	1%
#30	C47 <=>	C17 = -0.174 =>	1%
#31	C62 <=>	C5 = -0.055 =>	1%
#32	C12 <=>	C5 = -0.055 =>	1%
#33	O21 <=>	O2 = -0.245 =>	1%
#34	O14 <=>	O2 = -0.245 =>	1%
#35	O17 <=>	O3 = -0.445 =>	1%
#36	O2 <=>	O3 = -0.445 =>	1%
#37	C6 <=>	C18 = -0.061 =>	2%
#38	C17 <=>	C18 = -0.061 =>	2%
#39	C11 <=>	C11 = -0.120 =>	2%
#40	C14 <=>	C11 = -0.120 =>	2%
#41	C12 <=>	C12 = -0.096 =>	3%
#42	C15 <=>	C12 = -0.096 =>	3%
#43	O20 <=>	O21 = -0.250 =>	3%
#44	O22 <=>	O21 = -0.250 =>	3%
#45	H46 <=>	H4 = +0.080 =>	3%
#46	H10 <=>	H4 = +0.080 =>	3%
#47	C4 <=>	C19 = -0.071 =>	3%
#48	C26 <=>	C19 = -0.071 =>	3%
#49	C29 <=>	C10 = -0.061 =>	3%
#50	C3 <=>	C10 = -0.061 =>	3%
#51	H7 <=>	H17 = +0.110 =>	4%
#52	H14 <=>	H17 = +0.110 =>	4%
#53	C64 <=>	C8 = -0.172 =>	4%
#54	C31 <=>	C8 = -0.172 =>	4%
#55	C35 <=>	C14 = -0.053 =>	4%
#56	C28 <=>	C14 = -0.053 =>	4%
#57	C1 <=>	C1 = +0.052 =>	4%
#58	C42 <=>	C1 = +0.052 =>	4%
#59	H43 <=>	H15 = +0.081 =>	4%
#60	H32 <=>	H15 = +0.081 =>	4%
#61	C23 <=>	C23 = -0.057 =>	4%
#62	C46 <=>	C23 = -0.057 =>	4%
#63	C39 <=>	C59 = +0.093 =>	4%
#64	C55 <=>	C59 = +0.093 =>	4%
#65	C60 <=>	C3 = -0.058 =>	4%
#66	C10 <=>	C3 = -0.058 =>	4%
#67	C5 <=>	C25 = +0.055 =>	5%
#68	C27 <=>	C25 = +0.055 =>	5%
#69	C50 <=>	C7 = -0.030 =>	5%
#70	C9 <=>	C7 = -0.030 =>	5%
#71	C40 <=>	C12 = -0.056 =>	6%
#72	C15 <=>	C12 = -0.056 =>	6%
#73	H30 <=>	H13 = +0.085 =>	6%
#74	H22 <=>	H13 = +0.085 =>	6%
#75	C32 <=>	C24 = +0.006 =>	6%
#76	C24 <=>	C24 = +0.006 =>	6%
#77	H42 <=>	H14 = +0.092 =>	6%
#78	H31 <=>	H14 = +0.092 =>	6%

#79	C38 <=>	C26 = -0.171 =>	6%
#80	C63 <=>	C26 = -0.171 =>	6%
#81	C43 <=>	C9 = -0.063 =>	7%
#82	C2 <=>	C9 = -0.063 =>	7%
#83	H47 <=>	H1 = +0.077 =>	7%
#84	H11 <=>	H1 = +0.077 =>	7%
#85	H36 <=>	H25 = +0.079 =>	8%
#86	H51 <=>	H25 = +0.079 =>	8%
#87	C59 <=>	C58 = +0.042 =>	8%
#88	C54 <=>	C58 = +0.042 =>	8%
#89	H15 <=>	H18 = +0.049 =>	8%
#90	H8 <=>	H18 = +0.049 =>	8%
#91	H45 <=>	H3 = +0.087 =>	8%
#92	H9 <=>	H3 = +0.087 =>	8%
#93	C53 <=>	C57 = +0.063 =>	10%
#94	C58 <=>	C57 = +0.063 =>	10%
#95	C16 <=>	C13 = -0.131 =>	10%
#96	C13 <=>	C13 = -0.131 =>	10%
#97	H37 <=>	H12 = +0.065 =>	12%
#98	H13 <=>	H12 = +0.065 =>	12%
#99	H5 <=>	H19 = +0.046 =>	12%
#100	H20 <=>	H19 = +0.046 =>	12%
#101	H24 <=>	H11 = +0.076 =>	12%
#102	H4 <=>	H11 = +0.076 =>	12%
#103	C18 <=>	C20 = -0.025 =>	14%
#104	C37 <=>	C20 = -0.025 =>	14%
#105	C33 <=>	C27 = -0.028 =>	14%
#106	C25 <=>	C27 = -0.028 =>	14%
#107	C57 <=>	C56 = +0.090 =>	14%
#108	C52 <=>	C56 = +0.090 =>	14%
#109	H19 <=>	H27 = +0.079 =>	17%
#110	H29 <=>	H27 = +0.079 =>	17%
#111	H54 <=>	H7 = +0.081 =>	18%
#112	H27 <=>	H7 = +0.081 =>	18%
#113	C56 <=>	C55 = +0.063 =>	18%
#114	C51 <=>	C55 = +0.063 =>	18%
#115	H18 <=>	H26 = +0.082 =>	18%
#116	H28 <=>	H26 = +0.082 =>	18%
#117	C48 <=>	C6 = -0.020 =>	18%
#118	C8 <=>	C6 = -0.020 =>	18%
#119	C21 <=>	C16 = +0.023 =>	19%
#120	C14 <=>	C16 = +0.023 =>	19%
#121	H3 <=>	H10 = +0.042 =>	23%
#122	H23 <=>	H10 = +0.042 =>	23%
#123	H48 <=>	H2 = +0.068 =>	23%
#124	H12 <=>	H2 = +0.068 =>	23%
#125	H2 <=>	H9 = +0.092 =>	23%
#126	H39 <=>	H9 = +0.092 =>	23%
#127	H17 <=>	H22 = +0.070 =>	24%
#128	H41 <=>	H22 = +0.070 =>	24%
#129	H52 <=>	H5 = +0.081 =>	26%
#130	H25 <=>	H5 = +0.081 =>	26%
#131	H35 <=>	H24 = +0.081 =>	28%
#132	H50 <=>	H24 = +0.081 =>	28%
#133	C13 <=>	C11 = -0.025 =>	29%
#134	C30 <=>	C11 = -0.025 =>	29%
#135	H40 <=>	H21 = +0.062 =>	31%

#136	H16 <=>	H21 = +0.062 =>	31%
#137	H49 <=>	H23 = +0.080 =>	31%
#138	H34 <=>	H23 = +0.080 =>	31%
#139	H1 <=>	H8 = +0.043 =>	31%
#140	H38 <=>	H8 = +0.043 =>	31%
#141	H6 <=>	H20 = +0.043 =>	32%
#142	H21 <=>	H20 = +0.043 =>	32%
#143	C20 <=>	C15 = -0.012 =>	33%
#144	C16 <=>	C15 = -0.012 =>	33%
#145	C41 <=>	C13 = +0.004 =>	35%
#146	C34 <=>	C13 = +0.004 =>	35%
#147	C11 <=>	C4 = -0.000 =>	77%
#148	C61 <=>	C4 = -0.000 =>	77%
#149	C45 <=>	C22 = -0.002 =>	134%
#150	C22 <=>	C22 = -0.002 =>	134%
#151	C49 <=>	C2 = +0.003 =>	542%
#152	C7 <=>	C2 = +0.003 =>	542%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -142.927 eV = -13790.2 kJ.mol⁻¹

WinPacha retrosynthetic report for A (2B [#1]

Current molecular fragment is: [H27C31O12Ti2]*2 = 1374.68 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O5 <=>	O7 = -0.663 =>	0%
#2	O16 <=>	O7 = -0.663 =>	0%
#3	O19 <=>	O1 = -0.523 =>	0%
#4	O1 <=>	O1 = -0.523 =>	0%
#5	O6 <=>	O10 = -0.855 =>	0%
#6	O10 <=>	O10 = -0.855 =>	0%
#7	Ti2 <=>	Ti2 = +2.202 =>	0%
#8	Ti3 <=>	Ti2 = +2.202 =>	0%
#9	O7 <=>	O5 = -0.488 =>	0%
#10	O12 <=>	O5 = -0.488 =>	0%
#11	O13 <=>	O9 = -0.488 =>	0%
#12	O8 <=>	O9 = -0.488 =>	0%
#13	O9 <=>	O6 = -0.629 =>	0%
#14	O4 <=>	O6 = -0.629 =>	0%
#15	O18 <=>	O4 = -0.530 =>	0%
#16	O3 <=>	O4 = -0.530 =>	0%
#17	Ti1 <=>	Ti1 = +2.497 =>	0%
#18	Ti4 <=>	Ti1 = +2.497 =>	0%
#19	O15 <=>	O8 = -0.241 =>	1%
#20	O11 <=>	O8 = -0.241 =>	1%
#21	C62 <=>	C5 = -0.056 =>	1%
#22	C12 <=>	C5 = -0.056 =>	1%
#23	C6 <=>	C18 = -0.059 =>	1%
#24	C17 <=>	C18 = -0.059 =>	1%
#25	C1 <=>	C1 = +0.051 =>	1%
#26	C42 <=>	C1 = +0.051 =>	1%
#27	C57 <=>	C56 = +0.078 =>	1%
#28	C52 <=>	C56 = +0.078 =>	1%
#29	O17 <=>	O3 = -0.445 =>	2%
#30	O2 <=>	O3 = -0.445 =>	2%
#31	C47 <=>	C17 = -0.169 =>	2%

