ANNEXE A

TableauA1:Charges,cordonnées et la masse de chaque atome par la méthode :
Ab initio
(HyperChem7.0)du thiazole .

Atom	Coortinates(Angstrom)					Mass
	Z	charge	X	Y	Z	
1	16	0.262491	-0.97238142	-0.38248193	-0.00000015	32.06
2	6	-0.068902	0.76238366	-0.36341595	0.00000040	12.01
3	7	-0.246133	1.33799528	0.80180184	0.00000028	14.00
4	6	-0.008290	0.31770867	1.80380538	-0.00000025	12.01
5	6	-0.184823	-0.93413240	1.34687210	0.00000004	12.01
6	1	0.085144	1.32874838	-1.28808372	-0.00000030	1.008
7	1	0.076856	0.61586398	2.84388119	-0.00000001	1.008
8	1	0.083656	-1.8388517	1.93339810	-0.00000009	1.008

TableauA2:Charges,cordonnées et la masse de chaque atome par la méthode :

Ab initio

(HyperChem7.0)du Pénicilline .

Atom	Coordonates (Angstrom)					Mass
	Z	Charge	X	Y	Z	
1	16	0.270565	3.15748035	4.45193501	-2.31985443	32.0640
2	6	-0.680552	1.7637069	3.32829166	-2.97326426	12.0011
3	6	-0.184857	1.51548099	3.74742472	-4.44729741	12.0011
4	7	-0.758328	2.79361382	4.20520424	-4.96564323	14.0070
5	6	-0.247412	3.85323500	3.40384824	-5.42373951	12.0070
6	6	-0.541144	4.88515530	4.29776869	-4.69346914	12.0011
7	6	0.843325	3.64549622	5.00684886	-4.07074193	12.0011
8	8	-0.588046	3.85400307	2.40424757	-6.07833619	15.9999
9	1	0.276839	3.56555610	6.06640383	-4.15396558	1.00800
10	1	0.272773	5.46846269	4.91784116	-5.35801734	1.00800
11	1	0.263464	0.89876701	3.48187904	-2.34983030	1.00800
12	1	0.266473	2.10329941	2.30818706	-2.90565216	1.00800
13	1	0.269690	1.17487275	2.90917193	-5.03740876	1.00800
14	1	0.282140	5.51344324	3.76729737	-3.99744560	1.00800
15	1	0.255071	0.79338043	4.54775176	-4.49967284	1.00800

ANNEXE A

Tableau: A3 – Charges,cordonnées et la masse de chaque atome par la méthode :PM3 (HyperChem7.0)du thiazole .

Atom	Coordonates (Angstrom)					Mass
	Z	Charge	X	Y	Z	
1	16	0.280869	-0.987960	-0.338876	-0.000000	32.0640
2	6	-0.236160	0.761630	-0.396620	0.000000	12.0110
3	7	-0.059219	1.307290	0.808960	0.000000	14.0070
4	6	-0.106835	0.327600	1.821610	0.000000	12.0110
5	6	-0.332258	-0.952150	1.339070	0.000000	12.0110
6	1	0.155142	1.370710	-1.301000	0.000000	1.0080
7	1	0.143041	0.646420	2.866070	0.000000	1.0080
8	1	0.155423	-1.855560	1.946450	0.000000	1.0080

TableauA4 : Charges,cordonnées et la masse de chaque atome par la méthode :PM3 (HyperChem7.0)du Pénicilline .

Atom	Coordonates (Angstrom)					Mass
	Z	Charge	X	Y	Z	
1	16	-0.009473	3.116770	4.554670	-2.345620	32.0640
2	6	-0.195566	1.802130	3.418350	-2.909410	12.0110
3	6	-0.051150	1.542310	3.658060	-4.410590	12.0110
4	7	-0.118134	2.715310	4.293100	-5.040090	14.0070
5	6	-0.135433	3.639560	4.984450	-4.040880	12.0110
6	6	-0.151412	4.839050	4.227520	-4.663180	12.0110
7	6	0.282063	3.850570	3.499470	-5.571300	12.0110
8	8	-0.272845	3.865170	2.643230	-6.411380	15.9999
9	1	0.120783	3.666920	6.084000	-4.164680	1.00800
10	1	0.092256	5.572610	4.863610	-5.183410	1.00800
11	1	0.096448	0.888570	3.588760	-2.324060	1.00800

12	1	0.084416	2.101720	2.373190	-2.723720	1.00800
13	1	0.079933	1.293980	2.721050	-4.944390	1.00800
14	1	0.102034	5.401250	3.577360	-3.972380	1.00800
15	1	0.076080	0.690010	4.349870	-4.559260	1.00800