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THE NON-ADDITIVE POTENTIAL IN THE He_3 SYSTEM WITHIN THE LCAO-MO-SCF APPROXIMATION*

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ABSTRACT: The non-additive three body potential of the He_3 system for general linear and triangular geometrical configurations is calculated by using the Polyatom program based on the Roothaan LCAO-MO-SCF method with a Gaussian basis set formed by 6 s-type and 3 *p*-type functions for each center. Tables and Figures of numerical results are presented for linear, isosceles and scalene triangular configurations. A comparison with results of other authors is made.

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INTRODUCTION

Some physical properties of atomic and molecular systems like the free energy, specific heat, entropy, viscosity and thermal conductivity are usually calculated under certain approximations. One of these is known as "the pair-wise additivity of the molecular forces", which means that the interaction between atoms or molecules can be expressed as a sum of contributions referring to isolated pairs. The validity of this approximation has been studied by several authors. Per-Olov Löwdin[1], on investigating cohesive forces of certain of the alkali-halide ionic crystals, has shown that in this case, the cohesive energy is non-additive.

A convenient approach to the study of these non-additive interactions is by perturbation theory. Margenau[2] has pointed out that first order interactions do not have the property of pair-wise additivity. The long range forces between unexcited molecules like the dispersion forces are additive in second order of perturbation theory, if a simple product type of zero order wave function is used. Third order perturbation theory was applied to the Van der Waals type interaction between neutral atoms by Axilrod[3] in order to calculate three body non-additive interaction. Axilrod's results have been applied by Graben and Present[4] and Sherwood and Prausnitz[5] to the calculation of the third virial coefficient for Neon, Argon, Krypton, Xenon and other gases, obtaining a better agreement with experimental values than that afforded by additive Van der Waals' forces alone.

For short-range forces, Rosen[6] using the valence bond method has obtained formulae for the ratio of triple to pair-wise contributions for two types of geometrical configurations of the He_3 system: an equilateral triangle and a linear array of three atoms equally spaced. This problem has been investigated by Shostak[7], who employed molecular orbitals in this calculation. His results, evaluated only for linear configurations, while in general agreement with Rosen's conclusions, give increasingly larger non-additive contributions at shorter interatomic distances.

THE NON-ADDITIVE POTENTIAL IN THE He_3 SYSTEM

Bader, Beltrán-López and Novaro[8], have applied the Roothaan LCAO-MO-SCF method, using the Polyatom program in the Basch and Hornback version for calculating the non-additive energy of three Helium atoms in several linear and isosceles triangular-configurations. They used a basis set consisting of the optimized 6 s-type gaussians functions of Huzinaga[9] for the Helium atoms

TABLE I

Energies of linear configurations. (a.u.)

R_{ab} and R_{bc} are distances from central atom to the other two

R_{ab}	R_{bc}	Total energy of the He_3 system $E(He_3)$	Total two-body interaction ΣE_2	Total three-body interaction E_3	Non-additive energy ΔE_3
			$R_{ab} + R_{bc} = 6.0\ a_0$		
2.0	4.0	-8.460536	0.122485	0.122816	0.000331
2.1	3.9	-8.483438	0.099596	0.099915	0.000319
2.2	3.8	-8.501884	0.081156	0.081469	0.000313
2.3	3.7	-8.516659	0.066395	0.066694	0.000299
2.4	3.6	-8.528370	0.054690	0.054983	0.000293
2.5	3.5	-8.537526	0.045539	0.045826	0.000287
2.6	3.4	-8.544524	0.038545	0.038829	0.000284
2.7	3.3	-8.549670	0.033402	0.033683	0.000281
2.8	3.2	-8.553190	0.029883	0.030163	0.000280
2.9	3.1	-8.555240	0.027832	0.028112	0.000280
3.0	3.0	-8.555915	0.027158	0.027438	0.000280
			$R_{ab} + R_{bc} = 5.5\ a_0$		
2.0	3.5	-8.456990	0.125515	0.126363	0.000848
2.1	3.4	-8.479150	0.103386	0.104203	0.000817
2.2	3.3	-8.496666	0.085899	0.086687	0.000788
2.3	3.2	-8.510260	0.072327	0.073093	0.000766
2.4	3.1	-8.520502	0.062101	0.062851	0.000750
2.5	3.0	-8.527824	0.054795	0.055528	0.000734
2.6	2.9	-8.532538	0.050086	0.050815	0.000729
2.7	2.8	-8.534846	0.047782	0.048507	0.000725
			$R_{ab} + R_{bc} = 5.0\ a_0$		
2.0	3.0	-8.446463	0.134816	0.136890	0.002074
2.1	2.9	-8.466376	0.114980	0.116977	0.001997
2.2	2.8	-8.481081	0.100332	0.102272	0.001940
2.3	2.7	-8.491174	0.090279	0.092179	0.001900
2.4	2.6	-8.497068	0.084408	0.086285	0.001877
2.5	2.5	-8.499006	0.082488	0.084347	0.001859
			$R_{ab} + R_{bc} = 4.5\ a_0$		
2.0	2.5	-8.415844	0.162709	0.167508	0.004799
2.1	2.4	-8.429151	0.149509	0.154202	0.004693
2.2	2.3	-8.435677	0.143036	0.147676	0.004640

plus 3 p-type gaussian functions of exponents 0.25, 1.25, and 5.00 to account for the deformation of the charge cloud in the He_2 and He_3 systems. This basis set, while above the Hartree-Fock limit, is still good enough for extrapolating safely to it throughout the range of distances from $2.5\,a_0$ to $5\,a_0$.