#32	C36 <=>	C17 = -0.169 =>	2%
#33	C10 <=>	C3 = -0.060 =>	2%
#34	C60 <=>	C3 = -0.060 =>	2%
#35	C23 <=>	C23 = -0.058 =>	2%
#36	C46 <=>	C23 = -0.058 =>	2%
#37	O24 <=>	O22 = -0.261 =>	2%
#38	O23 <=>	O22 = -0.261 =>	2%
#39	C19 <=>	C21 = -0.061 =>	2%
#40	C44 <=>	C21 = -0.061 =>	2%
#41	O20 <=>	O21 = -0.251 =>	2%
#42	O22 <=>	O21 = -0.251 =>	2%
#43	C27 <=>	C25 = +0.053 =>	2%
#44	C5 <=>	C25 = +0.053 =>	2%
#45	O14 <=>	O2 = -0.254 =>	2%
#46	O21 <=>	O2 = -0.254 =>	2%
#47	C3 <=>	C10 = -0.061 =>	4%
#48	C29 <=>	C10 = -0.061 =>	4%
#49	C4 <=>	C19 = -0.071 =>	4%
#50	C26 <=>	C19 = -0.071 =>	4%
#51	H8 <=>	H18 = +0.043 =>	5%
#52	H15 <=>	H18 = +0.043 =>	5%
#53	C64 <=>	C8 = -0.169 =>	6%
#54	C31 <=>	C8 = -0.169 =>	6%
#55	C35 <=>	C14 = -0.054 =>	6%
#56	C28 <=>	C14 = -0.054 =>	6%
#57	H43 <=>	H15 = +0.073 =>	7%
#58	H32 <=>	H15 = +0.073 =>	7%
#59	C50 <=>	C7 = -0.029 =>	7%
#60	C9 <=>	C7 = -0.029 =>	7%
#61	C43 <=>	C9 = -0.062 =>	8%
#62	C2 <=>	C9 = -0.062 =>	8%
#63	C38 <=>	C26 = -0.169 =>	8%
#64	C63 <=>	C26 = -0.169 =>	8%
#65	H11 <=>	H1 = +0.066 =>	8%
#66	H47 <=>	H1 = +0.066 =>	8%
#67	C15 <=>	C12 = -0.057 =>	8%
#68	C40 <=>	C12 = -0.057 =>	8%
#69	H14 <=>	H17 = +0.096 =>	9%
#70	H7 <=>	H17 = +0.096 =>	9%
#71	H10 <=>	H4 = +0.074 =>	10%
#72	H46 <=>	H4 = +0.074 =>	10%
#73	H45 <=>	H3 = +0.072 =>	10%
#74	H9 <=>	H3 = +0.072 =>	10%
#75	C59 <=>	C58 = +0.041 =>	10%
#76	C54 <=>	C58 = +0.041 =>	10%
#77	H26 <=>	H6 = +0.080 =>	11%
#78	H53 <=>	H6 = +0.080 =>	11%
#79	H31 <=>	H14 = +0.076 =>	11%
#80	H42 <=>	H14 = +0.076 =>	11%
#81	H33 <=>	H16 = +0.081 =>	12%
#82	H44 <=>	H16 = +0.081 =>	12%
#83	C56 <=>	C55 = +0.060 =>	13%
#84	C51 <=>	C55 = +0.060 =>	13%
#85	H36 <=>	H25 = +0.072 =>	15%
#86	H51 <=>	H25 = +0.072 =>	15%
#87	C33 <=>	C27 = -0.027 =>	16%
#88	C25 <=>	C27 = -0.027 =>	16%

#89	H4 <=>	H11 = +0.073 =>	17%
#90	H24 <=>	H11 = +0.073 =>	17%
#91	H22 <=>	H13 = +0.067 =>	17%
#92	H30 <=>	H13 = +0.067 =>	17%
#93	H37 <=>	H12 = +0.060 =>	17%
#94	H13 <=>	H12 = +0.060 =>	17%
#95	C53 <=>	C57 = +0.058 =>	18%
#96	C58 <=>	C57 = +0.058 =>	18%
#97	H5 <=>	H19 = +0.042 =>	19%
#98	H20 <=>	H19 = +0.042 =>	19%
#99	C37 <=>	C20 = -0.027 =>	21%
#100	C18 <=>	C20 = -0.027 =>	21%
#101	H18 <=>	H26 = +0.078 =>	22%
#102	H28 <=>	H26 = +0.078 =>	22%
#103	H29 <=>	H27 = +0.075 =>	22%
#104	H19 <=>	H27 = +0.075 =>	22%
#105	C21 <=>	C16 = +0.022 =>	22%
#106	C14 <=>	C16 = +0.022 =>	22%
#107	H3 <=>	H10 = +0.041 =>	25%
#108	H23 <=>	H10 = +0.041 =>	25%
#109	H27 <=>	H7 = +0.073 =>	26%
#110	H54 <=>	H7 = +0.073 =>	26%
#111	H39 <=>	H9 = +0.089 =>	26%
#112	H2 <=>	H9 = +0.089 =>	26%
#113	H12 <=>	H2 = +0.065 =>	27%
#114	H48 <=>	H2 = +0.065 =>	27%
#115	C48 <=>	C6 = -0.021 =>	28%
#116	C8 <=>	C6 = -0.021 =>	28%
#117	H17 <=>	H22 = +0.066 =>	28%
#118	H41 <=>	H22 = +0.066 =>	28%
#119	H52 <=>	H5 = +0.075 =>	32%
#120	H25 <=>	H5 = +0.075 =>	32%
#121	H35 <=>	H24 = +0.076 =>	33%
#122	H50 <=>	H24 = +0.076 =>	33%
#123	H40 <=>	H21 = +0.058 =>	35%
#124	H16 <=>	H21 = +0.058 =>	35%
#125	H6 <=>	H20 = +0.041 =>	35%
#126	H21 <=>	H20 = +0.041 =>	35%
#127	H49 <=>	H23 = +0.075 =>	36%
#128	H34 <=>	H23 = +0.075 =>	36%
#129	C32 <=>	C24 = +0.004 =>	36%
#130	C24 <=>	C24 = +0.004 =>	36%
#131	C30 <=>	C11 = -0.027 =>	37%
#132	C13 <=>	C11 = -0.027 =>	37%
#133	H1 <=>	H8 = +0.040 =>	37%
#134	H38 <=>	H8 = +0.040 =>	37%
#135	C20 <=>	C15 = -0.016 =>	75%
#136	C16 <=>	C15 = -0.016 =>	75%
#137	C41 <=>	C13 = -0.001 =>	114%
#138	C34 <=>	C13 = -0.001 =>	114%
#139	C45 <=>	C22 = -0.005 =>	176%
#140	C22 <=>	C22 = -0.005 =>	176%
#141	C7 <=>	C2 = -0.000 =>	186%
#142	C49 <=>	C2 = -0.000 =>	186%
#143	C11 <=>	C4 = -0.004 =>	1021%
#144	C61 <=>	C4 = -0.004 =>	1021%

*** Total electrical charge on molecular fragment = 0 ***
Partial electrostatic balance: <EB> = -142.027 eV = -13703.4 kJ.mol-1

