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QUANTUM-CHEMICAL CALCULATION OF THE MODELS OF DEKACENE AND EICOCENE BY METHOD MNDO WITHIN THE FRAMEWORK OF MOLECULAR GRAPHENE MODEL

Keywords: quantum chemical calculation, method MNDO, dekacene, eicocene, acid strength.

Quantum-chemical calculation of molecules dekacene and eicocene was done by method MNDO. Optimized by all parameters geometric and electronic structures of these compounds was received. Each of these molecular models has a universal factor of acidity equal to 33 (pKa=33). They all pertain to class of very weak H-acids (pKa>14).

Ключевые слова: квантово-химический расчет, метод MNDO, декацен, эйкоцен, кислотная сила.

Впервые выполнен квантово-химический расчет молекул декацена и эйкоцена методом MNDO с оптимизацией геометрии по всем параметрам стандартным градиентным методом Получено оптимизированное геометрическое и электронное строение этих соединений. Теоретически оценена их кислотная сила (pKa=33). Установлено, что эти близкие к графену соединения относятся к классу очень слабых кислот (pKa>14).

Aims and backgrounds

The aim of this work is a study of electronic structure of molecules dekacene, eicocene and theoretical estimation its acid power by quantum-chemical method MNDO within the framework of molecular graphene model, which was dicovered by Novoselov and Game in 2004 [1].

Methodical part

The calculation was done with optimization of all parameters by standard gradient method built-in in PC GAMESS [2]. The calculation was executed in approach the insulated molecule in gas phase. Program MacMolPlt was used for visual presentation of the model of the molecule. [3].

The results of the calculation and discussion

Geometric and electronic structures, general and electronic energies of moleculaes dekacene, eicocene was received by method MNDO and are shown on fig. 1, fig. 2 and in tab.1-3 . The universal factor of acidity was calculated by formula: pKa = 49,4-134,61*$q_{max}H^+$ [4] (where, $q_{max}H^+$ − a maximum positive charge on atom of the hydrogen (by Milliken [1]) R=0.97, R− a coefficient of correlations, q_{max}^{H+}=+0,06). pKa=33. This formula was successfully used in the following articles: [5, 6, 7].

Quantum-chemical calculation of molecules dekacene, eicocene by method MNDO was executed for the first time. Optimized geometric and electronic structures of these compound was received. Acid power of molecules dekacene, eicocene was theoretically evaluated (pKa=33). These compounds pertain to class of very weak H-acids (pKa>14).

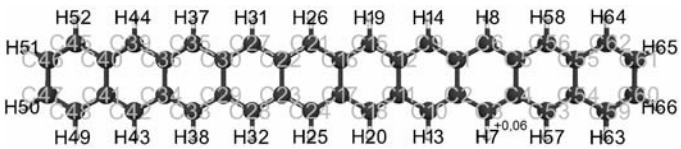

Fig. 1 - Geometric and electronic molecular structure of dekacene.
(E_0= -550105 kDg/mol, E_{el}= -4850841 kDg/mol).