Beltrán-López and Novaro[10] obtained an approximate energy surface for the three-body part in the He_3 by plotting points calculated as above, plus others found by linear interpolation. Their results were presented as potential surfaces for linear and isosceles triangle configurations. One of our objectives in this work is the calculation of more accurate potential surfaces for linear and isosceles triangles and other configurations.

Linear Configurations.- The potential surface for linear configurations obtained by Beltrán-López and Novaro presents certain "wiggles" which where not expected but could not be ignored in view of the results found by interpolation.

We investigated the reality of these "wiggles" by increasing the density of calculated points, rendering unnecessary the interpolation of results for obtaining the energy surface. The results thus obtained are presented in Table I and Figure 1. In these it is seen that the correct three body energy

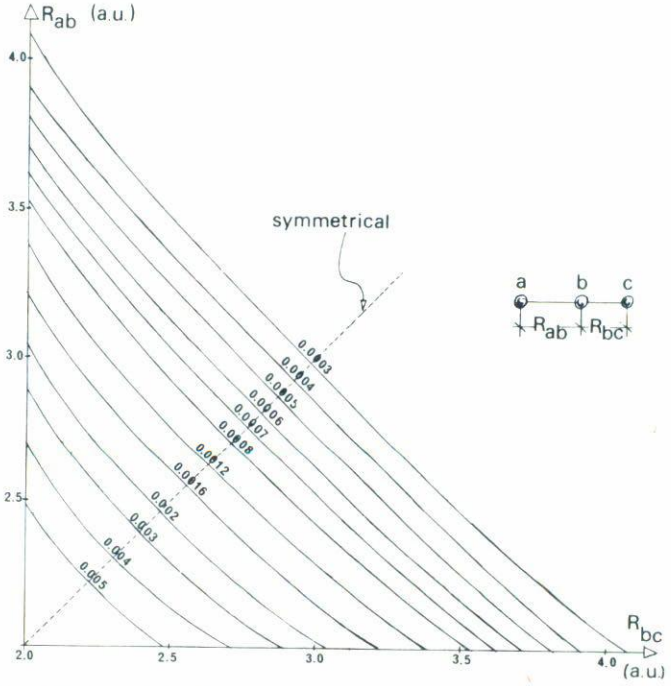

Figure 1. Equipotentials of the non-additive energy for linear configurations of the He_3 system [11]

for a linear configuration is very nearly a function of the sum of the distances between atoms, i.e., the equipotentials are very nearly straigth lines.

An analytical equation which closely fits our results has been obtained by the method of least squares. This equation is:

$$\Delta E_3 = 21.019424 \exp\left[-1.8783606\,(R_{ab} + R_{bc})\right] + \\ + \left\{\left[0.00363/(R_{ab} + R_{bc})\right] - 0.000588\right\}(R_{ab} - R_{bc})^2 \qquad (1)$$

where R_{ab} and R_{bc} are the distances between the outer and the central atoms. This expression is useful for the calculation of other physical properties such as the third virial coefficient. In Table II and Figure 2 the values given

TABLE II

Approximate non-additive energy of linear configurations calculated by using the empirical equation:

$$\Delta E_3 = 21.019424 \exp\left[-1.8783606\,(R_{ab} + R_{bc})\right] + \\ + \left[0.003630/(R_{ab} + R_{bc}) - 0.000588\right](R_{ab} - R_{bc})^2$$

R_{ab}	R_{bc}	ΔE_3	R_{ab}	R_{bc}	ΔE_3
	$R_{ab} + R_{bc} = 6.0$		2.3	3.2	0.000744
2.0	4.0	0.000336	2.4	3.1	0.000721
2.1	3.9	0.000323	2.5	3.0	0.000703
2.2	3.8	0.000312	2.6	2.9	0.000692
2.3	3.7	0.000301	2.7	2.8	0.000686
2.4	3.6	0.000292		$R_{ab} + R_{bc} = 5.0$	
2.5	3.5	0.000285	2.0	3.0	0.001891
2.6	3.4	0.000279	2.1	2.9	0.001841
2.7	3.3	0.000274	2.2	2.8	0.001803
2.8	3.2	0.000270	2.3	2.7	0.001775
2.9	3.1	0.000269	2.4	2.6	0.001759
3.0	3.0	0.000268	2.5	2.5	0.001753
	$R_{ab} + R_{bc} = 5.5$			$R_{ab} + R_{bc} = 4.5$	
2.0	3.5	0.000847	2.0	2.5	0.004534
2.1	3.4	0.000807	2.1	2.4	0.004504
2.2	3.3	0.000773	2.2	2.3	0.004487