WinPacha retrosynthetic report for A (2S [#1]
Current molecular fragment is: [H27C28O10Cl3Ti2]*2 = 1451.32 g.mol-1
#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O16 <=>	O7 = -0.663 =>	0%
#2	O5 <=>	O7 = -0.663 =>	0%
#3	O19 <=>	O1 = -0.523 =>	0%
#4	O1 <=>	O1 = -0.523 =>	0%
#5	O18 <=>	O4 = -0.529 =>	0%
#6	O3 <=>	O4 = -0.529 =>	0%
#7	H14 <=>	H17 = +0.106 =>	0%
#8	H7 <=>	H17 = +0.106 =>	0%
#9	C36 <=>	C17 = -0.173 =>	0%
#10	C47 <=>	C17 = -0.173 =>	0%
#11	O6 <=>	O10 = -0.858 =>	0%
#12	O10 <=>	O10 = -0.858 =>	0%
#13	O4 <=>	O6 = -0.629 =>	0%
#14	O9 <=>	O6 = -0.629 =>	0%
#15	O13 <=>	O9 = -0.489 =>	0%
#16	O8 <=>	O9 = -0.489 =>	0%
#17	O7 <=>	O5 = -0.489 =>	0%
#18	O12 <=>	O5 = -0.489 =>	0%
#19	O14 <=>	O2 = -0.249 =>	0%
#20	O21 <=>	O2 = -0.249 =>	0%
#21	Ti4 <=>	Ti1 = +2.489 =>	1%
#22	Ti1 <=>	Ti1 = +2.489 =>	1%
#23	Ti3 <=>	Ti2 = +2.184 =>	1%
#24	Ti2 <=>	Ti2 = +2.184 =>	1%
#25	C33 <=>	C27 = -0.032 =>	1%
#26	C25 <=>	C27 = -0.032 =>	1%
#27	Cl1 <=>	Cl1 = -0.124 =>	1%
#28	Cl4 <=>	Cl1 = -0.124 =>	1%
#29	H32 <=>	H15 = +0.079 =>	1%
#30	H43 <=>	H15 = +0.079 =>	1%
#31	H30 <=>	H13 = +0.081 =>	1%
#32	H22 <=>	H13 = +0.081 =>	1%
#33	C42 <=>	C1 = +0.049 =>	1%
#34	C1 <=>	C1 = +0.049 =>	1%
#35	H31 <=>	H14 = +0.088 =>	2%
#36	H42 <=>	H14 = +0.088 =>	2%
#37	C39 <=>	C59 = +0.091 =>	2%
#38	C55 <=>	C59 = +0.091 =>	2%
#39	O17 <=>	O3 = -0.447 =>	2%
#40	O2 <=>	O3 = -0.447 =>	2%
#41	C10 <=>	C3 = -0.059 =>	2%
#42	C60 <=>	C3 = -0.059 =>	2%
#43	C12 <=>	C5 = -0.057 =>	2%
#44	C62 <=>	C5 = -0.057 =>	2%
#45	C46 <=>	C23 = -0.061 =>	3%
#46	C23 <=>	C23 = -0.061 =>	3%
#47	C4 <=>	C19 = -0.072 =>	3%
#48	C26 <=>	C19 = -0.072 =>	3%
#49	C50 <=>	C7 = -0.030 =>	4%
#50	C9 <=>	C7 = -0.030 =>	4%

#51	C44 <=>	C21 = -0.062 =>	4%
#52	C19 <=>	C21 = -0.062 =>	4%
#53	H47 <=>	H1 = +0.075 =>	4%
#54	H11 <=>	H1 = +0.075 =>	4%
#55	H10 <=>	H4 = +0.079 =>	4%
#56	H46 <=>	H4 = +0.079 =>	4%
#57	C3 <=>	C10 = -0.060 =>	5%
#58	C29 <=>	C10 = -0.060 =>	5%
#59	C31 <=>	C8 = -0.171 =>	5%
#60	C64 <=>	C8 = -0.171 =>	5%
#61	C6 <=>	C18 = -0.063 =>	5%
#62	C17 <=>	C18 = -0.063 =>	5%
#63	C43 <=>	C9 = -0.064 =>	6%
#64	C2 <=>	C9 = -0.064 =>	6%
#65	H26 <=>	H6 = +0.084 =>	6%
#66	H53 <=>	H6 = +0.084 =>	6%
#67	C5 <=>	C25 = +0.049 =>	6%
#68	C27 <=>	C25 = +0.049 =>	6%
#69	H45 <=>	H3 = +0.086 =>	6%
#70	H9 <=>	H3 = +0.086 =>	6%
#71	C63 <=>	C26 = -0.170 =>	7%
#72	C38 <=>	C26 = -0.170 =>	7%
#73	O11 <=>	O8 = -0.257 =>	8%
#74	O15 <=>	O8 = -0.257 =>	8%
#75	C16 <=>	C13 = -0.135 =>	8%
#76	C13 <=>	C13 = -0.135 =>	8%
#77	H15 <=>	H18 = +0.049 =>	9%
#78	H8 <=>	H18 = +0.049 =>	9%
#79	H33 <=>	H16 = +0.083 =>	9%
#80	H44 <=>	H16 = +0.083 =>	9%
#81	H36 <=>	H25 = +0.076 =>	10%
#82	H51 <=>	H25 = +0.076 =>	10%
#83	C15 <=>	C12 = -0.110 =>	11%
#84	C12 <=>	C12 = -0.110 =>	11%
#85	H5 <=>	H19 = +0.046 =>	13%
#86	H20 <=>	H19 = +0.046 =>	13%
#87	C15 <=>	C12 = -0.060 =>	15%
#88	C40 <=>	C12 = -0.060 =>	15%
#89	H4 <=>	H11 = +0.073 =>	16%
#90	H24 <=>	H11 = +0.073 =>	16%
#91	H37 <=>	H12 = +0.061 =>	17%
#92	H13 <=>	H12 = +0.061 =>	17%
#93	C35 <=>	C14 = -0.059 =>	17%
#94	C28 <=>	C14 = -0.060 =>	17%
#95	H18 <=>	H26 = +0.082 =>	18%
#96	H28 <=>	H26 = +0.082 =>	18%
#97	H27 <=>	H7 = +0.079 =>	20%
#98	H54 <=>	H7 = +0.079 =>	20%
#99	H19 <=>	H27 = +0.074 =>	23%
#100	H29 <=>	H27 = +0.074 =>	23%
#101	H39 <=>	H9 = +0.090 =>	25%
#102	H2 <=>	H9 = +0.090 =>	25%
#103	C18 <=>	C20 = -0.028 =>	26%
#104	C37 <=>	C20 = -0.028 =>	26%
#105	H12 <=>	H2 = +0.065 =>	26%
#106	H48 <=>	H2 = +0.065 =>	26%
#107	H52 <=>	H5 = +0.078 =>	29%

#108	H25 <=>	H5 = +0.078 =>	29%
#109	H17 <=>	H22 = +0.065 =>	30%
#110	H41 <=>	H22 = +0.065 =>	30%
#111	H1 <=>	H8 = +0.042 =>	32%
#112	H38 <=>	H8 = +0.042 =>	32%
#113	H35 <=>	H24 = +0.076 =>	32%
#114	H50 <=>	H24 = +0.076 =>	32%
#115	H40 <=>	H21 = +0.060 =>	33%
#116	H16 <=>	H21 = +0.060 =>	33%
#117	H6 <=>	H20 = +0.042 =>	33%
#118	H21 <=>	H20 = +0.042 =>	33%
#119	H49 <=>	H23 = +0.076 =>	34%
#120	H34 <=>	H23 = +0.076 =>	34%
#121	H3 <=>	H10 = +0.036 =>	35%
#122	H23 <=>	H10 = +0.036 =>	35%
#123	C48 <=>	C6 = -0.023 =>	37%
#124	C8 <=>	C6 = -0.023 =>	37%
#125	C21 <=>	C16 = +0.017 =>	41%
#126	C14 <=>	C16 = +0.017 =>	41%
#127	C30 <=>	C11 = -0.031 =>	56%
#128	C13 <=>	C11 = -0.031 =>	56%
#129	C20 <=>	C15 = -0.020 =>	113%
#130	C16 <=>	C15 = -0.020 =>	113%
#131	C41 <=>	C13 = -0.003 =>	138%
#132	C34 <=>	C13 = -0.003 =>	138%
#133	C32 <=>	C24 = -0.003 =>	141%
#134	C24 <=>	C24 = -0.003 =>	141%
#135	C49 <=>	C2 = +0.001 =>	161%
#136	C7 <=>	C2 = +0.001 =>	161%
#137	C22 <=>	C22 = -0.006 =>	192%
#138	C45 <=>	C22 = -0.006 =>	192%
#139	C11 <=>	C4 = -0.003 =>	679%
#140	C61 <=>	C4 = -0.003 =>	679%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -140.862 eV = -13591.0 kJ.mol⁻¹

WinPacha retrosynthetic report for A (free) [#1]

Current molecular fragment is: [H27C27O10Ti2]*2 = 1214.60 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O16 <=>	O7 = -0.663 =>	0%
#2	O5 <=>	O7 = -0.663 =>	0%
#3	O1 <=>	O1 = -0.524 =>	0%
#4	O19 <=>	O1 = -0.524 =>	0%
#5	O18 <=>	O4 = -0.530 =>	0%
#6	O3 <=>	O4 = -0.530 =>	0%
#7	O10 <=>	O10 = -0.858 =>	0%
#8	O6 <=>	O10 = -0.858 =>	0%
#9	O9 <=>	O6 = -0.629 =>	0%
#10	O4 <=>	O6 = -0.629 =>	0%
#11	O8 <=>	O9 = -0.489 =>	1%
#12	O13 <=>	O9 = -0.489 =>	1%
#13	O12 <=>	O5 = -0.492 =>	1%
#14	O7 <=>	O5 = -0.492 =>	1%
#15	Ti1 <=>	Ti1 = +2.485 =>	1%