Table 1 - Optimised bond lengths, valent corners and atom charges of dekacene

Bond lengths	R,A	Valent corners	Grad	Atom	Charge (by Milliken)
1	2	3	4	5	6
C(1)-C(2)	1.46	C(3)-C(2)-C(1)	118	C(1)	-0.04
C(2)-C(3)	1.45	C(12)-C(9)-C(1)	122	C(2)	-0.04
C(3)-C(4)	1.38	C(4)-C(3)-C(2)	123	C(3)	-0.02
C(4)-C(5)	1.47	C(9)-C(1)-C(2)	119	C(4)	-0.06
C(5)-C(6)	1.38	C(5)-C(4)-C(3)	119	C(5)	-0.06
C(6)-C(1)	1.45	C(10)-C(2)-C(3)	123	C(6)	-0.02
H(7)-C(3)	1.09	C(6)-C(5)-C(4)	119	H(7)	**0.06**
H(8)-C(6)	1.09	C(54)-C(53)-C(4)	123	H(8)	0.06
C(9)-C(12)	1.44	C(1)-C(6)-C(5)	123	C(9)	-0.02
C(9)-C(1)	1.39	C(53)-C(4)-C(5)	118	C(10)	-0.02
C(10)-C(2)	1.39	C(2)-C(1)-C(6)	118	C(11)	-0.04
C(11)-C(10)	1.44	C(9)-C(1)-C(6)	123	C(12)	-0.04
C(12)-C(11)	1.46	C(4)-C(3)-H(7)	120	H(13)	0.06
H(13)-C(10)	1.38	C(1)-C(6)-H(8)	117	H(14)	0.06
H(14)-C(9)	1.45	C(11)-C(12)-C(9)	118	C(15)	-0.02
C(15)-C(16)	1.42	C(15)-C(12)-C(9)	123	C(16)	-0.04
C(15)-C(12)	1.41	C(1)-C(2)-C(10)	119	C(17)	-0.04
C(16)-C(17)	1.45	C(18)-C(11)-C(10)	123	C(18)	-0.02
C(17)-C(18)	1.42	C(2)-C(10)-C(11)	122	H(19)	0.06
C(18)-C(11)	1.41	C(15)-C(12)-C(11)	119	H(20)	0.06
H(19)-C(15)	1.09	C(10)-C(11)-C(12)	118	C(21)	-0.02
H(20)-C(18)	1.09	C(16)-C(15)-C(12)	122	C(22)	-0.04
C(21)-C(22)	1.41	C(2)-C(10)-H(13)	120	C(23)	-0.04
C(21)-C(16)	1.42	C(12)-C(9)-H(14)	118	C(24)	-0.02
C(22)-C(23)	1.46	C(17)-C(16)-C(15)	119	H(25)	0.06
C(23)-C(24)	1.40	C(21)-C(16)-C(15)	123	H(26)	0.06
C(24)-C(17)	1.42	C(18)-C(17)-C(16)	119	C(27)	-0.02
H(25)-C(24)	1.09	C(22)-C(21)-C(16)	122	C(28)	-0.02
H(26)-C(21)	1.09	C(11)-C(18)-C(17)	122	C(29)	-0.04
C(27)-C(30)	1.39	C(21)-C(16)-C(17)	119	C(30)	-0.04
C(27)-C(22)	1.44	C(12)-C(11)-C(18)	119	H(31)	0.06
C(28)-C(23)	1.44	C(24)-C(17)-C(18)	123	H(32)	0.06