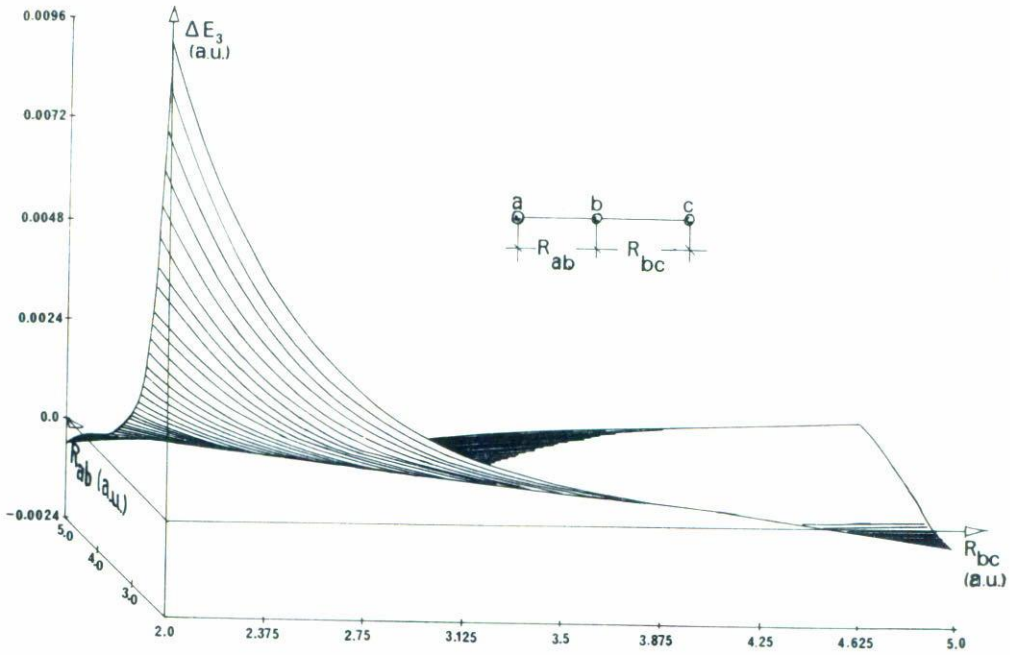

Figure 2. Non-additive potential energy surface for a He_3 system in linear configurations, as obtained by using the equation.

$$\Delta E_3 = 21.019424 \exp\left[-1.8783606\,(R_{ab} + R_{bc})\right] + \left[0.003630/(R_{ab} + R_{bc}) - 0.000588\right](R_{ab} - R_{bc})^2$$

by equation (1) are compared with those obtained with Polyatom. A comparison of our results with Shostak's results is made in Tables III and IV and Figure 3 and with Rosen's results in Table V and Figure 4.

Isosceles Configurations.- For isosceles triangular configurations, we find a smoother surface than that obtained by Beltrán-López and Novaro. This is shown in Table VI and Figure 5.

We have also calculated the non-additive energy for isosceles triangular configurations of constant base and varying sides. The results as a function of the length of the two equal sides are shown in Figures 6 and 7 and Tables VII and VIII. From these we see that the non-additive energy decreases from its zero value at $R \to \infty$, to a minimum near $R = 3a_0$ from which it increases again. The non-additive energy is then seen to contribute to the stability of certain geometrical configurations, whereas others, such as the linear configurations, are made more unstable.

A comparison of our results with Rosen's results is made in Table IX and Figure 8.

TABLE III

Comparison of our results for non-additive energies of symmetrical linear configurations and those calculated by Shostak[7].

R_{ab} = Distance between the central and the outer atoms

R_{ab}	*Shostak* non-additive energy	Polyatom non-additive energy
1.78	0.121646	
2.00		0.010870
2.37	0.018559	
2.50		0.001859
2.96	0.000048	
3.00		0.000280
3.50		0.000039
4.74	0.000000	

TABLE IV

Comparison of our results for the ratios of triple to pair-wise additive contributions of symmetrical linear configurations and those calculated by Shostak.