#16	Ti4 <=>	Ti1 = +2.485 =>	1%
#17	Ti3 <=>	Ti2 = +2.180 =>	1%
#18	Ti2 <=>	Ti2 = +2.180 =>	1%
#19	C10 <=>	C3 = -0.061 =>	1%
#20	C60 <=>	C3 = -0.061 =>	1%
#21	C17 <=>	C18 = -0.061 =>	2%
#22	C6 <=>	C18 = -0.061 =>	2%
#23	O17 <=>	O3 = -0.448 =>	2%
#24	O2 <=>	O3 = -0.448 =>	2%
#25	C33 <=>	C27 = -0.031 =>	2%
#26	C25 <=>	C27 = -0.031 =>	2%
#27	C47 <=>	C17 = -0.167 =>	3%
#28	C36 <=>	C17 = -0.167 =>	3%
#29	C4 <=>	C19 = -0.071 =>	4%
#30	C26 <=>	C19 = -0.071 =>	4%
#31	C50 <=>	C7 = -0.030 =>	4%
#32	C9 <=>	C7 = -0.030 =>	4%
#33	H8 <=>	H18 = +0.043 =>	5%
#34	H15 <=>	H18 = +0.043 =>	5%
#35	O21 <=>	O2 = -0.261 =>	5%
#36	O14 <=>	O2 = -0.261 =>	5%
#37	C42 <=>	C1 = +0.047 =>	5%
#38	C1 <=>	C1 = +0.047 =>	5%
#39	C29 <=>	C10 = -0.060 =>	5%
#40	C3 <=>	C10 = -0.060 =>	5%
#41	C12 <=>	C5 = -0.059 =>	5%
#42	C62 <=>	C5 = -0.059 =>	5%
#43	C46 <=>	C23 = -0.063 =>	5%
#44	C23 <=>	C23 = -0.063 =>	5%
#45	C44 <=>	C21 = -0.063 =>	6%
#46	C19 <=>	C21 = -0.063 =>	6%
#47	C43 <=>	C9 = -0.063 =>	6%
#48	C2 <=>	C9 = -0.063 =>	6%
#49	C31 <=>	C8 = -0.167 =>	7%
#50	C64 <=>	C8 = -0.167 =>	7%
#51	C63 <=>	C26 = -0.167 =>	9%
#52	C38 <=>	C26 = -0.167 =>	9%
#53	O11 <=>	O8 = -0.260 =>	9%
#54	O15 <=>	O8 = -0.260 =>	9%
#55	C27 <=>	C25 = +0.047 =>	10%
#56	C5 <=>	C25 = +0.047 =>	10%
#57	H43 <=>	H15 = +0.070 =>	11%
#58	H32 <=>	H15 = +0.070 =>	11%
#59	H10 <=>	H4 = +0.073 =>	12%
#60	H46 <=>	H4 = +0.073 =>	12%
#61	H11 <=>	H1 = +0.062 =>	13%
#62	H47 <=>	H1 = +0.062 =>	13%
#63	H45 <=>	H3 = +0.069 =>	14%
#64	H9 <=>	H3 = +0.069 =>	14%
#65	H14 <=>	H17 = +0.090 =>	15%
#66	H7 <=>	H17 = +0.090 =>	15%
#67	H53 <=>	H6 = +0.073 =>	17%
#68	H26 <=>	H6 = +0.073 =>	17%
#69	C15 <=>	C12 = -0.062 =>	18%
#70	C40 <=>	C12 = -0.062 =>	18%
#71	H51 <=>	H25 = +0.069 =>	19%
#72	H36 <=>	H25 = +0.069 =>	19%

#73	H42 <=>	H14 = +0.070 =>	19%
#74	H31 <=>	H14 = +0.070 =>	19%
#75	H5 <=>	H19 = +0.042 =>	20%
#76	H20 <=>	H19 = +0.042 =>	20%
#77	H4 <=>	H11 = +0.069 =>	21%
#78	H24 <=>	H11 = +0.069 =>	21%
#79	C28 <=>	C14 = -0.061 =>	21%
#80	C35 <=>	C14 = -0.061 =>	21%
#81	H18 <=>	H26 = +0.077 =>	23%
#82	H28 <=>	H26 = +0.077 =>	23%
#83	H33 <=>	H16 = +0.071 =>	23%
#84	H44 <=>	H16 = +0.071 =>	23%
#85	H37 <=>	H12 = +0.056 =>	24%
#86	H13 <=>	H12 = +0.056 =>	24%
#87	H22 <=>	H13 = +0.060 =>	25%
#88	H30 <=>	H13 = +0.060 =>	25%
#89	H29 <=>	H27 = +0.069 =>	28%
#90	H19 <=>	H27 = +0.069 =>	28%
#91	H39 <=>	H9 = +0.086 =>	29%
#92	H2 <=>	H9 = +0.086 =>	29%
#93	H54 <=>	H7 = +0.070 =>	29%
#94	H27 <=>	H7 = +0.070 =>	29%
#95	H48 <=>	H2 = +0.061 =>	31%
#96	H12 <=>	H2 = +0.061 =>	31%
#97	H41 <=>	H22 = +0.060 =>	35%
#98	H17 <=>	H22 = +0.060 =>	35%
#99	H52 <=>	H5 = +0.070 =>	36%
#100	H25 <=>	H5 = +0.070 =>	36%
#101	C18 <=>	C20 = -0.030 =>	36%
#102	C37 <=>	C20 = -0.030 =>	36%
#103	H40 <=>	H21 = +0.055 =>	38%
#104	H16 <=>	H21 = +0.055 =>	38%
#105	H1 <=>	H8 = +0.039 =>	38%
#106	H38 <=>	H8 = +0.039 =>	38%
#107	H50 <=>	H24 = +0.070 =>	38%
#108	H35 <=>	H24 = +0.070 =>	38%
#109	H6 <=>	H20 = +0.039 =>	38%
#110	H21 <=>	H20 = +0.039 =>	38%
#111	H3 <=>	H10 = +0.033 =>	40%
#112	H23 <=>	H10 = +0.033 =>	40%
#113	H49 <=>	H23 = +0.069 =>	40%
#114	H34 <=>	H23 = +0.069 =>	40%
#115	C21 <=>	C16 = +0.015 =>	46%
#116	C14 <=>	C16 = +0.015 =>	46%
#117	C48 <=>	C6 = -0.025 =>	50%
#118	C8 <=>	C6 = -0.025 =>	50%
#119	C30 <=>	C11 = -0.033 =>	68%
#120	C13 <=>	C11 = -0.033 =>	68%
#121	C16 <=>	C15 = -0.025 =>	168%
#122	C20 <=>	C15 = -0.025 =>	168%
#123	C24 <=>	C24 = -0.005 =>	182%
#124	C32 <=>	C24 = -0.005 =>	182%
#125	C41 <=>	C13 = -0.009 =>	236%
#126	C34 <=>	C13 = -0.009 =>	236%
#127	C45 <=>	C22 = -0.009 =>	245%
#128	C22 <=>	C22 = -0.009 =>	245%
#129	C49 <=>	C2 = -0.003 =>	781%

#130 C7 <=> C2 = -0.003 => 781%
#131 C11 <=> C4 = -0.007 => 2034%
#132 C61 <=> C4 = -0.007 => 2035%

*** Total electrical charge on molecular fragment = 0 ***
Partial electrostatic balance: <EB> = -139.835 eV = -13491.9 kJ.mol-1

WinPacha retrosynthetic report for B (free) [#1]
Current molecular fragment is: [C2O]*2 = 80.04 g.mol-1

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1 O2 <=> O22 = -0.231 => 10%
#2 O1 <=> O21 = -0.228 => 11%
#3 C3 <=> C56 = +0.118 => 50%
#4 C4 <=> C57 = +0.113 => 62%
#5 C1 <=> C55 = +0.114 => 113%
#6 C2 <=> C58 = +0.113 => 149%

*** Total electrical charge on molecular fragment = 0 ***
Partial electrostatic balance: <EB> = -0.847 eV = -81.8 kJ.mol-1

WinPacha retrosynthetic report for S (free) [#1]
Current molecular fragment is: [CCl3]*1 = 118.36 g.mol-1

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1 C1 <=> C59 = +0.114 => 27%
#2 Cl1 <=> Cl1 = -0.044 => 64%
#3 Cl3 <=> Cl3 = -0.044 => 70%
#4 Cl2 <=> Cl2 = -0.027 => 73%

*** Total electrical charge on molecular fragment = 0 ***
Partial electrostatic balance: <EB> = -0.087 eV = -8.4 kJ.mol-1

WinPacha retrosynthetic report for A (2(B+S) [#2]
Current molecular fragment is: [H27C32O12Cl3Ti2]*2 = 1611.40 g.mol-1

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1 O7 <=> O15 = -0.528 => 0%
#2 O13 <=> O15 = -0.528 => 0%
#3 O12 <=> O13 = -0.660 => 0%
#4 O2 <=> O13 = -0.660 => 0%
#5 Ti3 <=> Ti3 = +2.196 => 0%
#6 Ti1 <=> Ti3 = +2.196 => 0%
#7 O5 <=> O20 = -0.857 => 0%
#8 O6 <=> O20 = -0.857 => 0%
#9 Ti2 <=> Ti4 = +2.496 => 0%
#10 Ti4 <=> Ti4 = +2.496 => 0%
#11 O4 <=> O16 = -0.629 => 0%
#12 O10 <=> O16 = -0.629 => 0%
#13 C3 <=> C37 = -0.059 => 0%
#14 H29 <=> H41 = +0.089 => 0%
#15 H44 <=> H41 = +0.089 => 0%
#16 C20 <=> C37 = -0.059 => 0%
#17 O9 <=> O19 = -0.529 => 0%

