

QUANTUM MECHANICAL INVESTIGATIONS OF STRUCTUREAL AND THERMAL PROPERTIES OF SOME THIADIAZOL DERIVATIVES

دراسة ميكانيكا الكم للخصائص التركيبية والحرارية لبعض مشتقات الثياديازول

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Abstract:-

This study involved the adoption of the program (Gaussian 03) to use the method of calculating the total (Ab initio of method) according to the Hartree – Fock method (RHF), for the purpose of the expense of dimensional geometry (lengths and bond angles) when the geometry of a balanced, functions thermodynamic, some physical properties, charges for derivatives ring 4-(1,3,4-thiadiazol-2-yl)benzene-1,3-diols.

Have shown calculation results that the compound (R-SiH₃) has the highest value of thermodynamic functions (E^0, H^0, G^0, S^0, A^0) but the compound (R-AlH₂) has the highest value of heat capacity (C_V, C_P). The results showed that both nitrogen atoms (N_9, N_8) had the highest negative charge when the compound (R-AlH₂), which makes it a strong legend when Linked to metal and the formation of the complex.

For (R-AlH₂, R-SiH₃, R-PH₂, R-SH) molecules the calculated some of physical properties (dipole moment μ in Debye), orbital energies (E_{HOMO}, E_{LUMO} in eV), IP (in eV), (measurement stability Δ), hardness η and Electron Affinity E_A). Also For these molecules the calculated (ΔH_f^0 in KJ/mole) by using (semi-empirical method AM1 model in MOPAC program). Calculation results have shown that the compound (R-SiH₃) the lower value of the heat of formation (the more Stability) as well as has the highest value of ΔE and IP that means it's the less active between the compounds. This difference in the results come according to the difference of substituted groups.

Key words: RHF study, 4-(1,3,4-thiadiazol-2-yl) benzene-1,3-diols, thermodynamics functions.

الخلاصة:-

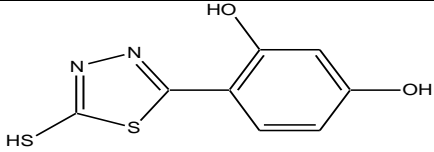
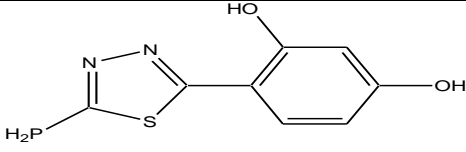
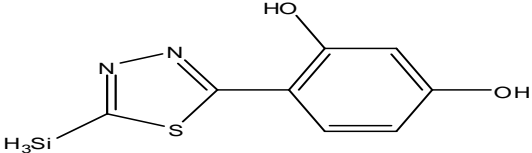
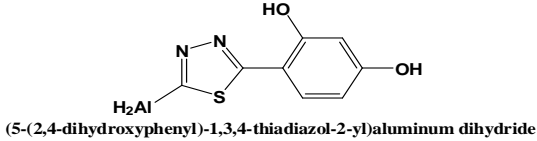
تضمنت هذه الدراسة اعتماد برنامج كاوس (Gaussian 03) لاستخدام طريقة الحساب التام على وفق طريقة هارترتي فوك (RHF\6-31G), وذلك لغرض حساب الأبعاد الهندسية (أطوال و زوايا التاصر) عند الشكل الهندسي المتوازن, الدوال الترموديناميكية (G^0, H^0, S^0, A^0, E^0) وكذلك تم حساب السعة الحرارية (C_p, C_v), بعض الخصائص الفيزيائية وكذلك الشحنات لمشتقات حلقة 4-(1,3,4-thiadiazol-2-yl)benzene-1,3-diol والتي يرمز لها اختصاراً (R-AlH₂, R-SiH₃, R-PH₂, R-SH) وقد أظهرت نتائج الحساب أن المركب (R-SiH₃) يمتلك أعلى قيمة من قيم الدوال الترموديناميكية (G^0, H^0, S^0, A^0, E^0). كما أظهرت النتائج أن المركب (R-AlH₂) يمتلك أعلى قيمة سعة حرارية (C_p, C_v), كما أظهرت نتائج الحساب بان لكل من ذرات النتروجين (N_8, N_9) قيمة شحنة سالبة عالية في المركب (R-AlH₂) مما يجعله ليكون قوي عند ارتباطه بالفلز وتكوين المعقد.

