УДК 547.854.83:544.183.25
ББК 24.5

QUANTUMCHEMICAL CALCULATION OF SOME DIOLS BY METHOD MNDO

Babkin Vladimir Aleksandrovich

Doctor of chemical sciences, professor of chair of mathematics and natural-science disciplines
Sebryakovsky branch of the Volgograd State Architectural and Construction University,
academician of the international academy of Sciences of "Kontenant"
Babkin_v.a@mail.ru
Michurina St. 21, 403343 Mikhailovka, Russian Federation

Ignatov Alexey Viktorovich

Student of Sebryakovsky branch
Volgograd State Architectural and Construction University
Babkin_v.a@mail.ru
Michurina St. 21, 403343 Mikhailovka, Russian Federation

Zakharov Dmitry Sergeyevich

Student of Sebryakovsky branch
Volgograd State Architectural and Construction University
Babkin_v.a@mail.ru
Michurina St. 21, 403343 Mikhailovka, Russian Federation

Zaikov Gennady Efremovich

Doctor of chemical sciences, Professor, Head of Division of biological and chemical physics
of Polymer of The Federal State Budget Institution
of Science N.M. Emanuel Institute of Biochemical Physics
chembio@sky.chph.ras.ru
Kosygina St. 4, 119334 Moscow, Russian Federation

Fomichev Valery Tarasovich

Doctor of Technical sciences, professor, head of the department of the general and applied chemistry
Volgograd State Architectural and Construction University
valerifomiche@yandex.ru
Akademicheskaia St. 1, 400074 Volgograd, Russian Federation

Belousov Andrey Sergeyevich

Engineer of Lytkarinsky plant of optical glass
referent@lzos.ru
Parkovaia St. 1, 140080 Lytkarino, Russian Federation

Gulyukin Mikhail Nikolaevich

Chief of design-technology bureau
Lytkarinsky plant of optical glass
referent@lzos.ru
Parkovaia St. 1, 140080 Lytkarino, Russian Federation

Ignatov Alexander Nikolaevich

Chief of scientific-industrial complex
Lytkarinsky plant of optical glass, Volgograd State Architecturally Building University,
Sebrykov departament
bartsimpson35@yandex.ru
Parkovaia St. 1, 140080 Lytkarino, Russian Federation

Titova Evgenia Stanislavovna

Candidate of chemical sciences, associate professor
Volgograd State Technical University
Babkin_v.a@mail.ru
Prospect Lenina, 28, 400005 Volgograd, Russian Federation

Abstract. Quantum chemical calculation of the molecules of 3,5-di(cyclo-trialumoxandiol)tetraalumoxantetraol-1,1,7,7and 1,7-di(cyclotrialumoxandiol)tetraalumoxantetraol-1,3,5,7 is executed for the first time by method MNDO with optimization of geometry on all parameters by standardgradient method. The optimized geometrical and electronic structure of these compounds is received. Acid force of 3,5-di(cyclo-trialumoxandiol) tetraalumoxantetraol-1,1,7,7and 1,7-di(cyclotrialumoxandiol)tetraalumoxantetraol-1,3,5,7 is theoretically appreciated. It is established, that it to relate to a class of very weak H-acids (pKa=14) where pKa-universal index of acidity).

Key words: quantum chemical calculation, method MNDO,3,5-di(cyclo-trialumoxandiol)tetraalumoxantetraol-1,1,7,7, 1,7-di(cyclotrialumoxandiol)tetraalumoxantetraol-1,3,5,7, acid force.

The Aim of this work is a quantum chemical calculation and theoretically determination of acid force of derivativesdioles3,5-di(cyclotrialumoxandiol) tetraalumoxantetra-ol-1,1,7,7and 1,7-di(cyclo trialumoxan-diol)tetraalumoxantetraol-1,3,5,7 by method MNDO with optimization of geometry on all parameters by standard gradient methodbuilt-in in PC GAMESS [10]. The calculation was executed in approach the insulated molecule in gas phase. Program MacMolPlt was used for visual presentation of models of molecules [9].These compounds can be fragments of polymermodels of optical glasses, such as «low-crownglass» and «heavyflint glass».

Results of the calculation

Optimized geometric and electronic structures, general and electronic energies of molecules3,5-di(cyclotrialumoxandiol)tetra-alumoxantetraol-1,1,7,7and 1,7-di(cyclo-trialumoxandiol)tetraalumoxantetraol-1,3,5,7 were received by method MNDO and are shown on fig. 1,2 and in tabl. 1–3. The universal factor of acidity was calculated for method MNDO by formula: $pKa=42.11-147.18q_{max}^{H+}$[1–8; 11] (where, q_{max}^{H+} " a maximum positive charge on atom of the hydrogenq_{max}^{H+}= 0.19pKa- pKa-universal index of acidity (tabl.1).pKa = 14.