#18	O17 <=>	O19 = -0.529 =>	0%
#19	C18 <=>	C28 = +0.055 =>	0%
#20	O15 <=>	O11 = -0.489 =>	0%
#21	O1 <=>	O11 = -0.489 =>	0%
#22	C1 <=>	C28 = +0.055 =>	0%
#23	O16 <=>	O14 = -0.488 =>	0%
#24	O3 <=>	O14 = -0.488 =>	0%
#25	H40 <=>	H54 = +0.076 =>	1%
#26	H23 <=>	H54 = +0.076 =>	1%
#27	C2 <=>	C36 = -0.068 =>	1%
#28	C19 <=>	C36 = -0.068 =>	1%
#29	C39 <=>	C29 = +0.007 =>	1%
#30	C7 <=>	C29 = +0.007 =>	1%
#31	O14 <=>	O17 = -0.438 =>	1%
#32	O8 <=>	O17 = -0.438 =>	1%
#33	O23 <=>	O24 = -0.266 =>	1%
#34	O24 <=>	O24 = -0.266 =>	1%
#35	H17 <=>	H36 = +0.041 =>	1%
#36	H2 <=>	H36 = +0.041 =>	1%
#37	C56 <=>	C64 = +0.106 =>	1%
#38	C60 <=>	C64 = +0.106 =>	1%
#39	C49 <=>	C44 = -0.175 =>	1%
#40	C34 <=>	C44 = -0.175 =>	1%
#41	C12 <=>	C32 = -0.059 =>	1%
#42	C43 <=>	C32 = -0.059 =>	1%
#43	H20 <=>	H48 = +0.070 =>	1%
#44	H47 <=>	H48 = +0.070 =>	1%
#45	C24 <=>	C48 = -0.054 =>	2%
#46	C50 <=>	C48 = -0.054 =>	2%
#47	O18 <=>	O12 = -0.239 =>	2%
#48	O19 <=>	O12 = -0.239 =>	2%
#49	C4 <=>	C46 = -0.061 =>	2%
#50	C35 <=>	C46 = -0.061 =>	2%
#51	H13 <=>	H39 = +0.073 =>	2%
#52	H38 <=>	H39 = +0.073 =>	2%
#53	H31 <=>	H43 = +0.082 =>	2%
#54	H46 <=>	H43 = +0.082 =>	2%
#55	C29 <=>	C41 = -0.055 =>	2%
#56	C33 <=>	C41 = -0.055 =>	2%
#57	O21 <=>	O23 = -0.240 =>	3%
#58	O22 <=>	O23 = -0.240 =>	3%
#59	C48 <=>	C53 = -0.172 =>	3%
#60	C62 <=>	C53 = -0.172 =>	3%
#61	C5 <=>	C52 = +0.055 =>	4%
#62	C36 <=>	C52 = +0.055 =>	4%
#63	C44 <=>	C39 = -0.054 =>	4%
#64	C15 <=>	C39 = -0.054 =>	4%
#65	C6 <=>	C45 = -0.060 =>	4%
#66	C17 <=>	C45 = -0.060 =>	4%
#67	O20 <=>	O18 = -0.252 =>	4%
#68	O11 <=>	O18 = -0.252 =>	4%
#69	C10 <=>	C30 = -0.056 =>	5%
#70	C41 <=>	C30 = -0.056 =>	5%
#71	C26 <=>	C50 = -0.057 =>	5%
#72	C52 <=>	C50 = -0.057 =>	5%
#73	C38 <=>	C47 = -0.019 =>	5%
#74	C23 <=>	C47 = -0.019 =>	5%

#75	C31 <=>	C35 = -0.172 =>	5%
#76	C53 <=>	C35 = -0.172 =>	5%
#77	H53 <=>	H51 = +0.089 =>	6%
#78	H42 <=>	H51 = +0.089 =>	6%
#79	C46 <=>	C54 = -0.028 =>	6%
#80	C28 <=>	C54 = -0.028 =>	6%
#81	C64 <=>	C61 = +0.101 =>	6%
#82	C63 <=>	C61 = +0.101 =>	6%
#83	C12 <=>	C18 = -0.107 =>	7%
#84	C15 <=>	C18 = -0.107 =>	7%
#85	H32 <=>	H46 = +0.093 =>	8%
#86	H5 <=>	H46 = +0.093 =>	8%
#87	C57 <=>	C65 = +0.024 =>	9%
#88	C61 <=>	C65 = +0.024 =>	9%
#89	H45 <=>	H42 = +0.101 =>	9%
#90	H30 <=>	H42 = +0.101 =>	9%
#91	H3 <=>	H37 = +0.097 =>	10%
#92	H18 <=>	H37 = +0.097 =>	10%
#93	H28 <=>	H40 = +0.068 =>	10%
#94	H24 <=>	H40 = +0.068 =>	10%
#95	H36 <=>	H28 = +0.074 =>	10%
#96	H11 <=>	H28 = +0.074 =>	10%
#97	H25 <=>	H32 = +0.084 =>	11%
#98	H49 <=>	H32 = +0.084 =>	11%
#99	H10 <=>	H31 = +0.080 =>	11%
#100	H35 <=>	H31 = +0.080 =>	11%
#101	C37 <=>	C33 = -0.026 =>	11%
#102	C8 <=>	C33 = -0.026 =>	11%
#103	H48 <=>	H49 = +0.073 =>	12%
#104	H21 <=>	H49 = +0.073 =>	12%
#105	C11 <=>	C17 = -0.124 =>	12%
#106	C14 <=>	C17 = -0.124 =>	12%
#107	H8 <=>	H45 = +0.077 =>	12%
#108	H15 <=>	H45 = +0.077 =>	12%
#109	H4 <=>	H38 = +0.046 =>	14%
#110	H19 <=>	H38 = +0.046 =>	14%
#111	C14 <=>	C43 = +0.021 =>	14%
#112	C22 <=>	C43 = +0.021 =>	14%
#113	C54 <=>	C62 = +0.066 =>	14%
#114	C58 <=>	C62 = +0.066 =>	14%
#115	H52 <=>	H50 = +0.083 =>	15%
#116	H41 <=>	H50 = +0.083 =>	15%
#117	C16 <=>	C42 = -0.025 =>	15%
#118	C21 <=>	C42 = -0.025 =>	15%
#119	H9 <=>	H30 = +0.083 =>	16%
#120	H34 <=>	H30 = +0.083 =>	16%
#121	H1 <=>	H35 = +0.043 =>	16%
#122	H16 <=>	H35 = +0.043 =>	16%
#123	C16 <=>	C19 = -0.111 =>	16%
#124	C13 <=>	C19 = -0.111 =>	16%
#125	H7 <=>	H44 = +0.042 =>	18%
#126	H14 <=>	H44 = +0.042 =>	18%
#127	H39 <=>	H53 = +0.079 =>	19%
#128	H22 <=>	H53 = +0.079 =>	19%
#129	C9 <=>	C34 = -0.028 =>	19%
#130	C40 <=>	C34 = -0.028 =>	19%
#131	H6 <=>	H47 = +0.042 =>	19%

#132	H33 <=>	H47 = +0.042 =>	19%
#133	C13 <=>	C38 = -0.016 =>	19%
#134	C30 <=>	C38 = -0.016 =>	19%
#135	H54 <=>	H52 = +0.081 =>	22%
#136	H43 <=>	H52 = +0.081 =>	22%
#137	H26 <=>	H33 = +0.085 =>	22%
#138	H50 <=>	H33 = +0.085 =>	22%
#139	C55 <=>	C63 = +0.079 =>	25%
#140	C59 <=>	C63 = +0.079 =>	25%
#141	H51 <=>	H34 = +0.079 =>	27%
#142	H27 <=>	H34 = +0.079 =>	27%
#143	H37 <=>	H29 = +0.062 =>	32%
#144	H12 <=>	H29 = +0.062 =>	32%
#145	C32 <=>	C40 = +0.004 =>	51%
#146	C47 <=>	C40 = +0.004 =>	51%
#147	C51 <=>	C49 = +0.000 =>	114%
#148	C25 <=>	C49 = +0.000 =>	115%
#149	C42 <=>	C31 = -0.001 =>	125%
#150	C11 <=>	C31 = -0.001 =>	125%
#151	C45 <=>	C51 = +0.001 =>	144%
#152	C27 <=>	C51 = +0.001 =>	144%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -142.691 eV = -13767.4 kJ.mol⁻¹

WinPacha retrosynthetic report for A (2B [#2]

