

Angle de bite

Table 1 – Analyse structurale et électronique (NBO) du complexe $\text{HCu}[\text{BiEt-H}]$ en fonction de l'angle de bite.

Bite angle (°)	Distance (Å)			Population (e)		Occupation (e) ⁱ		back-bonding (kcal.mol ⁻¹)	Interaction LP _p /# [*] _{Cu-H} E(2) (kcal.mol ⁻¹) r ⁻¹ (u.a.)F(i,j) (u.a.)		
	Cu-H	Cu-P1	Cu-P2	Cu	H	# _{Cu-H}	# _{Cu-H} [*]				
77	1.53	2.53	2.53	0.37	-0.42	1.97	0.15	4.71	69.00	0.56	0.25
78	1.53	2.52	2.51	0.38	-0.43	1.97	0.15	4.89	71.04	0.56	0.25
79	1.53	2.51	2.50	0.38	-0.43	1.97	0.16	5.04	73.08	0.56	0.26
80	1.53	2.50	2.49	0.39	-0.44	1.97	0.16	5.22	75.06	0.56	0.26
81	1.53	2.49	2.48	0.39	-0.44	1.97	0.16	5.33	76.95	0.56	0.26
82	1.53	2.48	2.47	0.39	-0.44	1.97	0.16	5.40	79.00	0.57	0.27
83	1.54	2.47	2.47	0.40	-0.45	1.97	0.17	5.49	80.97	0.57	0.27
84	1.54	2.45	2.46	0.40	-0.45	1.97	0.17	5.70	83.60	0.57	0.28
85	1.54	2.44	2.45	0.40	-0.46	1.97	0.17	5.75	85.43	0.57	0.28
86	1.54	2.44	2.45	0.41	-0.46	1.97	0.17	5.86	87.11	0.57	0.28
87	1.54	2.43	2.44	0.41	-0.46	1.97	0.18	5.98	88.83	0.57	0.29
88	1.54	2.42	2.43	0.41	-0.47	1.97	0.18	6.05	90.53	0.57	0.29
89	1.55	2.42	2.42	0.42	-0.47	1.96	0.18	6.22	92.09	0.57	0.29
90	1.55	2.41	2.42	0.42	-0.47	1.96	0.18	6.29	93.62	0.57	0.30
91	1.55	2.40	2.41	0.42	-0.48	1.96	0.18	6.38	95.16	0.57	0.30
92	1.55	2.39	2.42	0.43	-0.48	1.96	0.19	6.48	96.02	0.58	0.30
93	1.55	2.38	2.41	0.43	-0.48	1.96	0.19	6.61	97.34	0.58	0.30
94	1.55	2.38	2.40	0.43	-0.48	1.96	0.19	6.76	98.46	0.58	0.30

Table 2 – Analyse structurale et électronique (NBO) du complexe $\text{HCu}[\text{BiEt-Me}]$ en fonction de l'angle de bite.