كما تم حساب بعض الخصائص الفيزيائية عزم ثنائي القطب (μ in Debye), طاقة المدارات (E_{HOMO}, E_{LUMO}), طاقة التأين (IP in eV), فجوة الطاقة (ΔE in eV), الألفة الالكترونية و الصلابة (E_A, η , in eV) وكذلك تم اعتماد برنامج MOPAC لاستخدام الطريقة الشبه تجريبية AM1 لحساب حرارة التكوين للمركبات (ΔH_f^0 in kJ/mole). وقد أظهرت النتائج الحساب أن المركب (R-SiH₃) أكثر استقراراً لكونه يمتلك أقل قيمة في حرارة التكوين كذلك يمتلك أعلى قيمة لطاقة التأين ويمتلك أعلى قيمة لفرق الطاقة بين المدارات (E_{HOMO}, E_{LUMO}). بينما يمتلك المركب (R-SH) أقل قيمة لفجوة الطاقة (فرق الطاقة بين المدارين (HOMO, LUMO)) وهذا يعني أن هذا المركب هو أكثر المركبات فعالية لكونه يمتلك أقل قيمة لفجوة الطاقة. أن هذا التباين بالنتائج يعزى بصورة عامة لتأثير اختلاف المجموعة المعوضة على المركبات المدروسة في هذا البحث.

Introduction.

Fungicide commonly used in agriculture against phyta pathogenic filamentous fungi, include the compounds characterized by widely diverse chemical structure and functional group [1,2]. The compounds with the heterocyclic ring constituted an important group . In fungicides differently substituted five or six – membered heterocyclic (also fused with the homo aromatic ring) with one or some hetero atoms are used .these include pyridine , pyrimidine , piperidine , morpholine , azoles and others[3]. Particularly the derivative of azoles and benzimidazole exhibit useful properties in plant protection . However , the intensive use of these compounds lead to development of resistance in this field [4]. Therefore various structural modifications of heterocyclic based on the structure – activity studies are under taken to obtain compounds of higher efficacy[5-7].

Among azoles 1,3,4-thiadiazoles are an interesting group of fungi static compounds[8,9, 10] . Vikani reported p, p`- bis (2- substituted – benzalamino / benzolamino/sulphonamido-1,3,4-thiadiazol -5-yl-methylamino) diphenyl sulphones displaying good activity against *A. niger*[11]. Other sulphone derivatives containing a trimethoxyphenyl substituent were synthesized and evaluated for antifungal activities against *G. zeae* and *b. cinerea* [12]. 2- (3,4,5-Trimethoxyphenyl) -5- (substituted sulfinyl)-1,3,4-thiadiazoles act against *G. zeae* , *F. oxysporun*, *C. mandshurica*, 2-(substituted thio) -5-(2,4-dinitrophenylthio)-1,3,4-thiadiazoles against *V. inaequalis* , *B.cinerea* , *F. bulbigenum* and *C. melonis* [13]. For 2-(4-chloro-3-ethyl-1-methyl-1H-pyrazol-5-yl)- 5-(alkylthio)-1,3,4-thiadiazoles and 6- methyl -1-phenyl-3-ethyl-1-phenyl -3-(5-(phenylamino)-1,3,4-thiadiazol-2-yl) pyridazin-4(1H)-ones in vivo antifungal properties against *R.solani* and *P.recondita* also confirmed this compounds[15,16].