Current molecular fragment is: [H27C31O12Ti2]*2 = 1374.68 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O2 <=>	O13 = -0.660 =>	0%
#2	O12 <=>	O13 = -0.660 =>	0%
#3	O5 <=>	O20 = -0.857 =>	0%
#4	O6 <=>	O20 = -0.857 =>	0%
#5	Ti3 <=>	Ti3 = +2.194 =>	0%
#6	Ti1 <=>	Ti3 = +2.194 =>	0%
#7	O9 <=>	O19 = -0.530 =>	0%
#8	O17 <=>	O19 = -0.530 =>	0%
#9	O7 <=>	O15 = -0.529 =>	0%
#10	O13 <=>	O15 = -0.529 =>	0%
#11	Ti4 <=>	Ti4 = +2.493 =>	0%
#12	Ti2 <=>	Ti4 = +2.493 =>	0%
#13	O4 <=>	O16 = -0.629 =>	0%
#14	O10 <=>	O16 = -0.629 =>	0%
#15	O16 <=>	O14 = -0.489 =>	0%
#16	O3 <=>	O14 = -0.489 =>	0%
#17	O15 <=>	O11 = -0.490 =>	0%
#18	O1 <=>	O11 = -0.490 =>	0%
#19	O19 <=>	O12 = -0.241 =>	1%
#20	O18 <=>	O12 = -0.241 =>	1%
#21	O14 <=>	O17 = -0.439 =>	1%
#22	O8 <=>	O17 = -0.439 =>	1%
#23	H48 <=>	H49 = +0.066 =>	1%
#24	H21 <=>	H49 = +0.066 =>	1%
#25	C3 <=>	C37 = -0.058 =>	1%
#26	C20 <=>	C37 = -0.058 =>	1%
#27	C5 <=>	C52 = +0.053 =>	1%

#28	C36 <=>	C52 = +0.053 =>	1%
#29	C1 <=>	C28 = +0.054 =>	1%
#30	C18 <=>	C28 = +0.054 =>	1%
#31	O21 <=>	O23 = -0.243 =>	1%
#32	O22 <=>	O23 = -0.243 =>	1%
#33	C2 <=>	C36 = -0.068 =>	1%
#34	C19 <=>	C36 = -0.068 =>	1%
#35	O24 <=>	O24 = -0.273 =>	2%
#36	O23 <=>	O24 = -0.273 =>	2%
#37	C34 <=>	C44 = -0.169 =>	2%
#38	C49 <=>	C44 = -0.169 =>	2%
#39	C26 <=>	C50 = -0.059 =>	2%
#40	C52 <=>	C50 = -0.059 =>	2%
#41	C4 <=>	C46 = -0.061 =>	3%
#42	C35 <=>	C46 = -0.061 =>	3%
#43	C12 <=>	C32 = -0.060 =>	3%
#44	C43 <=>	C32 = -0.060 =>	3%
#45	O20 <=>	O18 = -0.256 =>	3%
#46	O11 <=>	O18 = -0.256 =>	3%
#47	C41 <=>	C30 = -0.057 =>	3%
#48	C10 <=>	C30 = -0.057 =>	3%
#49	H23 <=>	H54 = +0.073 =>	4%
#50	H40 <=>	H54 = +0.073 =>	4%
#51	C23 <=>	C47 = -0.020 =>	4%
#52	C38 <=>	C47 = -0.020 =>	4%
#53	C24 <=>	C48 = -0.056 =>	4%
#54	C50 <=>	C48 = -0.056 =>	4%
#55	H3 <=>	H37 = +0.092 =>	4%
#56	H18 <=>	H37 = +0.092 =>	4%
#57	H2 <=>	H36 = +0.039 =>	4%
#58	H17 <=>	H36 = +0.039 =>	4%
#59	C62 <=>	C53 = -0.169 =>	5%
#60	C48 <=>	C53 = -0.169 =>	5%
#61	H47 <=>	H48 = +0.066 =>	5%
#62	C59 <=>	C63 = +0.066 =>	5%
#63	C55 <=>	C63 = +0.066 =>	5%
#64	H20 <=>	H48 = +0.066 =>	5%
#65	C29 <=>	C41 = -0.056 =>	5%
#66	C33 <=>	C41 = -0.056 =>	5%
#67	C6 <=>	C45 = -0.059 =>	5%
#68	C17 <=>	C45 = -0.059 =>	5%
#69	H53 <=>	H51 = +0.080 =>	5%
#70	H42 <=>	H51 = +0.080 =>	5%
#71	C46 <=>	C54 = -0.027 =>	6%
#72	C28 <=>	C54 = -0.027 =>	6%
#73	C44 <=>	C39 = -0.055 =>	7%
#74	C15 <=>	C39 = -0.055 =>	7%
#75	C31 <=>	C35 = -0.169 =>	7%
#76	C53 <=>	C35 = -0.169 =>	7%
#77	H39 <=>	H53 = +0.072 =>	8%
#78	H22 <=>	H53 = +0.072 =>	8%
#79	C56 <=>	C64 = +0.097 =>	10%
#80	C60 <=>	C64 = +0.097 =>	10%
#81	C54 <=>	C62 = +0.063 =>	10%
#82	C58 <=>	C62 = +0.063 =>	10%
#83	H5 <=>	H46 = +0.089 =>	11%
#84	H32 <=>	H46 = +0.089 =>	11%

#85	H30 <=>	H42 = +0.082 =>	11%
#86	H45 <=>	H42 = +0.082 =>	11%
#87	H13 <=>	H39 = +0.066 =>	11%
#88	H38 <=>	H39 = +0.066 =>	11%
#89	H31 <=>	H43 = +0.073 =>	13%
#90	H46 <=>	H43 = +0.073 =>	13%
#91	H29 <=>	H41 = +0.076 =>	15%
#92	H44 <=>	H41 = +0.076 =>	15%
#93	H10 <=>	H31 = +0.075 =>	16%
#94	H35 <=>	H31 = +0.075 =>	16%
#95	H36 <=>	H28 = +0.069 =>	16%
#96	H11 <=>	H28 = +0.069 =>	16%
#97	C37 <=>	C33 = -0.027 =>	17%
#98	C8 <=>	C33 = -0.027 =>	17%
#99	C22 <=>	C43 = +0.020 =>	17%
#100	C14 <=>	C43 = +0.020 =>	17%
#101	H8 <=>	H45 = +0.073 =>	18%
#102	H15 <=>	H45 = +0.073 =>	18%
#103	H4 <=>	H38 = +0.043 =>	19%
#104	H19 <=>	H38 = +0.043 =>	19%
#105	H25 <=>	H32 = +0.076 =>	19%
#106	H49 <=>	H32 = +0.076 =>	19%
#107	H9 <=>	H30 = +0.080 =>	19%
#108	H34 <=>	H30 = +0.080 =>	19%
#109	H28 <=>	H40 = +0.061 =>	19%
#110	H24 <=>	H40 = +0.061 =>	19%
#111	C9 <=>	C34 = -0.028 =>	20%
#112	C40 <=>	C34 = -0.028 =>	20%
#113	H1 <=>	H35 = +0.040 =>	21%
#114	H16 <=>	H35 = +0.040 =>	21%
#115	H7 <=>	H44 = +0.040 =>	22%
#116	H14 <=>	H44 = +0.040 =>	22%
#117	H52 <=>	H50 = +0.076 =>	22%
#118	H41 <=>	H50 = +0.076 =>	22%
#119	C16 <=>	C42 = -0.027 =>	24%
#120	C21 <=>	C42 = -0.027 =>	24%
#121	H6 <=>	H47 = +0.039 =>	25%
#122	H33 <=>	H47 = +0.039 =>	25%
#123	C39 <=>	C29 = +0.005 =>	26%
#124	C7 <=>	C29 = +0.005 =>	26%
#125	H54 <=>	H52 = +0.073 =>	29%
#126	H43 <=>	H52 = +0.073 =>	29%
#127	H26 <=>	H33 = +0.077 =>	29%
#128	H50 <=>	H33 = +0.077 =>	29%
#129	H51 <=>	H34 = +0.073 =>	34%
#130	H27 <=>	H34 = +0.073 =>	34%
#131	C13 <=>	C38 = -0.018 =>	34%
#132	C30 <=>	C38 = -0.018 =>	34%
#133	H37 <=>	H29 = +0.058 =>	36%
#134	H12 <=>	H29 = +0.058 =>	36%
#135	C57 <=>	C65 = +0.015 =>	41%
#136	C61 <=>	C65 = +0.015 =>	41%
#137	C45 <=>	C51 = -0.001 =>	51%
#138	C27 <=>	C51 = -0.001 =>	51%
#139	C32 <=>	C40 = -0.001 =>	117%
#140	C47 <=>	C40 = -0.001 =>	117%
#141	C11 <=>	C31 = -0.004 =>	185%

#142	C42 <=>	C31 = -0.004 =>	185%
#143	C25 <=>	C49 = -0.004 =>	254%
#144	C51 <=>	C49 = -0.004 =>	254%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -141.798 eV = -13681.3 kJ.mol⁻¹

WinPacha retrosynthetic report for A (2S [#2]