End table 1

1	2	3	4	5	6
C(29)-C(28)	1.39	C(16)-C(15)-H(19)	118	C(33)	-0.02
C(30)-C(29)	1.46	C(11)-C(18)-H(20)	119	C(34)	-0.04
H(31)-C(27)	1.09	C(23)-C(22)-C(21)	119	C(35)	-0.02
H(32)-C(28)	1.09	C(27)-C(22)-C(21)	123	C(36)	-0.04
C(33)-C(29)	1.45	C(24)-C(23)-C(22)	119	H(37)	0.06
C(34)-C(33)	1.38	C(30)-C(27)-C(22)	122	H(38)	0.06
C(35)-C(36)	1.38	C(17)-C(24)-C(23)	122	C(39)	-0.02
C(35)-C(30)	1.45	C(27)-C(22)-C(23)	118	C(40)	-0.04
C(36)-C(34)	1.47	C(16)-C(17)-C(24)	119	C(41)	-0.04
H(37)-C(35)	1.09	C(28)-C(23)-C(24)	123	C(42)	-0.02
H(38)-C(33)	1.09	C(17)-C(24)-H(25)	119	H(43)	0.06
C(39)-C(40)	1.38	C(22)-C(21)-H(26)	119	H(44)	0.06
C(39)-C(36)	1.46	C(29)-C(30)-C(27)	119	C(45)	-0.04
C(40)-C(41)	1.48	C(35)-C(30)-C(27)	123	C(46)	-0.06
C(41)-C(42)	1.38	C(22)-C(23)-C(28)	118	C(47)	-0.06
C(42)-C(34)	1.46	C(33)-C(29)-C(28)	123	C(48)	-0.04
H(43)-C(42)	1.09	C(23)-C(28)-C(29)	122	H(49)	0.06
H(44)-C(39)	1.09	C(35)-C(30)-C(29)	118	H(50)	0.06
C(45)-C(46)	1.36	C(28)-C(29)-C(30)	119	H(51)	0.06
C(45)-C(40)	1.47	C(36)-C(35)-C(30)	124	H(52)	0.06
C(46)-C(47)	1.45	C(30)-C(27)-H(31)	120	C(53)	-0.02
C(47)-C(48)	1.36	C(23)-C(28)-H(32)	118	C(54)	-0.04
C(48)-C(41)	1.47	C(30)-C(29)-C(33)	118	C(55)	-0.04
H(49)-C(48)	1.09	C(42)-C(34)-C(33)	123	C(56)	-0.02
H(50)-C(47)	1.09	C(29)-C(33)-C(34)	123	H(57)	0.06
H(51)-C(46)	1.09	C(39)-C(36)-C(34)	118	H(58)	0.06
H(52)-C(45)	1.09	C(34)-C(36)-C(35)	119	C(59)	-0.04
C(53)-C(54)	1.38	C(39)-C(36)-C(35)	123	C(60)	-0.06
C(53)-C(4)	1.46	C(33)-C(34)-C(36)	119	C(61)	-0.06
C(54)-C(55)	1.48	C(40)-C(39)-C(36)	123	C(62)	-0.04
C(55)-C(56)	1.38	C(36)-C(35)-H(37)	120	H(63)	0.06
C(56)-C(5)	1.46	C(29)-C(33)-H(38)	117	H(64)	0.06
H(57)-C(53)	1.09	C(41)-C(40)-C(39)	119	H(65)	0.06
H(58)-C(56)	1.09	C(45)-C(40)-C(39)	123	H(66)	0.06
C(59)-C(60)	1.36	C(42)-C(41)-C(40)	119		
C(59)-C(54)	1.47	C(46)-C(45)-C(40)	122		
C(60)-C(61)	1.45	C(34)-C(42)-C(41)	123		
C(61)-C(62)	1.36	C(45)-C(40)-C(41)	118		
C(62)-C(55)	1.47	C(36)-C(34)-C(42)	118		
H(63)-C(59)	1.09	C(48)-C(41)-C(42)	123		
H(64)-C(62)	1.09	C(34)-C(42)-H(43)	117		
H(65)-C(61)	1.09	C(40)-C(39)-H(44)	120		
H(66)-C(60)	1.09	C(47)-C(46)-C(45)	121		
		C(48)-C(47)-C(46)	121		
		C(41)-C(48)-C(47)	122		
		C(40)-C(41)-C(48)	118		
		C(41)-C(48)-H(49)	118		
		C(48)-C(47)-H(50)	121		
		C(47)-C(46)-H(51)	118		
		C(46)-C(45)-H(52)	120		
		C(55)-C(54)-C(53)	119		
		C(3)-C(4)-C(53)	123		
		C(56)-C(55)-C(54)	119		
		C(60)-C(59)-C(54)	122		
		C(5)-C(56)-C(55)	123		
		C(59)-C(54)-C(55)	118		
		C(4)-C(5)-C(56)	118		
		C(6)-C(5)-C(56)	123		
		C(54)-C(53)-H(57)	120		
		C(5)-C(56)-H(58)	117		
		C(61)-C(60)-C(59)	121		
		C(53)-C(54)-C(59)	123		
		C(62)-C(61)-C(60)	121		
		C(55)-C(62)-C(61)	122		
		C(54)-C(55)-C(62)	118		
		C(56)-C(55)-C(62)	123		
		C(60)-C(59)-H(63)	120		
		C(55)-C(62)-H(64)	118		
		C(62)-C(61)-H(65)	121		
		C(61)-C(60)-H(66)	118		