Bite angle (°)	Distance (Å) †			Population (e) †		Occupation (e) †		back-bonding (kcal.mol ⁻¹) †	Interaction LP _P / _H /* _{Cu-H} † E(2) (kcal.mol ⁻¹) r ⁻¹ (u.a.) F(i,j) (u.a.)	
	Cu-H	Cu-P1	Cu-P2	Cu†	H†	# _{Cu-H}	#* _{Cu-H}			
82†	1.54†	2.53†	2.47†	0.38	-0.45†	1.97†	0.17†	5.40†	78.10†	0.54† 0.26†
83†	1.54†	2.51†	2.48†	0.39	-0.45†	1.97†	0.17†	5.60†	80.22†	0.54† 0.26†
84†	1.54†	2.49†	2.48†	0.39	-0.45†	1.97†	0.17†	5.79†	82.51†	0.54† 0.27†
85†	1.54†	2.47†	2.47†	0.39	-0.46†	1.97†	0.18†	5.94†	84.74†	0.54† 0.27†
86†	1.54†	2.45†	2.47†	0.40	-0.46†	1.97†	0.18†	6.07†	87.15†	0.54† 0.27†
87†	1.55†	2.44†	2.46†	0.40	-0.47†	1.97†	0.18†	6.25†	89.32†	0.54† 0.28†
88†	1.55†	2.43†	2.46†	0.40	-0.47†	1.97†	0.18†	6.38†	91.30†	0.54† 0.28†
89†	1.55†	2.42†	2.45†	0.41	-0.47†	1.97†	0.19†	6.44†	93.20†	0.54† 0.28†
90†	1.55†	2.42†	2.44†	0.41	-0.48†	1.97†	0.19†	6.64†	95.04†	0.54† 0.29†
91†	1.55†	2.41†	2.43†	0.42	-0.48†	1.96†	0.19†	6.75†	96.82†	0.54† 0.29†
92†	1.55†	2.40†	2.43†	0.42	-0.48†	1.96†	0.19†	6.86†	98.48†	0.54† 0.29†
93†	1.56†	2.40†	2.42†	0.42	-0.49†	1.96†	0.19†	7.01†	100.01†	0.54† 0.29†
94†	1.56†	2.39†	2.41†	0.43	-0.49†	1.96†	0.20†	7.12†	101.63†	0.54† 0.30†
95†	1.56†	2.39†	2.41†	0.43	-0.49†	1.96†	0.20†	7.28†	103.15†	0.54† 0.30†
96†	1.56†	2.38†	2.40†	0.43	-0.50†	1.96†	0.20†	7.42†	104.58†	0.54† 0.30†
97†	1.56†	2.37†	2.39†	0.44	-0.50†	1.96†	0.20†	7.54†	105.98†	0.54† 0.30†
98†	1.57†	2.37†	2.39†	0.44	-0.50†	1.96†	0.20†	7.62†	107.42†	0.54† 0.31†

Table 3 – Analyse structurale et électronique (NBO) du complexe $\text{HCu}[\text{BiEt-Ph}]$ en fonction de l'angle de bite.