R_{ab} = Distance between the central and the outer atoms

R_{ab}	Shostak's results	Polyatom results
1.78	0.260629	
2.00		0.044623
2.37	0.180035	
2.50		0.022538
2.96	0.001789	
3.0		0.010310
3.50		0.004479
4.74	0.000000	

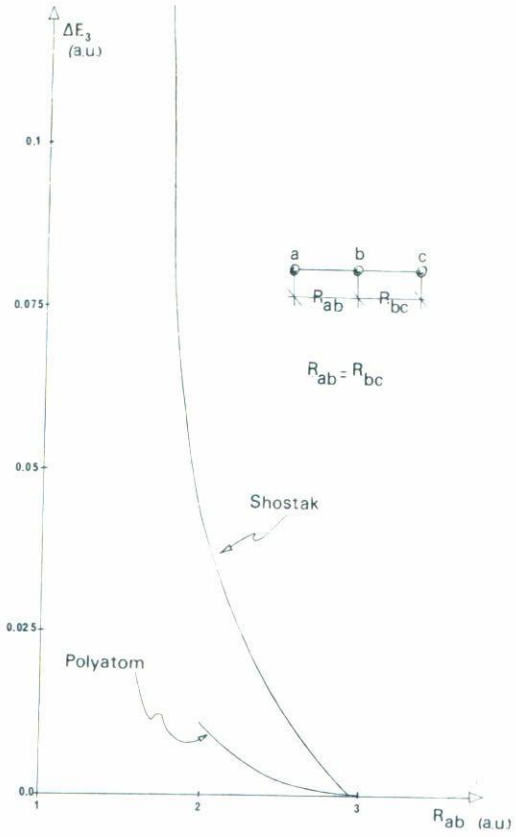

Figure 3. Comparison of our results for the non-additive energies of symmetrical linear configurations and those calculated by Shostak.

TABLE V

Comparison of our results for the ratios of triple to pair-wise additive contributions of symmetrical linear configurations and those calculated by using the Rosen's formula

R_{ab} = Distance between the central and the outer atoms

R_{ab}	Rosen's results	Polyatom results
2.0	0.049906	0.044623
2.5	0.013332	0.022538
3.0	0.003561	0.010310
3.5	0.000951	0.004479

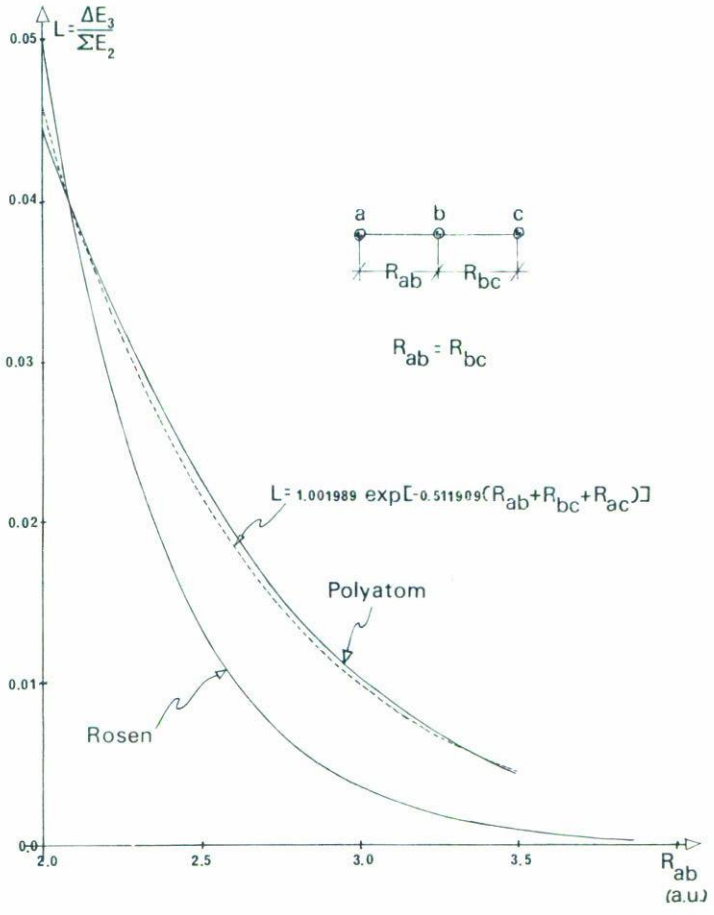

Figure 4. Comparison of our results for the ratios of triple to pair-wise additive contributions of symmetrical linear configurations and those calculated by using the Rosen's formula.

TABLE VI

Energies of some isosceles triangular configurations. (a.u.)

