

ANNEXE B

Tableau: B1 – Population électronique de chaque orbitale atomique par la méthode:

Ab initio (HyperChem) du thiazole.

S 1 S	S 1 S	S 1 Px	S 1 Py	S 1 Pz
1.995486	1.981213	1.981509	1.996174	1.999895
S 1 S	S 1 Px	S 1 Py	S 1 Pz	C 2 S
1.993433	1.759398	1.088378	1.102070	1.833385
C 2 S	C 2 Px	C 2 Py	C 2 Pz	N 3 S
1.996308	1.031438	0.951773	0.910500	1.181757
N 3 S	N 3 Px	N 3 Py	N 3 Pz	C 4 S
1.992984	1.090658	1.008532	1.483398	1.667237
C 4 S	C 4 Px	C 4 Py	C 4 Pz	C 5 S
1.993118	1.056328	0.950439	0.885921	1.122619
C 5 S	C 5 Px	C 5 Py	C 5 Pz	H 6 S
0.914856	1.066692	0.926770	1.008015	1.190228
H 7 S	H 8 S			
0.916344	0.923144			

TableauB2 :Population électronique de chaque orbitale atomique par la méthode:

Ab initio (HyperChem7.0) de la pénicilline

C 1 S	C 1 S	C 1 Px	C 1 Py	C 1 Pz
0.425371	0.573526	0.503869	0.343392	1.989274
C 1 S	C 1 Px	C 1 Py	C 1 Pz	C 2 S
1.989774	0.414558	0.535875	0.365541	1.096007
C 2 S	C 2 Px	C 2 Py	C 2 Pz	C 2 S
1.158455	0.535617	0.520033	0.560116	0.347129
C 2 Px	C 2 Py	C 2 Pz	C 3 S	C 3 S
0.417957	1.987977	0.511653	0.488304	0.430062
C 3 Px	C 3 Py	C 3 Pz	C 3 S	C 3 Px
0.271605	0.568497	0.438444	0.548320	0.525301
C 3 Py	C 3 Pz	N 4 S	N 4 S	N 4 Px

0.567223	0.349465	1.989489	0.296880	0.101696
N 4 Py	N 4 Pz	N 4 S	N 4 Px	N 4 Py
0.750377	0.641425	1.381140	0.647795	0.606575
N 4 Pz	S 5 S	S 5 S	S 5 Px	S 5 Py
1.964459	1.962174	1.963432	1.998654	0.824840
S 5 Pz	S 5 S	S 5 Px	S 5 Py	S 5 Pz
0.725631	0.843431	0.784494	0.991499	1.959581
S 5 S	S 5 Px	S 5 Py	S 5 Pz	C 6 S
1.988904	0.393202	0.679787	0.581678	0.881413
C 6 S	C 6 Px	C 6 Py	C 6 Pz	C 6 S
1.198336	0.528624	0.528083	0.493632	0.342975
C 6 Px	C 6 Py	C 6 Pz	C 7 S	C 7 S
0.356057	1.988803	0.425700	0.584674	0.589624
C 7 Px	C 7 Py	C 7 Pz	C 7 S	C 7 Px
0.309159	1.047907	0.517111	0.572442	0.494003
C 7 Py	C 7 Pz	O 8 S	O 8 S	O 8 Px
0.821464	0.429228	1.987447	0.356656	0.542719
O 8 Py	O 8 Pz	O 8 S	O 8 Px	O 8 Py
0.784365	0.960217	1.556427	0.613006	0.646119
O 8 Pz	H 9 S	H 9 S	H 10 S	H 10 S
0.264586	0.462641	0.244296	0.478865	0.789773
H 11 S	H 12 S	H 12 S	H 13 S	H 11 S
0.471118	0.262087	0.471441	0.266646	0.469890
H 13 S	H 14 S	H 14 S	H 15 S	H 15 S
0.267372	0.477557	0.255089	0.462770	0.259192

Tableau: B3 – Population électronique de chaque orbitale atomique par la méthode:
PM3 (HyperChem) du thiazole.

AO:	1 S S	1 Px S	1 Py S	1 Pz S	2 S C
	1.252713	1.727293	1.036529	1.074684	1.880625
AO:	2 Px C	2 Py C	2 Pz C	3 S N	3 Px N
	1.353173	1.633170	1.036641	1.013447	0.933360
AO:	3 Py N	3 Pz N	4 S C	4 Px C	4 Py C

	0.992297	0.894926	1.215120	1.106907	0.965969
AO:	4 Pz C	5 S C	5 Px C	5 Py C	5 Pz C
	1.124667	0.966158	1.022103	1.219331	1.004492
AO:	6 S H	7 S H	8 S H		
	0.844577	0.856959	0.844858		

Tableau: B4 – Population électronique de chaque orbitale atomique par la méthode:
PM3 (HyperChem) du pénicilline.

AO:	1 S C	1 Px C	1 Py C	1 Pz C	2 S C
	1.187158	0.913016	1.034766	0.961931	1.225720
AO:	2 Px C	2 Py C	2 Pz C	3 S C	3 Px C
	0.880460	1.235146	0.991265	0.997383	0.975607
AO:	3 Py C	3 Pz C	4 S N	4 Px N	4 Py N
	1.262768	1.042028	1.551171	0.808883	0.793447
AO:	4 Pz N	5 S S	5 Px S	5 Py S	5 Pz S
	1.105767	1.576663	1.414389	1.912654	1.262167
AO:	6 S C	6 Px C	6 Py C	6 Pz C	7 S C
	1.172681	0.984428	1.017262	1.009751	1.184124
AO:	7 Px C	7 Py C	7 Pz C	8 S O	8 Px O
	1.851332	1.856256	0.910014	1.015564	0.952892
AO:	8 Py O	8 Pz O	9 S H	10 S H	11 S H
	0.903552	0.907744	0.879217	1.280380	1.284876
AO:	12 S H	13 S H	14 S H	15 S H	
	0.923920	0.897966	0.920067	0.915584	