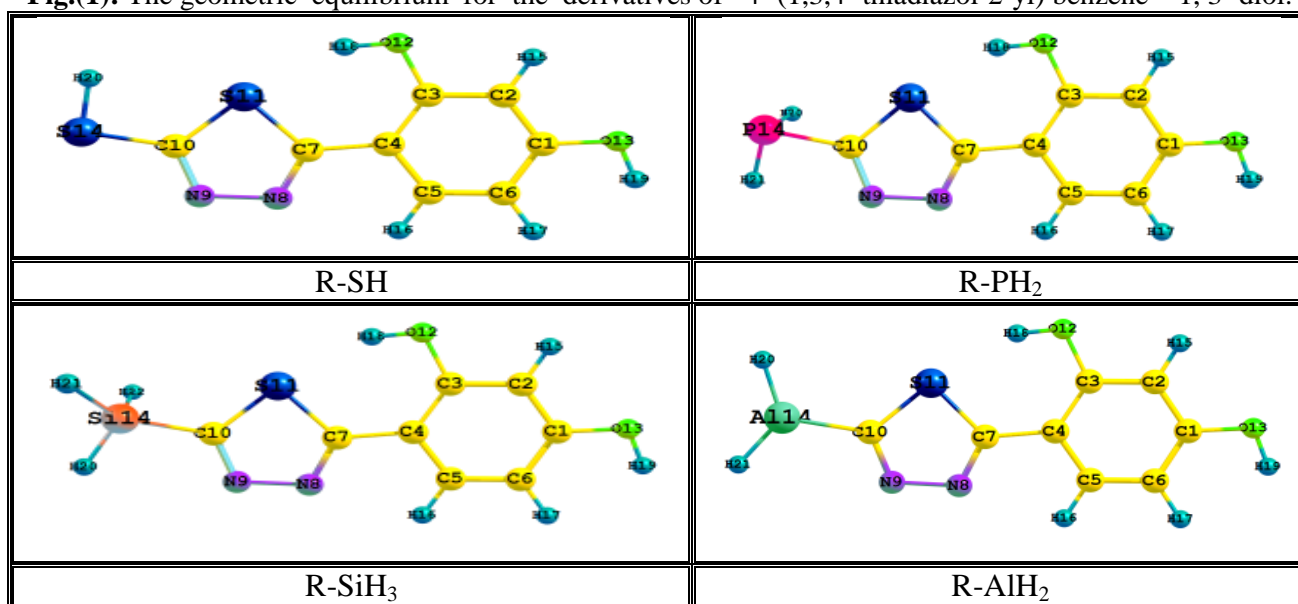
 <p>4-(5-Mercapto-[1,3,4]thiadiazol-2-yl)-benzene-1,3-diol</p>	 <p>4-(5-phosphino-1,3,4-thiadiazol-2-yl)benzene-1,3-diol</p>
<p>R-SH</p>	<p>R-PH₂</p>
 <p>4-(5-silyl-1,3,4-thiadiazol-2-yl)benzene-1,3-diol</p>	 <p>(5-(2,4-dihydroxyphenyl)-1,3,4-thiadiazol-2-yl)aluminum dihydride</p>
<p>R-SiH₃</p>	<p>R-AlH₂</p>

Results and Discussion :-

Geometrical parameter.

In this research calculated the geometry (bond lengths and bond angles) of the four molecules of derivatives 4-(1,3,4-thiadiazol-2-yl) benzene-1,3-diol (R-SH, R-PH₂, R-SiH₃, R-AlH₂), using the Ab initio method of according to the Hartree – Fock method (RHF). According to the results calculated and recorded in the (table 1 and fig. 1). Show that the bond (C₁₀-X₁₄, X= S, P, Si, Al) in compound R-SH has less value compared to other compounds studies it may be due to high electro – negative, whereas for the same bond length for each of the compound (R-PH₂, R-SiH₃, R-AlH₂) have highest value, may be caused by the large size group substituted (-P, -Si, -Al). The result showed that the bond length (C₁₀-S₁₁) in (R-PH₂) comp. has less value than the others, when the other compounds have high value this caused by electron pair on S atom in this bond length. When the bond length (C₁₀-N₉) in (R-AlH₂) has highest value compared with other compounds that's return to the Ion pair in nitrogen atom and electro – negative[17].

Fig.(1): The geometric equilibrium for the derivatives of 4-(1,3,4- thiadiazol-2-yl) benzene – 1, 3- diol.



Also the change of the group substituted had effect on the value of the angles of the compounds studied in this research, have shown calculation in the (table 1 and fig. 1). That the angle ($\angle S_{11}C_{10}N_9$) the compound R-SH has the highest value compared with other compound. The reason for the large size sulfur atom (-S). On the contrary, Aluminum atom is small size. The bond angle value which is located the group substituted X, (X=-S, -Si, -P, Al). have less value in compound (R- Al H₂). Also the angle ($\angle C_7S_{11} C_{10}$) the result showed that in compound R-SH has the less value when the compound R- Al H₂ this rearrangement return to difference in molecular weight of substituted groups on C₇ with the difference of electro-negative the substituted groups.

Table (1) : Calculated geometric parameters (bond lengths in Angstrom length angles in degree) of the derivatives 4- (1,3,4- thiadiazol-2-yl) benzene – 1, 3- diol.