Length of equal sides R	Length of Base X	Total energy of the He_3 system $E(He_3)$	Total two-body interaction ΣE_2	Total three-body interaction E_3	Non-additive energy ΔE_3
2.8	2.8	-8.527448	0.063700	0.055905	-0.007793
2.8	4.8	-8.540851	0.042666	0.042502	-0.000162
3.3	3.3	-8.564478	0.020650	0.018875	-0.001773
3.7	3.7	-8.575645	0.008219	0.007708	-0.000511
3.7	4.2	-8.577325	0.006324	0.006028	-0.000296
4.3	3.2	-8.573614	0.009971	0.009739	-0.000232
4.6	2.3	-8.519330	0.064294	0.064023	-0.000271

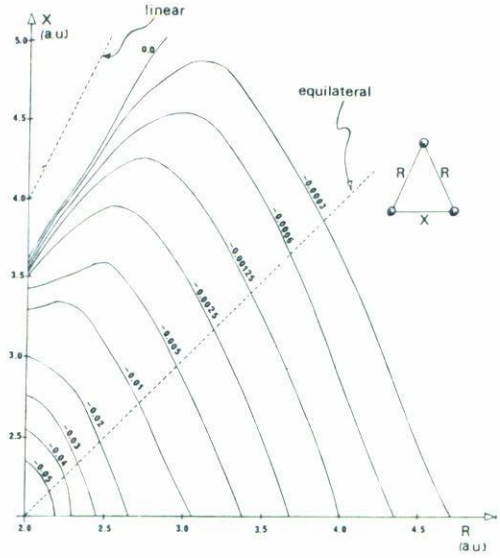

Figure 5. Equipotentials of the non-additive energy for isosceles triangular configurations of the He_3 system.[11]

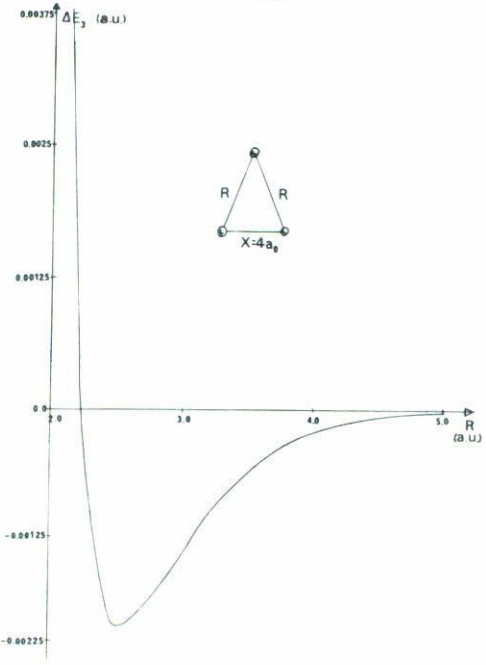

Figure 6. Non-additive energy of isosceles triangular configurations, with base constant at 4 a.u.

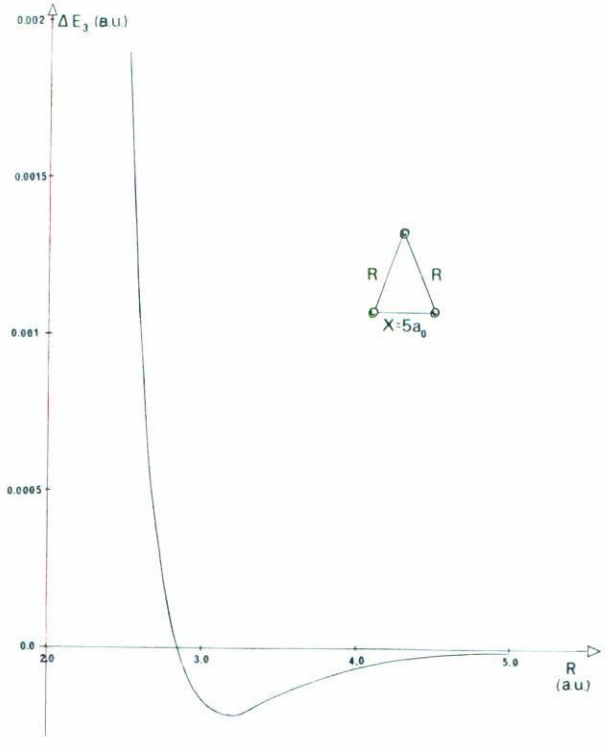

Figure 7. Non-additive energy of isosceles triangular configurations, with base constant at 5 a.u.

TABLE VII

at 4.a.u. Energies of isosceles triangular configurations, with base constant at 4 a.u.

Length of equal sides	Length of base	Total energy of the He_3 system	Total two-body interaction	Total three-body interaction	Non-additive energy
R	X	$E(He_3)$	ΣE_2	E_3	ΔE_3
2.0	4.0	-8.328887	0.243596	0.254466	0.010870
2.1	4.0	-8.381704	0.197098	0.201649	0.004551
2.2	4.0	-8.423000	0.159310	0.160353	0.001043
2.3	4.0	-8.455535	0.128650	0.127818	-0.000832
2.4	4.0	-8.481295	0.103808	0.102058	-0.001750
2.5	4.0	-8.501758	0.083712	0.081594	-0.002117
3.0	4.0	-8.556250	0.028505	0.027113	-0.001392
4.0	4.0	-8.579480	0.004068	0.003873	-0.000195
5.0	4.0	-8.581775	0.001599	0.001578	-0.000022

TABLE VIII

Energies of isosceles triangular configurations with base constant at 5 a.u.