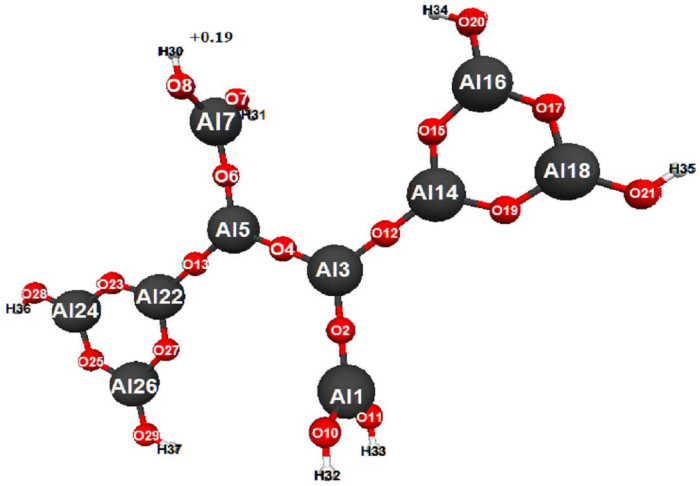

Fig.1. Geometric and electronic structure of molecule of 3,5-di(cyclotrialumoxandiol)tetraalumoxantetraol -1,1,7,7. (E_0 = -651635 kDg/mol, E_{el} = -3331183 kDg/mol)

Table 1

Optimized bond lengths, valence corners and charges on atoms of the molecul of 3,5-di(cyclotrialumoxandiol)tetraalumoxantetraol-1,1,7,7

Length of relations	R,A	Valent corners	Degree	Atom	Charges on atoms of a molecule
O(2)-Al(1)	1.62	Al(1)-O(2)-Al(3)	179	Al(1)	+1.08
Al(3)-O(2)	1.64	O(2)-Al(3)-O(4)	120	O(2)	-0.71
O(4)-Al(3)	1.63	Al(3)-O(4)-Al(5)	179	Al(3)	+1.15
Al(5)-O(4)	1.63	O(4)-Al(5)-O(6)	120	O(4)	-0.74
O(6)-Al(5)	1.64	Al(5)-O(6)-Al(7)	174	Al(5)	+1.15
Al(7)-O(6)	1.62	O(6)-Al(7)-O(8)	121	O(6)	-0.72
O(8)-Al(7)	1.67	O(6)-Al(7)-O(9)	122	Al(7)	+1.07
O(9)-Al(7)	1.68	O(2)-Al(1)-O(10)	120	O(8)	-0.55
O(10)-Al(1)	1.68	O(2)-Al(1)-O(11)	120	O(9)	-0.56
O(11)-Al(1)	1.68	O(2)-Al(3)-O(12)	120	O(10)	-0.56
O(12)-Al(3)	1.64	O(4)-Al(5)-O(13)	121	O(11)	-0.56
O(13)-Al(5)	1.64	Al(3)-O(12)-Al(14)	179	O(12)	-0.72
Al(14)-O(12)	1.62	O(12)-Al(14)-O(15)	126	O(13)	-0.72
O(15)-Al(14)	1.68	Al(14)-O(15)-Al(16)	131	Al(14)	+1.07
Al(16)-O(15)	1.66	O(15)-Al(16)-O(17)	110	O(15)	-0.71
O(17)-Al(16)	1.67	Al(16)-O(17)-Al(18)	129	Al(16)	+1.02
Al(18)-O(17)	1.67	O(17)-Al(18)-O(19)	110	O(17)	-0.70
O(19)-Al(18)	1.66	O(15)-Al(16)-O(20)	125	Al(18)	+1.02
O(20)-Al(16)	1.67	O(17)-Al(18)-O(21)	125	O(19)	-0.70
O(21)-Al(18)	1.67	Al(5)-O(13)-Al(22)	179	O(20)	-0.53
Al(22)-O(13)	1.62	O(13)-Al(22)-O(23)	126	O(21)	-0.53
O(23)-Al(22)	1.67	Al(22)-O(23)-Al(24)	131	Al(22)	+1.07
Al(24)-O(23)	1.66	O(23)-Al(24)-O(25)	110	O(23)	-0.70
O(25)-Al(24)	1.67	Al(24)-O(25)-Al(26)	129	Al(24)	+1.03
Al(26)-O(25)	1.67	O(25)-Al(26)-O(27)	110	O(25)	-0.70
O(27)-Al(26)	1.66	O(23)-Al(24)-O(28)	125	Al(26)	+1.02
O(28)-Al(24)	1.67	O(25)-Al(26)-O(29)	125	O(27)	-0.71
O(29)-Al(26)	1.67	Al(7)-O(8)-H(30)	122	O(28)	-0.53
H(30)-O(8)	0.93	Al(7)-O(9)-H(31)	123	O(29)	-0.53
H(31)-O(9)	0.93	Al(1)-O(10)-H(32)	124	H(30)	+0.19
H(32)-O(10)	0.93	Al(1)-O(11)-H(33)	124	H(31)	+0.19
H(33)-O(11)	0.93	Al(16)-O(20)-H(34)	122	H(32)	+0.18
H(34)-O(20)	0.93	Al(18)-O(21)-H(35)	122	H(33)	+0.18
H(35)-O(21)	0.93	Al(24)-O(28)-H(36)	122	H(34)	+0.19
H(36)-O(28)	0.93	Al(26)-O(29)-H(37)	122	H(35)	+0.19