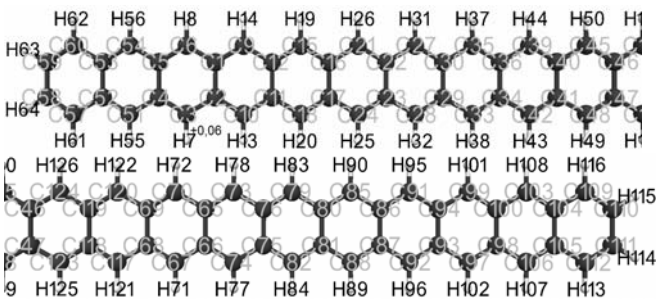

Fig. 2 - Geometric and electronic molecular structure of eicocene.
(E_0= -1069853 kDg/mol, E_{el}= -11719827 kDg/mol)

Table 2 - Optimised bond lengths, valent corners and atom charges of eicocene

Bond lengths	R,A	Valence corners	Grad	Atom	Charge (by Milliken)
1	2	3	4	5	6
C(2)-C(1)	1.46	C(5)-C(6)-C(1)	122	C(1)	-0.03
C(3)-C(2)	1.44	C(11)-C(10)-C(2)	122	C(2)	-0.04
C(4)-C(3)	1.39	C(1)-C(2)-C(3)	118	C(3)	-0.02
C(4)-C(5)	1.47	C(10)-C(2)-C(3)	123	C(4)	-0.04
C(5)-C(54)	1.46	C(5)-C(4)-C(3)	119	C(5)	-0.04
C(6)-C(5)	1.39	C(2)-C(3)-C(4)	122	C(6)	-0.02
C(6)-C(1)	1.44	C(54)-C(5)-C(4)	118	**H(7)**	**+0.06**
H(7)-C(3)	1.09	C(6)-C(5)-C(4)	119	H(8)	+0.06
H(8)-C(6)	1.09	C(53)-C(54)-C(5)	123	C(9)	-0.02
C(9)-C(1)	1.40	C(54)-C(5)-C(6)	123	C(10)	-0.02
C(10)-C(2)	1.40	C(2)-C(1)-C(6)	118	C(11)	-0.03
C(10)-C(11)	1.43	C(2)-C(3)-H(7)	118	C(12)	-0.03
C(11)-C(18)	1.42	C(5)-C(6)-H(8)	120	H(13)	+0.06
C(11)-C(12)	1.45	C(1)-C(6)-H(8)	118	H(14)	+0.06
C(12)-C(9)	1.43	C(2)-C(1)-C(9)	119	C(15)	-0.02
H(13)-C(10)	1.09	C(1)-C(2)-C(10)	119	C(16)	-0.04
H(14)-C(9)	1.09	C(18)-C(11)-C(10)	123	C(17)	-0.04
C(15)-C(12)	1.42	C(12)-C(11)-C(10)	119	C(18)	-0.02
C(16)-C(15)	1.41	C(17)-C(18)-C(11)	122	H(19)	+0.06
C(16)-C(17)	1.45	C(9)-C(12)-C(11)	119	H(20)	+0.06
C(17)-C(24)	1.44	C(15)-C(12)-C(11)	119	C(21)	-0.02
C(18)-C(17)	1.41	C(1)-C(9)-C(12)	122	C(22)	-0.04
H(19)-C(15)	1.09	C(18)-C(11)-C(12)	119	C(23)	-0.04
H(20)-C(18)	1.09	C(2)-C(10)-H(13)	119	C(24)	-0.02
C(21)-C(16)	1.44	C(11)-C(10)-H(13)	118	H(25)	+0.06
C(22)-C(21)	1.39	C(1)-C(9)-H(14)	119	H(26)	+0.06
C(23)-C(22)	1.46	C(9)-C(12)-C(15)	123	C(27)	-0.02
C(24)-C(23)	1.39	C(17)-C(16)-C(15)	119	C(28)	-0.02
H(25)-C(24)	1.09	C(12)-C(15)-C(16)	122	C(29)	-0.04
H(26)-C(21)	1.09	C(24)-C(17)-C(16)	118	C(30)	-0.04