Bite angle (°)	Distance (Å) [†]			Population (e)		Occupation (e) [†]		back-bonding (kcal.mol ⁻¹) [†]	Interaction $\text{LP}_i/\#_{\text{Cu-H}}^*$		
	Cu-H	Cu-P1	Cu-P2	Cu [†]	H [†]	# _{Cu-H}	#* _{Cu-H}		E(2) (kcal.mol ⁻¹)	r _i (u.a.)	F(i,j) (u.a.)
84 [†]	1.54 [†]	2.54 [†]	2.45 [†]	0.42 [†]	-0.47 [†]	1.96 [†]	0.18 [†]	5.33 [†]	88.07 [†]	0.53 [†]	0.27 [†]
85 [†]	1.55 [†]	2.51 [†]	2.46 [†]	0.42 [†]	-0.47 [†]	1.96 [†]	0.18 [†]	5.36 [†]	89.87 [†]	0.54 [†]	0.28 [†]
86 [†]	1.55 [†]	2.48 [†]	2.47 [†]	0.43 [†]	-0.48 [†]	1.96 [†]	0.18 [†]	5.62 [†]	91.85 [†]	0.54 [†]	0.28 [†]
87 [†]	1.55 [†]	2.47 [†]	2.46 [†]	0.43 [†]	-0.48 [†]	1.96 [†]	0.18 [†]	5.78 [†]	93.77 [†]	0.54 [†]	0.28 [†]
88 [†]	1.55 [†]	2.46 [†]	2.45 [†]	0.43 [†]	-0.48 [†]	1.95 [†]	0.19 [†]	5.92 [†]	95.93 [†]	0.54 [†]	0.29 [†]
89 [†]	1.55 [†]	2.45 [†]	2.44 [†]	0.44 [†]	-0.49 [†]	1.95 [†]	0.19 [†]	6.10 [†]	98.02 [†]	0.54 [†]	0.29 [†]
90 [†]	1.56 [†]	2.44 [†]	2.43 [†]	0.44 [†]	-0.49 [†]	1.95 [†]	0.19 [†]	6.23 [†]	99.92 [†]	0.54 [†]	0.29 [†]
91 [†]	1.56 [†]	2.43 [†]	2.43 [†]	0.45 [†]	-0.49 [†]	1.95 [†]	0.19 [†]	6.33 [†]	101.47 [†]	0.54 [†]	0.30 [†]
92 [†]	1.56 [†]	2.42 [†]	2.42 [†]	0.45 [†]	-0.50 [†]	1.95 [†]	0.19 [†]	6.56 [†]	103.26 [†]	0.54 [†]	0.30 [†]
93 [†]	1.56 [†]	2.41 [†]	2.42 [†]	0.45 [†]	-0.50 [†]	1.95 [†]	0.19 [†]	6.71 [†]	104.86 [†]	0.54 [†]	0.30 [†]
94 [†]	1.56 [†]	2.40 [†]	2.41 [†]	0.46 [†]	-0.50 [†]	1.95 [†]	0.20 [†]	6.88 [†]	106.34 [†]	0.54 [†]	0.30 [†]
95 [†]	1.56 [†]	2.40 [†]	2.40 [†]	0.46 [†]	-0.51 [†]	1.95 [†]	0.20 [†]	7.03 [†]	107.77 [†]	0.54 [†]	0.31 [†]
96 [†]	1.57 [†]	2.39 [†]	2.40 [†]	0.46 [†]	-0.51 [†]	1.95 [†]	0.20 [†]	7.17 [†]	109.19 [†]	0.54 [†]	0.31 [†]
97 [†]	1.57 [†]	2.39 [†]	2.39 [†]	0.47 [†]	-0.51 [†]	1.95 [†]	0.20 [†]	7.29 [†]	110.61 [†]	0.54 [†]	0.31 [†]
98 [†]	1.57 [†]	2.38 [†]	2.39 [†]	0.47 [†]	-0.52 [†]	1.95 [†]	0.20 [†]	7.43 [†]	112.09 [†]	0.54 [†]	0.31 [†]
99 [†]	1.57 [†]	2.37 [†]	2.38 [†]	0.47 [†]	-0.52 [†]	1.94 [†]	0.20 [†]	7.56 [†]	113.53 [†]	0.54 [†]	0.31 [†]
100 [†]	1.57 [†]	2.37 [†]	2.37 [†]	0.48 [†]	-0.52 [†]	1.94 [†]	0.20 [†]	7.68 [†]	115.14 [†]	0.54 [†]	0.32 [†]
101 [†]	1.58 [†]	2.36 [†]	2.36 [†]	0.48 [†]	-0.53 [†]	1.94 [†]	0.21 [†]	7.83 [†]	116.55 [†]	0.54 [†]	0.32 [†]
102 [†]	1.58 [†]	2.36 [†]	2.36 [†]	0.49 [†]	-0.53 [†]	1.94 [†]	0.21 [†]	7.95 [†]	117.84 [†]	0.54 [†]	0.32 [†]