R	X	$E(He_3)$	ΣE_2	E_3	ΔE_3
2.5	5.0	-8.499006	0.082488	0.084347	0.001859
2.6	5.0	-8.516148	0.066242	0.067205	0.000963
2.7	5.0	-8.529796	0.053142	0.053557	0.000415
2.8	5.0	-8.540669	0.042588	0.042684	0.000096
2.9	5.0	-8.549336	0.034096	0.034017	-0.000079
3.0	5.0	-8.556248	0.027271	0.027104	-0.000166
4.0	5.0	-8.580581	0.002834	0.002772	-0.000062
5.0	5.0	-8.582996	0.000365	0.000357	-0.000009

TABLE IX

Comparison of our results for the ratios of triple to pair-wise additive contributions of equilateral triangular configurations and those calculated by using the Rosen formula

R_{ab} = Length of sides of equilateral triangle

R_{ab}	Rosen' results	Polyatom results
2.0	-0.158780	-0.185692
2.5	-0.096787	-0.146629
2.8	-0.071917	-0.122339
3.0	-0.058999	-0.106961
3.3	-0.043839	-0.085860
3.5	-0.035964	-0.073589
3.7	-0.029504	-0.062173
4.0	-0.021923	-0.047935
4.5	-0.013363	-0.030819
5.0	-0.008146	-0.024590

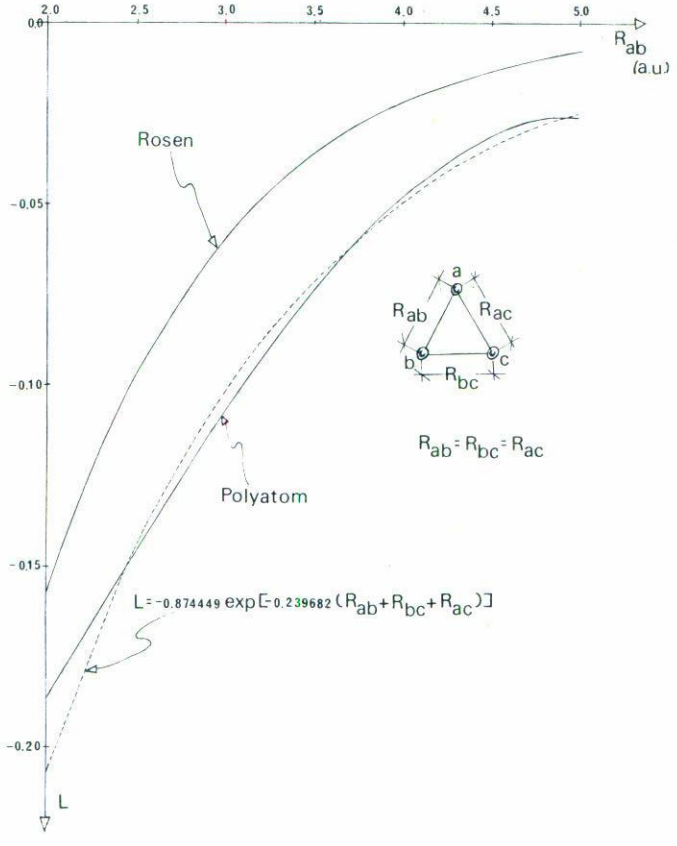

Figure 8. Comparison of our results for the ratios of triple to pair-wise additive contributions of equilateral triangular configurations and those calculated by using the Rosen' formula.

Scalene Configurations.— For scalene triangular configurations, we calculate the non-additive energy as a function of the angle between two sides whose lengths are kept constant. The corresponding results are shown in Tables, X, XI, XII, XIII, XIV, XV and XVI and Figures 9 and 10.

Axilrod's long-range formulae predicts positive energies when one of the inside angles is greater than 117°. From our results at shorter ranges we find that, as R increases, this critical angle decreases from 128° at $R = 2a_0$ towards Axilrod's value.

TABLE X

Energies of scalene triangular configurations with two sides constant at 2.0 and 2.0 a.u. R_{ab}, R_{bc} and R_{ac} are the lengths of the sides of the atomic triangle

R_{ab}	R_{bc}	R_{ac}	$E(He_3)$	ΣE_2	E_3	ΔE_3
2.0	2.0	2.0	-8.287465	0.363360	0.295888	-0.067473
2.0	2.0	2.5	-8.341791	0.282418	0.241562	-0.041856
2.0	2.0	3.0	-8.348048	0.255815	0.235305	-0.020510
2.0	2.0	3.5	-8.339750	0.246592	0.243603	-0.002990
2.0	2.0	4.0	-8.328887	0.243596	0.254466	0.010870

TABLE XI

Energies of scalene triangular configurations with two sides constant at 2.0 and 2.5 a.u.