Continuation table 2

1	2	3	4	5	6
C(27)-C(22)	1.45	C(18)-C(17)-C(16)	119	H(31)	+0.06
C(28)-C(23)	1.45	C(23)-C(24)-C(17)	122	H(32)	+0.06
C(29)-C(28)	1.38	C(24)-C(17)-C(18)	123	C(33)	-0.02
C(29)-C(30)	1.47	C(12)-C(15)-H(19)	119	C(34)	-0.04
C(30)-C(27)	1.38	C(17)-C(18)-H(20)	119	C(35)	-0.02
H(31)-C(27)	1.09	C(15)-C(16)-C(21)	123	C(36)	-0.04
H(32)-C(28)	1.09	C(17)-C(16)-C(21)	118	H(37)	+0.06
C(33)-C(29)	1.46	C(16)-C(21)-C(22)	122	H(38)	+0.06
C(34)-C(33)	1.38	C(21)-C(22)-C(23)	119	C(39)	-0.02
C(34)-C(36)	1.48	C(27)-C(22)-C(23)	118	C(40)	-0.04
C(34)-C(42)	1.46	C(22)-C(23)-C(24)	119	C(41)	-0.04
C(35)-C(30)	1.46	C(28)-C(23)-C(24)	123	C(42)	-0.02
C(36)-C(35)	1.38	C(23)-C(24)-H(25)	120	H(43)	+0.06
H(37)-C(35)	1.09	C(16)-C(21)-H(26)	118	H(44)	+0.06
H(38)-C(33)	1.09	C(21)-C(22)-C(27)	123	C(45)	-0.02
C(39)-C(36)	1.46	C(22)-C(23)-C(28)	118	C(46)	-0.03
C(40)-C(39)	1.38	C(30)-C(29)-C(28)	119	C(47)	-0.03
C(40)-C(41)	1.48	C(23)-C(28)-C(29)	123	C(48)	-0.02
C(41)-C(48)	1.45	C(27)-C(30)-C(29)	119	H(49)	+0.05
C(42)-C(41)	1.38	C(35)-C(30)-C(29)	118	H(50)	+0.05
H(43)-C(42)	1.09	C(22)-C(27)-C(30)	123	C(51)	-0.02
H(44)-C(39)	1.09	C(22)-C(27)-H(31)	117	C(52)	-0.04
C(45)-C(40)	1.45	C(23)-C(28)-H(32)	117	C(53)	-0.04
C(46)-C(45)	1.39	C(28)-C(29)-C(33)	123	C(54)	-0.02
C(47)-C(46)	1.49	C(30)-C(29)-C(33)	118	H(55)	+0.06
C(48)-C(47)	1.39	C(36)-C(34)-C(33)	120	H(56)	+0.06
H(49)-C(48)	1.09	C(42)-C(34)-C(33)	123	C(57)	-0.04
H(50)-C(45)	1.09	C(29)-C(33)-C(34)	123	C(58)	-0.06
C(51)-C(4)	1.46	C(35)-C(36)-C(34)	120	C(59)	-0.06
C(52)-C(51)	1.38	C(41)-C(42)-C(34)	123	C(60)	-0.04
C(52)-C(53)	1.48	C(39)-C(36)-C(34)	118	H(61)	+0.06
C(53)-C(60)	1.47	C(27)-C(30)-C(35)	123	H(62)	+0.06
C(54)-C(53)	1.38	C(30)-C(35)-C(36)	123	H(63)	+0.06
H(55)-C(51)	1.09	C(42)-C(34)-C(36)	118	H(64)	+0.06
H(56)-C(54)	1.09	C(30)-C(35)-H(37)	117	C(65)	-0.04
C(57)-C(52)	1.47	C(29)-C(33)-H(38)	117	C(66)	-0.04
C(58)-C(57)	1.36	C(35)-C(36)-C(39)	123	C(67)	-0.02
C(59)-C(58)	1.45	C(41)-C(40)-C(39)	119	C(68)	-0.04
C(60)-C(59)	1.36	C(36)-C(39)-C(40)	123	C(69)	-0.04
H(61)-C(57)	1.09	C(48)-C(41)-C(40)	118	C(70)	-0.02
H(62)-C(60)	1.09	C(42)-C(41)-C(40)	119	H(71)	+0.06
H(63)-C(59)	1.09	C(47)-C(48)-C(41)	124	H(72)	+0.06