Table 2

Optimized bond lengths, valence corners and charges on atoms of the molecule of 1,7-di(cyclotrialumoxandiol)tetraalumoxantetraol-1,3,5,7

Length of relations	R,A	Valent corners	Degree	Atom	Charges on atoms of a molecule
O(2)-Al(1)	1.63	Al(1)-O(2)-Al(3)	178	Al(1)	+1.11
Al(3)-O(2)	1.63	O(2)-Al(3)-O(4)	121	O(2)	-0.73
O(4)-Al(3)	1.64	Al(3)-O(4)-Al(5)	170	Al(3)	+1.10
Al(5)-O(4)	1.64	O(4)-Al(5)-O(6)	121	O(4)	-0.74
O(6)-Al(5)	1.63	Al(5)-O(6)-Al(7)	175	Al(5)	+1.10
Al(7)-O(6)	1.64	O(6)-Al(7)-O(8)	121	O(6)	-0.73
O(8)-Al(7)	1.63	O(6)-Al(7)-O(9)	120	Al(7)	+1.11
O(9)-Al(7)	1.68	O(2)-Al(1)-O(10)	121	O(8)	-0.70
O(10)-Al(1)	1.63	O(2)-Al(1)-O(11)	121	O(9)	-0.56
O(11)-Al(1)	1.68	O(2)-Al(3)-O(12)	119	O(10)	-0.70
O(12)-Al(3)	1.68	O(4)-Al(5)-O(13)	120	O(11)	-0.56
O(13)-Al(5)	1.68	Al(1)-O(10)-Al(14)	178	O(12)	-0.56
Al(14)-O(10)	1.62	O(10)-Al(14)-O(15)	126	O(13)	-0.56
O(15)-Al(14)	1.68	Al(14)-O(15)-Al(16)	131	Al(14)	+1.08
Al(16)-O(15)	1.67	O(15)-Al(16)-O(17)	110	O(15)	-0.71
O(17)-Al(16)	1.67	Al(16)-O(17)-Al(18)	130	Al(16)	+1.02
Al(18)-O(17)	1.67	O(17)-Al(18)-O(19)	110	O(17)	-0.70
O(19)-Al(18)	1.66	O(15)-Al(16)-O(20)	125	Al(18)	+1.03
O(20)-Al(16)	1.67	O(17)-Al(18)-O(21)	125	O(19)	-0.70
O(21)-Al(18)	1.67	Al(7)-O(8)-Al(22)	177	O(20)	-0.53
Al(22)-O(8)	1.62	O(8)-Al(22)-O(23)	125	O(21)	-0.53
O(23)-Al(22)	1.67	Al(22)-O(23)-Al(24)	131	Al(22)	+1.08
Al(24)-O(23)	1.66	O(23)-Al(24)-O(25)	110	O(23)	-0.70
O(25)-Al(24)	1.67	Al(24)-O(25)-Al(26)	130	Al(24)	+1.03
Al(26)-O(25)	1.67	O(25)-Al(26)-O(27)	110	O(25)	-0.70
O(27)-Al(26)	1.67	O(23)-Al(24)-O(28)	125	Al(26)	+1.03
O(28)-Al(24)	1.67	O(25)-Al(26)-O(29)	125	O(27)	-0.71
O(29)-Al(26)	1.67	Al(5)-O(13)-H(30)	123	O(28)	-0.53
H(30)-O(13)	0.93	Al(7)-O(9)-H(31)	123	O(29)	-0.53
H(31)-O(9)	0.93	Al(3)-O(12)-H(32)	123	H(30)	+0.18
H(32)-O(12)	0.93	Al(1)-O(11)-H(33)	123	H(31)	+0.18
H(33)-O(11)	0.93	Al(16)-O(20)-H(34)	122	H(32)	+0.18
H(34)-O(20)	0.93	Al(18)-O(21)-H(35)	122	H(33)	+0.19
H(35)-O(21)	0.93	Al(24)-O(28)-H(36)	122	H(34)	+0.19
H(36)-O(28)	0.93	Al(26)-O(29)-H(37)	122	H(35)	+0.19