R_{ab}	R_{bc}	R_{ac}	$E(He_3)$	ΣE_2	E_3	ΔE_3
2.0	2.5	2.0	-8.341791	0.282418	0.241562	-0.041856
2.0	2.5	2.5	-8.407598	0.203476	0.175755	-0.027721
2.0	2.5	3.5	-8.423550	0.166654	0.159803	-0.006851
2.0	2.5	4.5	-8.415844	0.162709	0.167508	0.004799

TABLE XII

Energies of scalene triangular configurations with two sides constant at 2.0 and 3.0 a.u.

R_{ab}	R_{bc}	R_{ac}	$E(He_3)$	ΣE_2	E_3	ΔE_3
2.0	3.0	2.0	-8.348048	0.255815	0.235305	-0.020510
2.0	3.0	3.0	-8.445586	0.148262	0.137767	-0.011495
2.0	3.0	4.0	-8.449450	0.136051	0.133903	-0.002148
2.0	3.0	4.5	-8.447841	0.135106	0.135512	0.000406
2.0	3.0	4.8	-8.446956	0.134895	0.136397	0.001502
2.0	3.0	5.0	-8.446463	0.134816	0.136890	0.002074

TABLE XIII

Energies of scalene triangular configurations with two sides constant at 2.0 and 3.5 a.u.

R_{ab}	R_{bc}	R_{ac}	$E(He_3)$	ΣE_2	E_3	ΔE_3
2.0	3.5	2.0	-8.339750	0.246592	0.243603	-0.002990
2.0	3.5	2.5	-8.423550	0.166654	0.159803	-0.006851
2.0	3.5	3.5	-8.457296	0.129825	0.126056	-0.003786
2.0	3.5	4.5	-8.458098	0.125884	0.125255	-0.000629
2.0	3.5	5.0	-8.457472	0.125594	0.125881	0.000287
2.0	3.5	5.4	-8.457070	0.125519	0.126283	0.000764
2.0	3.5	5.5	-8.456990	0.125515	0.126363	0.000848

TABLE XIV

Energies of scalene triangular configurations with two sides constant at 2.0 and 4.0 a.u.

R_{ab}	R_{bc}	R_{ac}	$E(He_3)$	ΣE_2	E_3	ΔE_3
2.0	4.0	2.0	-8.328887	0.243596	0.254466	0.010870
2.0	4.0	3.0	-8.449450	0.136051	0.133903	-0.002148
2.0	4.0	4.0	-8.460816	0.123832	0.122536	-0.001296
2.0	4.0	6.0	-8.460536	0.122485	0.122816	0.000332

TABLE XV

Energies of scalene triangular configurations with two sides constant at 2.0 and 4.5 a.u.

R_{ab}	R_{bc}	R_{ac}	$E(He_3)$	ΣE_2	E_3	ΔE_3
2.0	4.5	2.5	-8.415844	0.162709	0.167508	0.004799
2.0	4.5	3.0	-8.447841	0.135106	0.135512	0.000406
2.0	4.5	3.5	-8.458098	0.125884	0.125255	-0.000629
2.0	4.5	4.5	-8.461841	0.121942	0.121511	-0.000432

TABLE XVI

Non-additive energies of scalene triangular configurations. R_{ab}, R_{bc} and R_{ac} are the lengths of the sides of the atomic triangle ΔE_3 is the non-additive energy.