H(64)-C(58)	1.09	C(48)-C(41)-C(42)	123	C(73)	-0.02
C(65)-C(70)	1.46	C(41)-C(42)-H(43)	120	C(74)	-0.02
C(66)-C(65)	1.47	C(36)-C(39)-H(44)	117	C(75)	-0.04
C(67)-C(66)	1.46	C(39)-C(40)-C(45)	123	C(76)	-0.04
C(68)-C(67)	1.37	C(41)-C(40)-C(45)	118	H(77)	+0.06
C(68)-C(69)	1.48	C(40)-C(45)-C(46)	124	H(78)	+0.06
C(69)-C(120)	1.46	C(45)-C(46)-C(47)	119	C(79)	-0.02
C(70)-C(69)	1.38	C(124)-C(46)-C(47)	118	C(80)	-0.04
H(71)-C(67)	1.09	C(46)-C(47)-C(48)	119	C(81)	-0.04
H(72)-C(70)	1.09	C(123)-C(47)-C(48)	123	C(82)	-0.02
C(73)-C(65)	1.38	C(47)-C(48)-H(49)	119	H(83)	+0.06
C(74)-C(66)	1.38	C(40)-C(45)-H(50)	117	H(84)	+0.06
C(75)-C(74)	1.46	C(3)-C(4)-C(51)	123	C(85)	-0.02
C(75)-C(76)	1.47	C(5)-C(4)-C(51)	118	C(86)	-0.03
C(76)-C(73)	1.46	C(53)-C(52)-C(51)	119	C(87)	-0.04
H(77)-C(74)	1.09	C(4)-C(51)-C(52)	123	C(88)	-0.02
H(78)-C(73)	1.09	C(60)-C(53)-C(52)	118	H(89)	+0.06
C(79)-C(76)	1.39	C(54)-C(53)-C(52)	119	H(90)	+0.06
C(80)-C(79)	1.45	C(59)-C(60)-C(53)	122	C(91)	-0.02
C(80)-C(81)	1.46	C(60)-C(53)-C(54)	123	C(92)	-0.02
C(81)-C(82)	1.45	C(4)-C(51)-H(55)	117	C(93)	-0.04
C(82)-C(75)	1.39	C(53)-C(54)-H(56)	120	C(94)	-0.04
H(83)-C(79)	1.09	C(51)-C(52)-C(57)	123	H(95)	+0.06
H(84)-C(82)	1.09	C(53)-C(52)-C(57)	118	H(96)	+0.06
C(85)-C(80)	1.40	C(52)-C(57)-C(58)	122	C(97)	-0.02
C(86)-C(85)	1.43	C(57)-C(58)-C(59)	121	C(98)	-0.04
C(86)-C(87)	1.45	C(58)-C(59)-C(60)	121	C(99)	-0.02
C(87)-C(88)	1.43	C(52)-C(57)-H(61)	118	C(100)	-0.04
C(88)-C(81)	1.40	C(59)-C(60)-H(62)	120	H(101)	+0.06
H(89)-C(88)	1.09	C(58)-C(59)-H(63)	118	H(102)	+0.06
H(90)-C(85)	1.09	C(57)-C(58)-H(64)	121	C(103)	-0.02
C(91)-C(86)	1.42	C(69)-C(70)-C(65)	123	C(104)	-0.04
C(92)-C(87)	1.42	C(70)-C(65)-C(66)	118	C(105)	-0.04
C(93)-C(92)	1.41	C(73)-C(65)-C(66)	119	C(106)	-0.02
C(93)-C(94)	1.45	C(65)-C(66)-C(67)	118	H(107)	+0.06
C(94)-C(91)	1.41	C(74)-C(66)-C(67)	123	H(108)	+0.06
H(95)-C(91)	1.09	C(69)-C(68)-C(67)	120	C(109)	-0.04
H(96)-C(92)	1.09	C(66)-C(67)-C(68)	123	C(110)	-0.06
C(97)-C(93)	1.44	C(120)-C(69)-C(68)	118	C(111)	-0.06
C(98)-C(97)	1.39	C(70)-C(69)-C(68)	120	C(112)	-0.04
C(98)-C(100)	1.46	C(119)-C(120)-C(69)	123	H(113)	+0.06