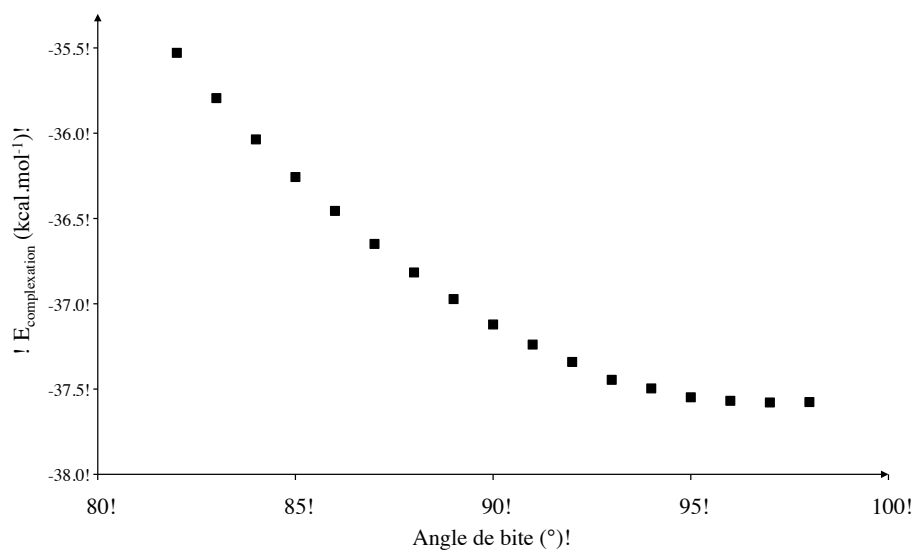


Figure 1 – $\Delta E_{\text{complexation}}$ en fonction de l'angle de bite pour le complexe HCu[BiEt-Me].

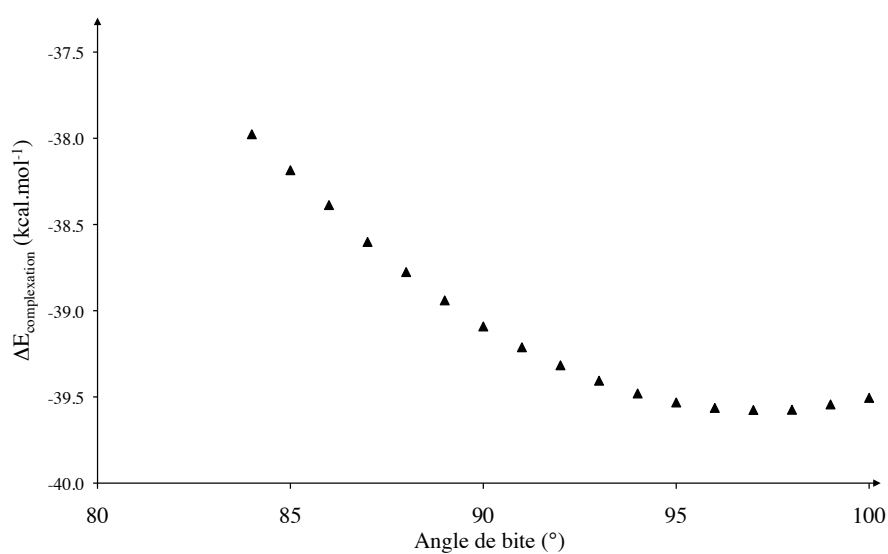


Figure 2 – $\Delta E_{\text{complexation}}$ en fonction de l'angle de bite pour le complexe HCu[BiEt-Ph].

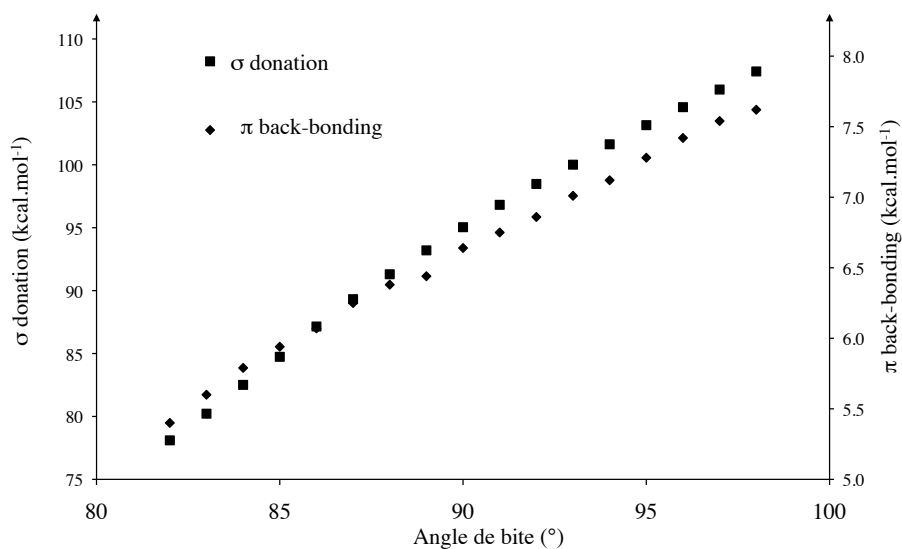


Figure 3 – Energie d'interaction LP_P/σ_{Cu-H}^* (σ donation) et π back-bonding d_{Cu}/σ_{P-R}^* pour le complexe $HCu[BiEt-Me]$.

