

Aims and backgrounds The aim of this work is a study of electronic structure of molecules deakacene, 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 deakacene, 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: $pK_a = 49,4 - 134,61 \cdot q_{maxH^+}$ [4] (where, q_{maxH^+} – a maximum positive charge on atom of the hydrogen (by Milliken [1]) $R=0.97$, R – a coefficient of correlations, $q_{maxH^+}=+0,06$). $pK_a=33$. This formula was successfully used in the following articles: [5, 6, 7]. Quantum-chemical calculation of molecules deakacene, eicocene by method MNDO was executed for the first time. Optimized geometric and electronic structures of these compound was received. Acid power of molecules deakacene, eicocene was theoretically evaluated ($pK_a=33$). These compounds pertain to class of very weak H-acids ($pK_a>14$). Fig. 1 - Geometric and electronic molecular structure of deakacene. ($E_0 = -550105$ kDg/mol, $E_{el} = -4850841$ kDg/mol). Table 1 - Optimised bond lengths, valent corners and atom charges of deakacene

Bond lengths	R, Å	Valent corners Grad	Atom Charge (by Milliken)
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
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. (E0= -1069853 kDg/mol, Eel= -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 (E0), maximal
 charge on the hydrogen atom (qmaxH+) and universal factor of acidity (pKa) of
 molecules dekacene and eicocene Molecules E0 (kDg/mol) qmaxH+ pKa Dekacene -
 550105 +0.06 33 Eicocene -1069853 +0.06 33