C(98)-C(106)	1.45	C(120)-C(69)-C(70)	123	H(114)	+0.06
C(99)-C(94)	1.44	C(66)-C(67)-H(71)	117	H(115)	+0.06
C(100)-C(99)	1.39	C(69)-C(70)-H(72)	120	H(116)	+0.06
H(101)-C(99)	1.09	C(70)-C(65)-C(73)	123	C(117)	-0.02
H(102)-C(97)	1.09	C(65)-C(66)-C(74)	119	C(118)	-0.04
C(103)-C(100)	1.45	C(76)-C(75)-C(74)	118	C(119)	-0.04
C(104)-C(103)	1.38	C(66)-C(74)-C(75)	123	C(120)	-0.02
C(104)-C(105)	1.47	C(73)-C(76)-C(75)	118	H(121)	+0.05
C(105)-C(112)	1.47	C(79)-C(76)-C(75)	119	H(122)	+0.05
C(106)-C(105)	1.38	C(65)-C(73)-C(76)	123	C(123)	-0.02
H(107)-C(106)	1.09	C(66)-C(74)-H(77)	120	C(124)	-0.02
H(108)-C(103)	1.09	C(65)-C(73)-H(78)	120	H(125)	+0.05
C(109)-C(104)	1.47	C(73)-C(76)-C(79)	123	H(126)	+0.05
C(110)-C(109)	1.36	C(81)-C(80)-C(79)	118		
C(111)-C(110)	1.45	C(76)-C(79)-C(80)	122		
C(112)-C(111)	1.36	C(82)-C(81)-C(80)	118		
H(113)-C(112)	1.09	C(88)-C(81)-C(80)	119		
H(114)-C(111)	1.09	C(75)-C(82)-C(81)	122		
H(115)-C(110)	1.09	C(74)-C(75)-C(82)	123		
H(116)-C(109)	1.09	C(76)-C(75)-C(82)	119		
C(117)-C(68)	1.46	C(76)-C(79)-H(83)	120		
C(118)-C(117)	1.38	C(75)-C(82)-H(84)	120		
C(118)-C(119)	1.49	C(79)-C(80)-C(85)	123		
C(118)-C(123)	1.44	C(81)-C(80)-C(85)	119		
C(119)-C(124)	1.44	C(87)-C(86)-C(85)	119		
C(120)-C(119)	1.38	C(80)-C(85)-C(86)	122		
H(121)-C(117)	1.09	C(88)-C(87)-C(86)	119		
H(122)-C(120)	1.09	C(92)-C(87)-C(86)	119		
C(123)-C(47)	1.42	C(81)-C(88)-C(87)	122		
C(124)-C(46)	1.42	C(82)-C(81)-C(88)	123		
H(125)-C(123)	1.09	C(81)-C(88)-H(89)	119		
H(126)-C(124)	1.09	C(80)-C(85)-H(90)	119		
		C(85)-C(86)-C(91)	123		
		C(87)-C(86)-C(91)	119		
		C(88)-C(87)-C(92)	123		
		C(94)-C(93)-C(92)	119		
		C(87)-C(92)-C(93)	122		
		C(91)-C(94)-C(93)	119		
		C(99)-C(94)-C(93)	118		
		C(86)-C(91)-C(94)	122		
		C(86)-C(91)-H(95)	119		
		C(87)-C(92)-H(96)	119		
		C(92)-C(93)-C(97)	123		
		C(94)-C(93)-C(97)	118		
		C(100)-C(98)-C(97)	119		
		C(106)-C(98)-C(97)	123		
		C(93)-C(97)-C(98)	122		
		C(99)-C(100)-C(98)	119		
		C(105)-C(106)-C(98)	123		
		C(103)-C(100)-C(98)	118		
		C(91)-C(94)-C(99)	123		
		C(94)-C(99)-C(100)	122		
		C(106)-C(98)-C(100)	118		
		C(94)-C(99)-H(101)	118		
		C(93)-C(97)-H(102)	118		
		C(99)-C(100)-C(103)	123		
		C(105)-C(104)-C(103)	119		