Current molecular fragment is: [H27C28O10Cl3Ti2]*2 = 1451.32 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O12 <=>	O13 = -0.660 =>	0%
#2	O2 <=>	O13 = -0.660 =>	0%
#3	O7 <=>	O15 = -0.528 =>	0%
#4	O13 <=>	O15 = -0.528 =>	0%
#5	C2 <=>	C36 = -0.069 =>	0%
#6	C19 <=>	C36 = -0.069 =>	0%
#7	O9 <=>	O19 = -0.530 =>	0%
#8	O17 <=>	O19 = -0.530 =>	0%
#9	O16 <=>	O14 = -0.489 =>	0%
#10	O3 <=>	O14 = -0.489 =>	0%
#11	O5 <=>	O20 = -0.859 =>	0%
#12	O6 <=>	O20 = -0.859 =>	0%
#13	O10 <=>	O16 = -0.629 =>	0%
#14	O4 <=>	O16 = -0.629 =>	0%
#15	H40 <=>	H54 = +0.075 =>	0%
#16	H23 <=>	H54 = +0.075 =>	0%
#17	Ti4 <=>	Ti4 = +2.487 =>	0%
#18	Ti2 <=>	Ti4 = +2.487 =>	0%
#19	O15 <=>	O11 = -0.491 =>	1%
#20	O1 <=>	O11 = -0.491 =>	1%
#21	C4 <=>	C46 = -0.062 =>	1%
#22	C35 <=>	C46 = -0.062 =>	1%
#23	Ti3 <=>	Ti3 = +2.181 =>	1%
#24	Ti1 <=>	Ti3 = +2.181 =>	1%
#25	C49 <=>	C44 = -0.175 =>	1%
#26	C34 <=>	C44 = -0.175 =>	1%
#27	H17 <=>	H36 = +0.041 =>	1%
#28	H2 <=>	H36 = +0.041 =>	1%
#29	C36 <=>	C52 = +0.052 =>	1%
#30	C5 <=>	C52 = +0.052 =>	1%
#31	C20 <=>	C37 = -0.059 =>	1%
#32	C3 <=>	C37 = -0.059 =>	1%
#33	H42 <=>	H51 = +0.085 =>	1%
#34	H53 <=>	H51 = +0.085 =>	1%
#35	O14 <=>	O17 = -0.440 =>	1%
#36	O8 <=>	O17 = -0.440 =>	1%
#37	H47 <=>	H48 = +0.067 =>	3%
#38	H20 <=>	H48 = +0.067 =>	3%
#39	C10 <=>	C30 = -0.060 =>	3%
#40	C41 <=>	C30 = -0.060 =>	3%
#41	C26 <=>	C50 = -0.058 =>	3%
#42	C52 <=>	C50 = -0.058 =>	3%
#43	O11 <=>	O18 = -0.255 =>	3%
#44	O20 <=>	O18 = -0.255 =>	3%
#45	H29 <=>	H41 = +0.086 =>	3%

#46	H44 <=>	H41 = +0.086 =>	3%
#47	C48 <=>	C53 = -0.171 =>	3%
#48	C62 <=>	C53 = -0.171 =>	3%
#49	H45 <=>	H42 = +0.096 =>	4%
#50	H30 <=>	H42 = +0.096 =>	4%
#51	H31 <=>	H43 = +0.081 =>	4%
#52	H46 <=>	H43 = +0.081 =>	4%
#53	C15 <=>	C18 = -0.120 =>	4%
#54	C12 <=>	C18 = -0.120 =>	4%
#55	C46 <=>	C54 = -0.028 =>	5%
#56	C28 <=>	C54 = -0.028 =>	5%
#57	C12 <=>	C32 = -0.061 =>	5%
#58	C43 <=>	C32 = -0.061 =>	5%
#59	O19 <=>	O12 = -0.255 =>	5%
#60	O18 <=>	O12 = -0.255 =>	5%
#61	C24 <=>	C48 = -0.056 =>	5%
#62	C50 <=>	C48 = -0.056 =>	5%
#63	C6 <=>	C45 = -0.059 =>	5%
#64	C17 <=>	C45 = -0.059 =>	5%
#65	C31 <=>	C35 = -0.171 =>	6%
#66	C53 <=>	C35 = -0.171 =>	6%
#67	C9 <=>	C34 = -0.032 =>	6%
#68	C40 <=>	C34 = -0.032 =>	6%
#69	H13 <=>	H39 = +0.070 =>	6%
#70	H38 <=>	H39 = +0.070 =>	6%
#71	C14 <=>	C17 = -0.133 =>	6%
#72	C11 <=>	C17 = -0.133 =>	6%
#73	H3 <=>	H37 = +0.094 =>	6%
#74	H18 <=>	H37 = +0.094 =>	6%
#75	C64 <=>	C61 = +0.087 =>	9%
#76	C63 <=>	C61 = +0.087 =>	9%
#77	H48 <=>	H49 = +0.071 =>	9%
#78	H21 <=>	H49 = +0.071 =>	9%
#79	C1 <=>	C28 = +0.049 =>	10%
#80	C18 <=>	C28 = +0.049 =>	10%
#81	C38 <=>	C47 = -0.021 =>	10%
#82	C23 <=>	C47 = -0.021 =>	10%
#83	C29 <=>	C41 = -0.059 =>	10%
#84	C33 <=>	C41 = -0.059 =>	10%
#85	H5 <=>	H46 = +0.090 =>	10%
#86	H32 <=>	H46 = +0.090 =>	10%
#87	C16 <=>	C19 = -0.119 =>	10%
#88	C13 <=>	C19 = -0.119 =>	10%
#89	C44 <=>	C39 = -0.058 =>	12%
#90	C15 <=>	C39 = -0.058 =>	12%
#91	H4 <=>	H38 = +0.046 =>	13%
#92	H19 <=>	H38 = +0.046 =>	13%
#93	H28 <=>	H40 = +0.065 =>	14%
#94	H24 <=>	H40 = +0.065 =>	14%
#95	H25 <=>	H32 = +0.080 =>	14%
#96	H49 <=>	H32 = +0.080 =>	14%
#97	H8 <=>	H45 = +0.075 =>	15%
#98	H15 <=>	H45 = +0.075 =>	15%
#99	H10 <=>	H31 = +0.076 =>	16%
#100	H35 <=>	H31 = +0.076 =>	16%
#101	H22 <=>	H53 = +0.077 =>	16%
#102	H39 <=>	H53 = +0.077 =>	16%

#103	H9 <=>	H30 = +0.082 =>	16%
#104	H34 <=>	H30 = +0.082 =>	16%
#105	H36 <=>	H28 = +0.068 =>	17%
#106	H11 <=>	H28 = +0.068 =>	17%
#107	H41 <=>	H50 = +0.080 =>	18%
#108	H52 <=>	H50 = +0.080 =>	18%
#109	H1 <=>	H35 = +0.042 =>	18%
#110	H16 <=>	H35 = +0.042 =>	18%
#111	H6 <=>	H47 = +0.042 =>	20%
#112	H33 <=>	H47 = +0.042 =>	20%
#113	C37 <=>	C33 = -0.029 =>	23%
#114	C8 <=>	C33 = -0.029 =>	23%
#115	H43 <=>	H52 = +0.079 =>	24%
#116	H54 <=>	H52 = +0.079 =>	24%
#117	H26 <=>	H33 = +0.081 =>	26%
#118	H50 <=>	H33 = +0.081 =>	26%
#119	H51 <=>	H34 = +0.078 =>	29%
#120	H27 <=>	H34 = +0.078 =>	29%
#121	H7 <=>	H44 = +0.037 =>	29%
#122	H14 <=>	H44 = +0.037 =>	29%
#123	C14 <=>	C43 = +0.016 =>	32%
#124	C22 <=>	C43 = +0.016 =>	32%
#125	H37 <=>	H29 = +0.060 =>	34%
#126	H12 <=>	H29 = +0.060 =>	34%
#127	C16 <=>	C42 = -0.030 =>	38%
#128	C21 <=>	C42 = -0.030 =>	38%
#129	C13 <=>	C38 = -0.021 =>	53%
#130	C30 <=>	C38 = -0.021 =>	53%
#131	C45 <=>	C51 = -0.000 =>	82%
#132	C27 <=>	C51 = -0.000 =>	82%
#133	C47 <=>	C40 = -0.001 =>	116%
#134	C32 <=>	C40 = -0.001 =>	116%
#135	C25 <=>	C49 = -0.002 =>	123%
#136	C51 <=>	C49 = -0.002 =>	123%
#137	C39 <=>	C29 = -0.002 =>	127%
#138	C7 <=>	C29 = -0.002 =>	127%
#139	C11 <=>	C31 = -0.005 =>	194%
#140	C42 <=>	C31 = -0.005 =>	194%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -140.688 eV = -13574.2 kJ.mol⁻¹

WinPacha retrosynthetic report for A (free) [#2]

Current molecular fragment is: [H27C27O10Ti2]*2 = 1214.60 g.mol⁻¹

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O12 <=>	O13 = -0.660 =>	0%
#2	O2 <=>	O13 = -0.660 =>	0%
#3	O17 <=>	O19 = -0.531 =>	0%
#4	O9 <=>	O19 = -0.531 =>	0%
#5	O16 <=>	O14 = -0.491 =>	0%
#6	O3 <=>	O14 = -0.491 =>	0%
#7	O13 <=>	O15 = -0.529 =>	0%
#8	O7 <=>	O15 = -0.529 =>	0%
#9	O5 <=>	O20 = -0.859 =>	0%
#10	O6 <=>	O20 = -0.859 =>	0%