Table 3

General energy (E_0), electronic energy (E_{el}), maximum positive charge on atom of the hydrogen (q_{max}^{H+}), the universal factor of acidityderivativesdioles-monomersofcationicpolymerization

№	Monomer	E_0kDg/mol	E_{el}= kDg/mol	q_{max}^{H+}	pKa
1	3,5-di(cyclotrialumoxandiol) tetraalumoxantetraol-1,1,7,7	-651 635	-3 331 183	+0,19	14
2	1,7- di cyclotrialumoxandiol) tetraalumoxantetraol -1,3,5,7	-651 646	-3 399 236	+0,19	14

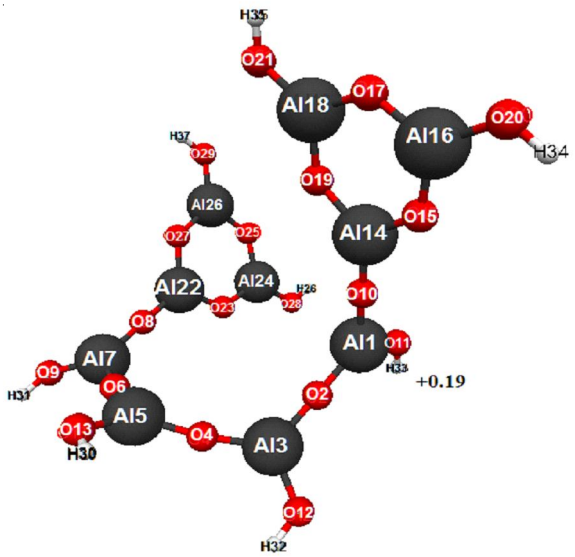

Fig. 2. Geometric and electronic structure of molecule of 1,7-di(cyclotrialumoxandiol) tetraalumoxantetraol-1,3,5,7 (E_0 = -651646 kDg/mol, E_{el} = -3399236 kDg/mol)

Quantum-chemical calculation of molecules 3,5-di(cyclotrialumoxandiol)tetra-alumoxantetraol-1,1,7,7 and 1,7-di(cyclotrialumoxandiol)tetraalumoxantetraol-1,3,5,7 by method MNDO was executed for the first time. Optimized geometric and electronic structures of these compounds were received. Acid power of moleculesterpenes was theoretically evaluated (pKa = 14). These compounds pertain to class of very weak H-acids (pKa = 14).

REFERENCES

1. *Babkin V.A., Andreev D. S., Titova E. S., Dmitriev V.U., Fomichev V.T., Zaikov G. E.* Theoretical Estimation of Acidic Force of Linear Olefins of Cationic Polymerization. N. Y., Nova Publisher, 2011, 65 p.

2. *Babkin V.A., Andreev D.S.* Quantum-chemical calculation of molecule 2-ethylbutene-1 by method MNDO. Collection of research paper: Quantum-chemical calculation of unique molecular systems. Volgograd, VolGU publ., 2010, vol. 1, p. 176-185.

3. *Babkin V.A., Andreev D.S., Fomichev V.T., Dmitriev V.Yu.* Quantum-chemical calculation of linear and branchy monomers of cationic polymerization. Volgograd, VolGU publ., 2011, 65 p.

4. *Babkin V.A., Andreev D.S., Titovav E.S., Sangalov Yu.A., Denisov A.A.* Quantum-chemical calculation of alicyclicolefins and their derivations. Volgograd, VolGU publ., 2012, 100 p.

5. *Babkin V.A., Andreev D.S., Titova E. S., Potapov S.S., Sangalov Yu.A.* Quantum-chemical calculation of isoolefinsanddienes. Volgograd, VolGU publ., 2011, 71 p.

6. *Babkin V.A., Dmitriev V.Yu., Savin G.A., Zaikov G.E., Rakhimov A.I.* Quantum-chemical aspects of mechanism acylation of bicyclophosphits by chloranhydrides of carboxylic acid. Volgograd, VolGU publ., 2011, 91 p.