End table 2

1	2	3	4	5	6
		C(100)-C(103)-C(104)	123		
		C(112)-C(105)-C(104)	118		
		C(106)-C(105)-C(104)	119		
		C(111)-C(112)-C(105)	122		
		C(112)-C(105)-C(106)	123		
		C(105)-C(106)-H(107)	120		
		C(100)-C(103)-H(108)	117		
		C(103)-C(104)-C(109)	123		
		C(105)-C(104)-C(109)	118		
		C(104)-C(109)-C(110)	122		
		C(109)-C(110)-C(111)	121		
		C(110)-C(111)-C(112)	121		
		C(111)-C(112)-H(113)	120		
		C(110)-C(111)-H(114)	118		
		C(109)-C(110)-H(115)	121		
		C(104)-C(109)-H(116)	118		
		C(67)-C(68)-C(117)	123		
		C(69)-C(68)-C(117)	118		
		C(119)-C(118)-C(117)	119		
		C(123)-C(118)-C(117)	123		
		C(68)-C(117)-C(118)	123		
		C(124)-C(119)-C(118)	118		
		C(47)-C(123)-C(118)	124		
		C(120)-C(119)-C(118)	119		
		C(46)-C(124)-C(119)	124		
		C(123)-C(118)-C(119)	118		
		C(124)-C(119)-C(120)	123		
		C(68)-C(117)-H(121)	117		
		C(119)-C(120)-H(122)	120		
		C(46)-C(47)-C(123)	118		
		C(45)-C(46)-C(124)	123		
		C(47)-C(123)-H(125)	118		
		C(46)-C(124)-H(126)	118		

Table 3 - Total energy (E_0), maximal charge on the hydrogen atom (q_{max}^{H+}) and universal factor of acidity (pKa) of molecules dekacene and eicocene

Molecules	E_0 (kDg/mol)	q_{max}^{H+}	pKa
Dekacene	-550105	+0.06	33
Eicocene	-1069853	+0.06	33

References

1. K. S. Novoselov, et al. Electric Field Effect in Atomically Thin Carbon Films, Science 306, 666 (2004);DOI:10.1126/science.1102896
2. M.W.Shmidt, K.K.Baldrosge, J.A. Elbert, M.S. Gordon, J.H. Enseh, S.Koseki, N.Matsvnaga., K.A. Nguyen, S. J. Su, And Anothers. J. Comput. Chem.14, 1347-1363, (1993).
3. Bode, B. M. and Gordon, M. S. *J. Mol. Graphics Mod., 16*, 1998, 133-138
4. Babkin V.A., Fedunov R.G., Minsker K.S. and anothers. Oxidation communication, 2002, №1, 25, 21-47.
5. V.A. Babkin, A.V. Ignatov, A.N. Ignatov, M.N. Gulyukin, V.Yu. Dmitriev, O.V. Stoyanov, G.E. Zaikov. Quantum-chemical Calculation of some molecules of triboratols. Kazan. "Vestnik" of Kazan State Technological University. 2013., Vol. 16, N2, p. 15-17
6. V.A. Babkin, A.V. Ignatov, O.V. Stoyanov, G.E. Zaikov. Quantum-chemical Calculation of some monomers of cationic polymerisation with small cycles. Kazan. "Vestnik" of Kazan State Technological University. 2013., Vol. 16, N 4, p.21-22
7. V.A. Babkin, V.V. Trifonov B.B., N.G. Lebedev, V.Yu. Dmitriev, D.S. Andreev, O.V. Stoyanov, G.E. Zaikov. Quantum-chemical Calculation of tetracene and pentacene by MNDO in approximation of the linear molecular model of graphene. Kazan. "Vestnik" of Kazan State Technological University. 2013., Vol. 16, N 7, p.16-18.

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