R-SH		R-PH ₂		R- SiH ₃		R- AlH ₂	
Para.Geo.	Bond length and Angle	Para.Geo.	Bond length and Angle	Para.Geo.	Bond length and Angle	Para.Geo.	Bond length and Angle
R(7-8)	1.310	R(7-8)	1.311	R(7-8)	1.311	R(7-8)	1.312
R(7-11)	1.748	R(7-11)	1.744	R(7-11)	1.742	R(7-11)	1.739
R(8-9)	1.425	R(8-9)	1.427	R(8-9)	1.426	R(8-9)	1.427
R(9-10)	1.303	R(9-10)	1.302	R(9-10)	1.304	R(9-10)	1.307
R(10-11)	1.745	R(10-11)	1.743	R(10-11)	1.744	R(10-11)	1.751
R(10-14)	1.764	R(10-14)	1.831	R(10-14)	1.864	R(10-14)	1.908
R(12-18)	0.985	R(12-18)	0.985	R(12-18)	0.985	R(12-18)	0.985
R(13-19)	0.989	R(13-19)	0.989	R(13-19)	0.989	R(13-19)	0.989
R(14-20)	1.332	R(14-20)	1.383	R(14-20)	1.421	R(14-20)	1.473
A(2-1-6)	119.5	A(2-1-6)	119.5	A(2-1-6)	119.6	R(14-21)	1.470
A(1-6-5)	119.3	A(1-6-5)	119.3	A(1-6-5)	119.3	A(1-6-5)	119.3
A(1-6-17)	120.1	A(1-6-17)	120.1	A(1-6-17)	120.1	A(1-6-17)	120.1
A(1-13-19)	105.5	A(1-13-19)	105.4	A(1-13-19)	105.4	A(1-13-19)	105.4
A(3-12-18)	107.4	A(3-12-18)	107.4	A(3-12-18)	107.4	A(3-12-18)	107.2
A(5-4-7)	116.3	A(5-4-7)	116.5	A(5-4-7)	116.5	A(5-4-7)	116.7
A(4-5-6)	122.7	A(4-5-6)	122.7	A(4-5-6)	122.7	A(4-5-6)	122.7
A(4-5-16)	117.5	A(4-5-16)	117.4	A(4-5-16)	117.4	A(4-5-16)	117.4
A(4-7-8)	120.3	A(4-7-8)	120.2	A(4-7-8)	120.2	A(4-7-8)	120.1
A(4-7-11)	125.9	A(2-1-6)	119.5	A(4-7-11)	126.0	A(4-7-11)	126.1
A(8-7-11)	113.8	A(8-7-11)	113.8	A(8-7-11)	113.8	A(8-7-11)	113.8
A(7-8-9)	112.4	A(7-8-9)	112.0	A(7-8-9)	111.9	A(7-8-9)	111.6
A(7-11-10)	87.3	A(7-11-10)	87.7	A(7-11-10)	88.0	A(7-11-10)	88.5
A(8-9-10)	111.9	A(8-9-10)	112.5	A(8-9-10)	112.9	A(8-9-10)	113.7
A(9-10-11)	114.5	A(9-10-11)	114.0	A(9-10-11)	113.5	A(9-10-11)	112.4
A(9-10-14)	120.9	A(9-10-14)	122.8	A(9-10-14)	121.8	A(9-10-14)	120.9
A(11-10-14)	124.6	---	----	A(11-10-14)	124.7	---	----
A(10-14-20)	95.1	---	----	A(10-14-20)	108.9	---	----
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Physical properties.

Depending on the Ab initio physical properties have been calculated by using of method according to the Hartree – Fock method (RHF) , is calculated some physical properties of the molecules were calculated to get on ; Dipole moments (μ in Debye) , energies (e V) of the high Occupied Molecular Orbital (E_{HOMO}) and the Lower Unoccupied Molecular Orbital (E_{LUMO}) and according Koopmans theorem (the negative E_{HOMO} is equal to the ionization potential) the calculation has been ionization energies (e V) , Also calculated the energy difference (ΔE , e V), And finally calculated (Molecular Hardness) $Hardness(\eta) = \frac{1}{2}(E_{HOMO} - E_{LUMO})$, (Electron Affinity) $EA = - E_{LUMO}$ according Koopmans theorem for N system of electrons.