#11	O4 <=>	O16 = -0.629 =>	0%
#12	O10 <=>	O16 = -0.629 =>	0%
#13	C3 <=>	C37 = -0.059 =>	0%
#14	C20 <=>	C37 = -0.059 =>	0%
#15	O11 <=>	O18 = -0.262 =>	1%
#16	O20 <=>	O18 = -0.262 =>	1%
#17	Ti4 <=>	Ti4 = +2.482 =>	1%
#18	Ti2 <=>	Ti4 = +2.482 =>	1%
#19	O15 <=>	O11 = -0.491 =>	1%
#20	O1 <=>	O11 = -0.491 =>	1%
#21	C2 <=>	C36 = -0.068 =>	1%
#22	C19 <=>	C36 = -0.068 =>	1%
#23	Ti3 <=>	Ti3 = +2.177 =>	1%
#24	Ti1 <=>	Ti3 = +2.176 =>	1%
#25	H18 <=>	H37 = +0.087 =>	1%
#26	H3 <=>	H37 = +0.087 =>	1%
#27	C52 <=>	C50 = -0.061 =>	1%
#28	C26 <=>	C50 = -0.061 =>	1%
#29	C4 <=>	C46 = -0.061 =>	2%
#30	C35 <=>	C46 = -0.061 =>	2%
#31	O8 <=>	O17 = -0.442 =>	2%
#32	O14 <=>	O17 = -0.442 =>	2%
#33	H22 <=>	H53 = +0.068 =>	3%
#34	H39 <=>	H53 = +0.068 =>	3%
#35	C34 <=>	C44 = -0.167 =>	4%
#36	C49 <=>	C44 = -0.167 =>	4%
#37	C46 <=>	C54 = -0.028 =>	4%
#38	C28 <=>	C54 = -0.028 =>	4%
#39	H21 <=>	H49 = +0.062 =>	5%
#40	H48 <=>	H49 = +0.062 =>	5%
#41	C36 <=>	C52 = +0.050 =>	5%
#42	C5 <=>	C52 = +0.050 =>	5%
#43	H40 <=>	H54 = +0.071 =>	6%
#44	H23 <=>	H54 = +0.071 =>	6%
#45	C62 <=>	C53 = -0.167 =>	6%
#46	C48 <=>	C53 = -0.167 =>	6%
#47	C9 <=>	C34 = -0.032 =>	6%
#48	C40 <=>	C34 = -0.032 =>	6%
#49	H2 <=>	H36 = +0.038 =>	6%
#50	H17 <=>	H36 = +0.038 =>	6%
#51	C41 <=>	C30 = -0.063 =>	6%
#52	C10 <=>	C30 = -0.063 =>	6%
#53	C6 <=>	C45 = -0.058 =>	7%
#54	C17 <=>	C45 = -0.058 =>	7%
#55	O19 <=>	O12 = -0.259 =>	7%
#56	O18 <=>	O12 = -0.259 =>	7%
#57	C12 <=>	C32 = -0.063 =>	8%
#58	C43 <=>	C32 = -0.063 =>	8%
#59	C53 <=>	C35 = -0.167 =>	8%
#60	C31 <=>	C35 = -0.167 =>	8%
#61	C24 <=>	C48 = -0.058 =>	9%
#62	C50 <=>	C48 = -0.058 =>	9%
#63	H47 <=>	H48 = +0.061 =>	11%
#64	H20 <=>	H48 = +0.061 =>	11%
#65	C1 <=>	C28 = +0.047 =>	13%
#66	C18 <=>	C28 = +0.047 =>	13%
#67	H53 <=>	H51 = +0.073 =>	13%

#68	H42 <=>	H51 = +0.073 =>	13%
#69	H5 <=>	H46 = +0.086 =>	15%
#70	H32 <=>	H46 = +0.086 =>	15%
#71	C33 <=>	C41 = -0.062 =>	15%
#72	C29 <=>	C41 = -0.062 =>	15%
#73	H31 <=>	H43 = +0.069 =>	18%
#74	H46 <=>	H43 = +0.069 =>	18%
#75	C44 <=>	C39 = -0.061 =>	18%
#76	C15 <=>	C39 = -0.061 =>	18%
#77	H13 <=>	H39 = +0.060 =>	19%
#78	H38 <=>	H39 = +0.060 =>	19%
#79	H4 <=>	H38 = +0.043 =>	20%
#80	H19 <=>	H38 = +0.043 =>	20%
#81	H9 <=>	H30 = +0.079 =>	20%
#82	H34 <=>	H30 = +0.079 =>	20%
#83	H29 <=>	H41 = +0.070 =>	21%
#84	H44 <=>	H41 = +0.070 =>	21%
#85	H8 <=>	H45 = +0.069 =>	22%
#86	H15 <=>	H45 = +0.069 =>	22%
#87	H10 <=>	H31 = +0.069 =>	23%
#88	H35 <=>	H31 = +0.069 =>	23%
#89	H30 <=>	H42 = +0.071 =>	23%
#90	H45 <=>	H42 = +0.071 =>	23%
#91	C38 <=>	C47 = -0.024 =>	24%
#92	C23 <=>	C47 = -0.024 =>	24%
#93	H1 <=>	H35 = +0.038 =>	24%
#94	H16 <=>	H35 = +0.038 =>	24%
#95	H25 <=>	H32 = +0.070 =>	25%
#96	H49 <=>	H32 = +0.070 =>	25%
#97	H36 <=>	H28 = +0.061 =>	26%
#98	H11 <=>	H28 = +0.061 =>	26%
#99	H28 <=>	H40 = +0.056 =>	26%
#100	H24 <=>	H40 = +0.056 =>	26%
#101	H41 <=>	H50 = +0.071 =>	27%
#102	H52 <=>	H50 = +0.071 =>	27%
#103	H6 <=>	H47 = +0.038 =>	27%
#104	H33 <=>	H47 = +0.038 =>	27%
#105	H54 <=>	H52 = +0.070 =>	33%
#106	H43 <=>	H52 = +0.070 =>	33%
#107	C37 <=>	C33 = -0.031 =>	33%
#108	C8 <=>	C33 = -0.031 =>	33%
#109	H26 <=>	H33 = +0.070 =>	36%
#110	H50 <=>	H33 = +0.070 =>	36%
#111	H51 <=>	H34 = +0.069 =>	37%
#112	H27 <=>	H34 = +0.069 =>	37%
#113	H7 <=>	H44 = +0.032 =>	38%
#114	H14 <=>	H44 = +0.032 =>	38%
#115	H37 <=>	H29 = +0.055 =>	40%
#116	H12 <=>	H29 = +0.055 =>	40%
#117	C14 <=>	C43 = +0.014 =>	40%
#118	C22 <=>	C43 = +0.014 =>	40%
#119	C21 <=>	C42 = -0.033 =>	54%
#120	C16 <=>	C42 = -0.033 =>	54%
#121	C27 <=>	C51 = -0.005 =>	64%
#122	C45 <=>	C51 = -0.005 =>	64%
#123	C13 <=>	C38 = -0.025 =>	79%
#124	C30 <=>	C38 = -0.025 =>	79%

#125	C39 <=>	C29 = -0.005 =>	174%
#126	C7 <=>	C29 = -0.005 =>	174%
#127	C32 <=>	C40 = -0.009 =>	209%
#128	C47 <=>	C40 = -0.009 =>	209%
#129	C42 <=>	C31 = -0.009 =>	289%
#130	C11 <=>	C31 = -0.009 =>	289%
#131	C25 <=>	C49 = -0.007 =>	634%
#132	C51 <=>	C49 = -0.007 =>	634%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -139.577 eV = -13467.0 kJ.mol-1

WinPacha retrosynthetic report for B (free) [#2]

Current molecular fragment is: [C2O]*2 = 80.04 g.mol-1

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	O2 <=>	O24 = -0.242 =>	10%
#2	O1 <=>	O23 = -0.212 =>	14%
#3	C4 <=>	C64 = +0.149 =>	38%
#4	C3 <=>	C63 = +0.109 =>	72%
#5	C1 <=>	C62 = +0.120 =>	108%
#6	C2 <=>	C65 = +0.077 =>	195%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -0.851 eV = -82.1 kJ.mol-1

WinPacha retrosynthetic report for S (free) [#2]

Current molecular fragment is: [CCl3]*1 = 118.36 g.mol-1

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	C1 <=>	C61 = +0.116 =>	22%
#2	Cl2 <=>	Cl8 = -0.037 =>	68%
#3	Cl3 <=>	Cl9 = -0.038 =>	71%
#4	Cl1 <=>	Cl7 = -0.040 =>	71%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -0.090 eV = -8.6 kJ.mol-1

WinPacha retrosynthetic report for S (free) [#3]

Current molecular fragment is: [CCl3]*1 = 118.36 g.mol-1

#n Mol symb <=> Net symb = fragment PC => Retrosynthetic index(%)

#1	C1 <=>	C60 = +0.115 =>	54%
#2	Cl1 <=>	Cl4 = -0.039 =>	71%
#3	Cl2 <=>	Cl5 = -0.038 =>	72%
#4	Cl3 <=>	Cl6 = -0.038 =>	74%

*** Total electrical charge on molecular fragment = 0 ***

Partial electrostatic balance: <EB> = -0.086 eV = -8.3 kJ.mol-1