7. *Babkin V.A., Dmitriev V.Yu., Zaikov G.E.* Quantum-chemical calculation of molecule monomer of cationic polymerizationhexene-1 by method MNDO. Collection of research paper: Quantum-chemical calculation of unique molecular systems. Volgograd, VolGU publ., 2010, vol. 1, p. 93-104.

8. *Babkin V.A., Fedunov R.G., Minsker K.S.* Oxidation communication, 2002, № 1, 25, p. 21-47.

9. *Bode B.M., Gordon M.S., Mol J.* Graphics Mod, 1998, 16, p. 133-138.

10. *Shmidt M.W., Baldrosge K.K., Elbert J.A., Gordon M.S., Enseh J.H., Koseki N., Matsvnaga K.A. Nguyen S.J.* SU, and anothers. *J. Comput. Chem.14*, 1993, p. 1347-1363.

11. *Babkin V.A., Zaikov G.E.* Nobel laureats and nanotechnologgy of the applaed quantum chemistry. USA. N.Y., Nova Science Publisher, 2010, pp. 351

КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ НЕКОТОРЫХ ДИОЛОВ МЕТОДОМ MNDO

Бабкин Владимир Александрович

Доктор химических наук, профессор кафедры математики и естественнонаучных дисциплин
Себряковского филиала Волгоградского государственного архитектурно-строительного
университета, академик международной академии наук «Контенант»
Babkin_v.a@mail.ru
ул. Мичурина, 21, 403343 г. Михайловка, Российская Федерация

Игнатов Алексей Викторович

Студент Себряковского филиала
Волгоградского государственного архитектурно-строительного университета
bartsimpson35@yandex.ru
ул. Мичурина, 21, 403343 г. Михайловка, Российская Федерация

Захаров Дмитрий Сергеевич

Студент Себряковского филиала
Волгоградского государственного архитектурно-строительного университета
Babkin_v.a@mail.ru
ул. Мичурина, 21, 403343 г. Михайловка, Российская Федерация

Заиков Геннадий Ефремович

Доктор химических наук, профессор,
заведующий отделом биологической и химической физики полимеров
Федерального государственного бюджетного учреждения науки
Институт биохимической физики им. Н.М. Эмануэля РАН
chembio@sky.chph.ras.ru
ул. Косыгина, 4, 119334 г. Москва, Российская Федерация

Фомичев Валерий Тарасович

Доктор технических наук, профессор, заведующий кафедрой общей и прикладной химии
Волгоградского государственного архитектурно-строительного университета
Babkin_v.a@mail.ru
ул. Академическая, 1, 400074 г. Волгоград, Российская Федерация

Белоусов Андрей Сергеевич

Инженер Лыткаринского завода оптического стекла
referent@lzos.ru
ул. Парковая, 1, 140080 г. Лыткарино, Российская Федерация

Гулюкин Михаил Николаевич

Начальник конструкторско-технологического бюро
Лыткаринского завода оптического стекла
referent@lzos.ru
ул. Парковая, 1, 140080 г. Лыткарино, Российская Федерация

Игнатов Александр Николаевич

Начальник научно-производственного комплекса
Лыткаринского завода оптического стекла
referent@lzos.ru
ул. Парковая, 1, 140080 г. Лыткарино, Российская Федерация

Титова Евгения Станиславовна

Кандидат химических наук, доцент
Волгоградского государственного технического университета
Babkin_v.a@mail.ru
Проспект Ленина, 28, 400005 г. Волгоград, Российская Федерация

Аннотация. Квантово-химическое вычисление молекул 3,5-di (cyclo-trialumoxandiol) tetraalumoxantetraol-1,1,7,7 и 1,7-di (cyclotrialumoxandiol) tetraalumoxantetraol-1,3,5,7 выполнен впервые методом MNDO с оптимизацией геометрии на всех параметрах предлагаемым методом. Получена оптимизированная геометрическая и электронная структура этих составов. Теоретически оценена кислотная сила 3,5-di (cyclo-trialumoxandiol) tetraalumoxantetraol-1,1,7,7 и 1,7-di (cyclotrialumoxandiol) tetraalumoxantetraol-1,3,5,7. Установлено, что эта молекула относится к классу очень слабых кислот (pKa>14) , где pKa-универсальный индекс кислотности).

Ключевые слова: квантово- химическое вычисление, метод MNDO, 3,5-di (cyclo-trialumoxandiol) tetraalumoxantetraol-1,1,7,7, 1,7-di (cyclotrialumoxandiol) tetraalumoxantetraol-1,3,5,7, кислотная сила.