The shown this results (**table 2:**) that compound R-AlH₂ has high value for each of (Dipole moments , E_{LUMO}), And less value in ionization potential (IP) and this indicates that the compound R-AlH₂ has less ability to gain electrons compared to other compounds. While we note that this compound has highest value of E_{HOMO} (less the value of a negative energy) , and has a lower value for the ionization potential (IP), and this means that this compound has more ability to lose electrons and be easier ionization compared to other compounds. Result also showed that the compound (R-SiH₃) has highest value of (ΔE), sense of activity of this compound is few. Also this compound has highest values for each of (Hardness η) and (Electron Affinity E_A)[18-21] .

Also , The MOPAC computational packages (semi-empirical method , AM1 model) employed to compute physical properties; heats of formation (ΔH_f , kJ.mol⁻¹),the results showed[22,23] (**Table2:**) for each of compound (R-SiH₃ , R-AlH₂) have lower heat of formation (more stability), Whereas the compound (R-PH₂) has a higher heat of formation (less stability), Perhaps due this result to the effect of the group substitutes for the stability the compound , as previously mentioned reason.

Table 2: Calculated ΔH_f (kJ.mol⁻¹) , μ (in Debye) ,orbital energies (E_{HOMO} , E_{LUOM} , ΔE in eV) , IP(in eV) , E_A (in eV) , and η (in eV) for the derivatives of 4-(1,3,4- thiadiazol-2-yl) benzene – 1, 3- diol.

Comp.	ΔH_f KJ/Mol	Debye	E_{HOMO}	E_{LOMO}	ΔE	IP	EA	η
R-SH	-6.3647	2.0085	-6.3368	5.2804	11.6172	6.3368	-5.2804	-3.1684
R-PH2	65.317	1.5061	-6.4198	5.3327	11.7524	6.4198	-5.3327	-3.2099
R-SiH ₃	-42.456	1.6989	-6.4535	5.3329	11.9864	6.4535	-5.3329	-3.2267
R-ALH3	-24.753	2.3113	-6.2927	5.3525	11.6452	6.2927	-5.3525	-3.1463

Thermodynamics functions

The fundamental vibration frequencies for the (R-SH, R-SiH₃, R-PH₂, R-AlH₂) molecules along with the rotational constants, obtained in this study, where used to calculate the vibration and rotation contributions to the thermodynamic functions according to the statistical thermodynamic equations.

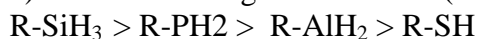
$$U_{vib}^0 = \sum_{i=1}^{3N-6} \frac{RTX_i}{e^{X_i} - 1} \qquad X_i = \frac{1.44\nu}{T}$$

$$S_{vib}^0 = R \sum_{i=1}^{3N-6} \left[\frac{X_i}{e^{X_i} - 1} - \ln(1 - e^{-X_i}) \right]$$

$$S_{rot}^0 = R \left[\frac{3}{2} + \ln \frac{8\pi^2 (8\pi^2 I_x I_y I_z)^{\frac{1}{2}} (KT)^{\frac{3}{2}}}{\sigma h^3} \right]$$

””

These two contributions along with the others contributions, for the translation, electronic, and nuclear motions, were used to calculate E^0 , H^0 , S^0 , A^0 , and G^0 thermodynamic functions . Standard thermodynamics functions and heat capacity for the studied molecules were listed, **Table 3** : looking at the calculation results show that each of the thermodynamic functions (G^0 , A^0 , E^0 , H^0 , S^0) have the same gradient values (different the group substitutes),



Where , compound (R-SiH₃) has the highest value for each of the above functions, while compound (R-SH) has the lowest value .

In addition , compound (R-SH) has the lowest value for each of the functions (C_p , C_v) , while the compound (R-AlH₂) has the highest value for the same functions last,



The deferent thermodynamics functions values due to deferent substituted groups(X), viz, the sulfur atom a high electro-negative in addition to its high size which makes restricted movement.

Table 3: The calculated standard thermodynamics functions at 298.15K of the derivatives of 4-(1,3,4- thiadiazol-2-yl) benzene – 1, 3- diol.

