Electronic supplementary materials *Mendeleev Commun.*, 2020, **30**, 91–93

Fullerene compounds with general formulae $C_{60}O_x$ (x = 1–3): isomerism, stability and polarizability

Denis Sh. Sabirov

Computational details

The Perdew–Burke–Ernzerhof (PBE) density functional theory method with the 3ζ split-valence basis set was used in the computations. The orbital basis sets for calculating the electronic configurations of C and O atoms in the PBE/3ζ method are following:

(a) contracted Gaussian-type functions: (11*s*6*p*2*d*)/[6*s*3*p*2*d*];
(b) uncontracted Gaussian-type functions: 10*s*3*p*3*d*1*f*.

After DFT-optimization and vibration modes solving (to prove that all the stationary points, respective to the molecules under study, are minima of the potential energy surfaces) using standard techniques, the components of polarizability tensors **α** were calculated in terms of the finite field approach as the second order derivatives of the total energy *E* with respect to the homogenous external electric field ***F***:

$$\alpha_{ij} = -\frac{\partial^2 E}{\partial F_i \partial F_j} .$$

Tensors **α** were calculated in the arbitrary coordinate system and then diagonalized. Their eigenvalues were used for the calculation of the mean polarizabilities:

$$\alpha = \frac{1}{3}\left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right).$$

Table S1 The energy effects of reactions (1) and mean polarizabilities of the formed $C_{60}O_2$ diepoxides*†

Regioisomer	**Δ*E* / kJ mol^{-1}**	**α / Å^3**
cis-1	**–133.4**	83.67
cis-2	**–103.9**	83.79
cis-3	–108.7	83.79
e	–116.3	83.73
trans-1	–113.6	**83.64**
trans-2	–114.7	83.76
trans-3	–115.3	83.80
trans-4	–113.5	83.68

* Hereinafter, blue and orange colorings correspond respectively to highest and lowest absolute values of the quantities.

† Schematic indication of the second oxygen position

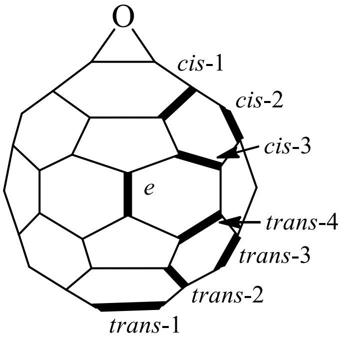

Table S2 The energy effects of reactions (1) and mean polarizabilities of the formed $C_{60}O_3$ epoxy diketones*

Regioisomer	**ΔE / kJ mol^{-1}**	**α / Å^3**
cis-1	**−220.0**	86.44
cis-2	**−175.5**	**86.75**
cis-3	−179.7	86.63
e_{edge}	−191.5	86.59
e_{face}	−188.2	86.65
trans-1	−182.5	**86.36**
trans-2	−186.0	86.64
trans-3	−188.0	86.70
trans-4	−179.7	86.50

* Schematic indication of the epoxide oxygen position

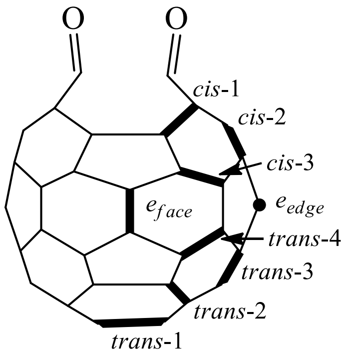

Table S3 The energy effects of reactions (1) and mean polarizabilities of the formed $C_{60}O_3$ epoxy dioxetanes*

Regioisomer	**Δ*E* / kJ mol^{-1}**	**α / Å^3**
cis-1	**−71.8**	**84.92**
cis-2	**−40.2**	**85.22**
cis-3	−40.6	85.15
e_{edge}	−50.2	85.09
e_{face}	−50.6	85.12
trans-1	−45.8	84.94
trans-2	−47.2	85.14
trans-3	−48.5	85.19
trans-4	−45.9	85.02

* Schematic indication of the epoxide oxygen position

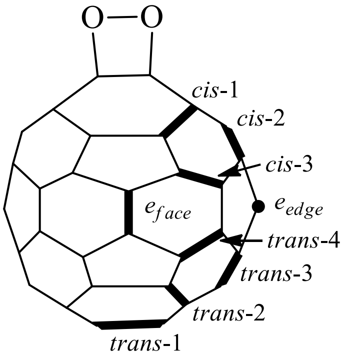

Table S4 The energy effects of reactions (1) and mean polarizabilities of the formed $C_{60}O_3$ triepoxides

Regioisomer designation by three functionalized 6,6 bonds*	**Δ*E* / kJ mol^{-1}**	**α / Å^3**
(1,2) (3,5) (4,6)	**−216.8**	84.18
(1,2) (3,5) (7,9)	−202.8	84.06
(1,2) (3,5) (8,10)	−206.7	84.05
(1,2) (3,5) (11,13)	−177.0	84.18
(1,2) (3,5) (12,14)	−180.8	84.21
(1,2) (3,5) (15,16)	−190.2	84.09
(1,2) (3,5) (17,19)	−190.6	84.26
(1,2) (3,5) (18,20)	−190.5	84.22
(1,2) (3,5) (25,27)	−164.4	84.26
(1,2) (3,5) (30,32)	−192.7	84.17
(1,2) (3,5) (31,33)	−189.8	84.14
(1,2) (3,5) (35,49)	−188.3	84.14
(1,2) (3,5) (22,50)	−188.7	84.08
(1,2) (3,5) (55,56)	−184.7	84.21
(1,2) (3,5) (58,59)	−183.5	84.19
(1,2) (3,5) (52,60)	−190.1	84.15
(1,2) (15,16) (30,32)	−173.6	84.28
(1,2) (15,16) (23,36)	−172.8	84.08
(1,2) (15,16) (34,38)	−171.3	84.14
(1,2) (15,16) (41,42)	−176.1	84.20
(1,2) (15,16) (40,48)	−172.5	84.21
(1,2) (17,19) (30,32)	−171.7	84.27
(1,2) (17,19) (31,33)	−173.3	84.39
(1,2) (24,26) (11,13)	**−146.3**	84.23
(1,2) (24,26) (12,14)	−149.5	84.34
(1,2) (24,26) (15,16)	−161.5	84.23
(1,2) (24,26) (17,19)	−160.8	84.34
(1,2) (24,26) (18,20)	−159.8	84.21
(1,2) (24,26) (45,39)	−158.5	84.13
(1,2) (24,26) (46,47)	−155.8	84.34
(1,2) (24,26) (22,50)	−159.6	84.28
(1,2) (24,26) (55,56)	−147.6	**84.41**
(1,2) (24,26) (51,57)	−161.8	84.19
(1,2) (24,26) (58,59)	−156.0	84.39
(1,2) (24,26) (52,60)	−159.5	84.24
(1,2) (21,37) (51,57)	−169.4	84.14
(1,2) (43,44) (15,16)	−168.0	84.32
(1,2) (43,44) (17,19)	−164.9	84.27
(1,2) (43,44) (18,20)	−165.8	84.34
(1,2) (43,44) (21,37)	−167.2	84.27
(1,2) (43,44) (22,50)	−165.9	84.36
(1,2) (43,44) (55,56)	−158.9	84.26
(1,2) (43,44) (58,59)	−161.0	84.36
(1,2) (43,44) (52,60)	−164.0	84.16

(1,2) (39,45) (52,60)	–167.9	**84.03**

* Atom numbering used in the present work for automatically generating the triepoxide structures