R_{ab}	R_{bc}	R_{ac}	ΔE_3	R_{ab}	R_{bc}	R_{ac}	ΔE_3
Constant sides = $2.5a_0$ & $2a_0$				Constant sides = $2.5a_0$ & $3a_0$			
2.5	2.0	2.0	-0.041856	2.5	3.0	2.5	-0.010943
2.5	2.0	2.5	-0.027721	2.5	3.0	3.0	-0.006924
2.5	2.0	3.5	-0.006851	2.5	3.0	5.5	0.000734
2.5	2.0	4.5	0.004799	Constant sides = $2.5a_0$ & $3.5a_0$			
Constant sides = $2.5a_0$ & $2.5a_0$				2.5	3.5	2.0	-0.006851
2.5	2.5	2.0	-0.027721	2.5	3.5	2.5	-0.005750
2.5	2.5	2.5	-0.018115	2.5	3.5	3.5	-0.002485
2.5	2.5	3.0	-0.010943	2.5	3.5	6.0	0.000287
2.5	2.5	3.5	-0.005750	Constant sides = $2.5a_0$ & $4a_0$			
2.5	2.5	4.0	-0.002117	2.5	4.0	2.5	-0.002117
2.5	2.5	4.5	0.000332	2.5	4.0	4.0	-0.000854
2.5	2.5	5.0	0.001859	Constant sides = $2.5a_0$ & $4.5a_0$			
				2.5	4.5	2.0	0.004799
				2.5	4.5	2.5	0.000332
				2.5	4.5	4.5	-0.000284
Constant sides = $3a_0$ & $2a_0$				Constant sides = $3a_0$ & $3.5a_0$			
3.0	2.0	2.0	-0.020510	3.0	3.5	3.0	-0.002582
3.0	2.0	3.0	-0.010495	3.0	3.5	3.5	0.020704
3.0	2.0	4.0	-0.002148	Constant sides = $3a_0$ & $4a_0$			
3,0	2.0	4.5	0.000406	3.0	4.0	2.0	-0.002148
3.0	2.0	4.8	0.001502	3.0	4.0	3.0	-0.001392
3.0	2.0	5.0	0.002074	3.0	4.0	4.0	-0.000541
Constant sides = $3a_0$ & $2.5a_0$				3.0	4.0	5.0	-0.000153
3.0	2.5	2.5	-0.010943	Constant sides = $3a_0$ & $4.5a_0$			
3.0	2.5	3.0	-0.006924	3.0	4.5	2.0	0.000406
3.0	2.5	5.5	0.000734	3.0	4.5	3.0	-0.000642
Constant sides = $3a_0$ & $3a_0$				Constant sides = $3a_0$ & $5a_0$			
3.0	3.0	2.0	-0.010495	3.0	5.0	2.0	0.002074
3.0	3.0	2.5	-0.006924	3.0	5.0	3.0	-0.000166
3.0	3.0	3.0	-0.004356	3.0	5.0	4.0	-0.000153
3.0	3.0	3.5	-0.002582	3.0	5.0	5.0	-0.000058
3.0	3.0	4.0	-0.001392	Constant sides = $3a_0$ & $5.5a_0$			
3.0	3.0	4.5	-0.000642	3.0	5.5	2.5	0.000734
3.0	3.0	5.0	-0.000166	3.0	5.5	3.0	0.000113
3.0	3.0	5.5	0.000113				
3.0	3.0	6.0	0.000280				

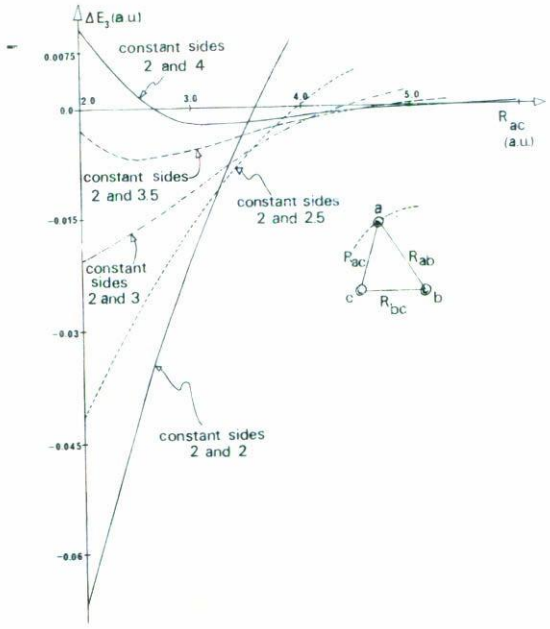

Figure 9. Non-additive energy of scalene triangular configurations with two sides constant. Here one side is always equal to 2 a_0.

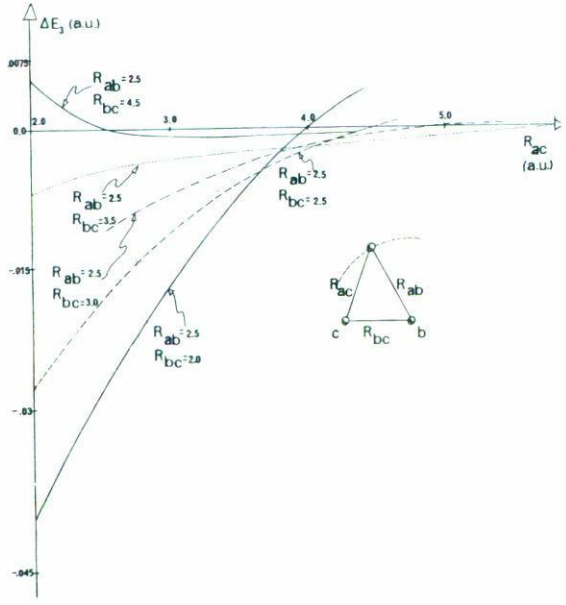

Figure 10. Non-additive energy of scalene triangular configurations with two sides constant. Here one side is always equal to 2.5 a_0.

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RESUMEN

Se calcula el potencial no aditivo de tres cuerpos del sistema He_3 para configuraciones geométricas lineales y triangulares en general, usando el programa Polyatom, basado en el método LCAO-MO-SCF de Roothaan, con una base gaussiana formada por 6 funciones tipo "*s*" y 3 tipo "*p*" para cada centro. Se presentan tablas y figuras con resultados numéricos para configuraciones lineales lo mismo que para triángulos isósceles y escalenos. Se hace una comparación con los resultados de otros autores.