Comp.	E KJ/Mol	H KJ/mol	G KJ/mol	S KJ/mol.deg	A KJ/mol	Cp KJ/mol.deg	Cv KJ/mol.deg
R_SH	426.4081	429.0960	298.1564	0.4389	295.6774	0.1815	0.1732
R_PH2	458.2023	460.6809	328.7184	0.4422	326.2398	0.1840	0.1757
R_SIH3	482.9884	485.4670	350.0066	0.4539	347.5276	0.1899	0.1815
R_AL	446.6671	449.1457	314.9200	0.4497	321.4414	0.1903	0.1820

The Charges:

The Calculated for all charges atoms of the molecules studied according to the method (RHF), have shown (**Table: 4**), are each of the (N_8 , N_9) has lower value of charge (the highest density electronic) in the charge case of compound (R-AlH₂, R-PH₂) , while it has the highest value of charge (less density electronic) when the compound (R-SH), Perhaps the reason for this difference in electrical negative and molecular weight which increase the electronic density on nitrogen atom (N_8 , N_9) As in the case of compound (R-SH , R-SiH₃).

This scientific fact indicates that the compound (R-AlH₂, R-PH₂) can be strong legand when it linked to metal complex formation , as a result of higher giving electronic to nitrogen atoms(N_8 , N_9) compared to other compounds ,and on the contrary , the compound (R-SiH₃).

It also found that the amount of charge of the atom(S_{11} , C_{10}) has gradient opposite to the value of charge ((N_8 , N_9)).

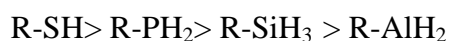


Table:4 Calculated charge for the derivatives of 4- (1,3,4- thiadiazol-2-yl) benzene – 1, 3- diol by using Hartree – Fock method.

R-SH			R-PH ₂			R-SiH ₃			R-AlH ₂		
Atom e	charge	density	Atom e	charge	density	Atom e	charge	density	Atom e	charge	density
C1	0.1416	3.8583	C1	0.1414	3.8586	C1	0.1413	3.8586	C1	0.1397	3.8603
C2	-0.1059	4.1059	C2	-0.1064	4.1064	C2	-0.1067	4.1066	C2	-0.1074	4.1073
C3	0.1357	3.8643	C3	0.1363	3.8637	C3	0.1364	3.8636	C3	0.1353	3.8647
C4	-0.0504	4.0504	C4	-0.0509	4.0509	C4	-0.0510	4.0510	C4	-0.0510	4.0510
C5	-0.0293	4.0299	C5	-0.0294	4.0294	C5	-0.0293	4.0293	C5	-0.0305	4.0305
C6	-0.1129	4.1129	C6	-0.1136	4.1135	C6	-0.1138	4.1138	C6	-0.1145	4.1145
C7	-0.0104	4.0108	C7	-0.0113	4.0013	C7	-0.0117	4.0117	C7	-0.0177	4.0177
N8	-0.1796	5.1795	N8	-0.1865	5.1865	N8	-0.1899	5.1899	N8	-0.1967	5.1960
N9	-0.1855	5.1854	N9	-0.1946	5.1845	N9	-0.1785	5.1785	N9	-0.1941	5.1941
C10	-0.1067	4.1067	C10	-0.1627	4.1627	C10	-0.1998	4.1997	C10	-0.2679	4.2678
S11	0.2213	5.7786	S11	0.2156	5.7844	S11	0.2087	5.7912	S11	0.1813	5.8187
O12	-0.2763	6.2762	O12	-0.2774	6.2774	O12	0.2779-	6.2779	O12	-0.2805	6.2805
O13	-0.2702	6.2702	O13	-0.2705	5.2704	O13	-0.2705	6.2705	O13	-0.2714	6.2713
S14	0.2086	5.7914	P14	0.4399	4.5600	Si14	0.7341	3.2659	Al14	0.9668	2.0332
H15	0.0831	0.9168	H15	0.0828	0.9172	H15	0.0825	0.9174	H15	0.0813	0.9867
H16	0.0992	0.9008	H16	0.0985	0.9015	H16	0.0985	0.9014	H16	0.0975	0.9025
H17	0.0598	0.9401	H17	0.0592	0.9408	H17	0.0590	0.9404	H17	0.0577	0.9422
H18	0.1976	0.8023	H18	0.1998	0.8002	H18	0.2002	0.7998	H18	0.2015	0.7985
H19	0.2032	0.7968	H19	0.2028	0.7972	H19	0.2027	0.7973	H19	0.2016	0.7984
H20	-0.0229	1.0229	H20	-0.1007	1.1007	H20	-0.1342	1.1341	H20	-0.2729	1.2728
			H21	-0.0819	1.0819	H21	-0.1499	1.1499	H21	-0.2578	1.2578
						H22	-0.1499	1.1499			

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