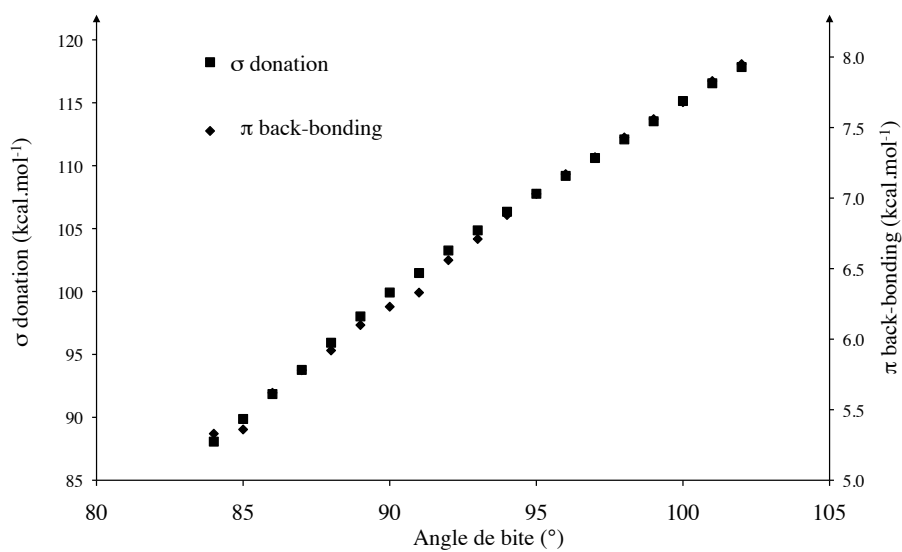


Figure 4 – Energie d'interaction LP_P/σ_{Cu-H}^* (σ donation) et π back-bonding d_{Cu}/σ_{P-R}^* pour le complexe $HCu[BiEt-Ph]$.

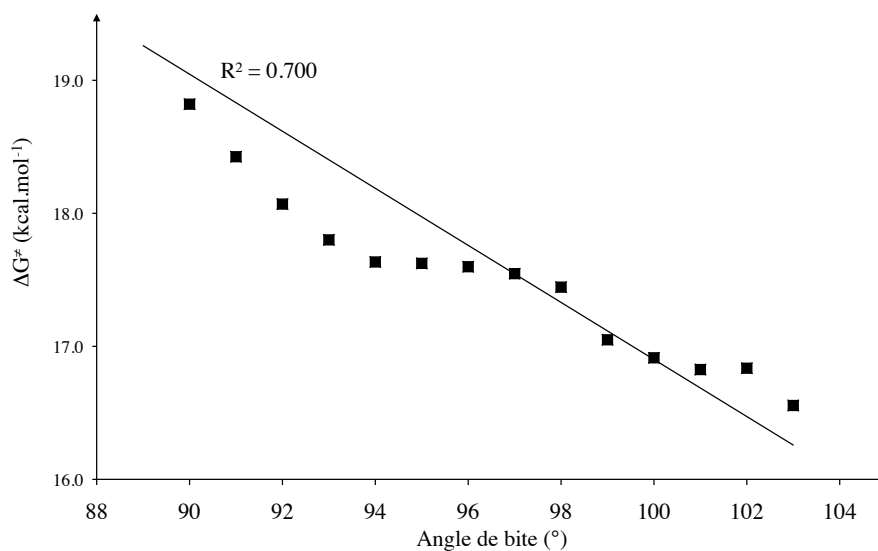


Figure 5 – Influence de l'angle de bite sur la barrière d'activation de la première étape du cycle catalytique pour les réactifs HCu[BiEt-Me] et Me₂CO.

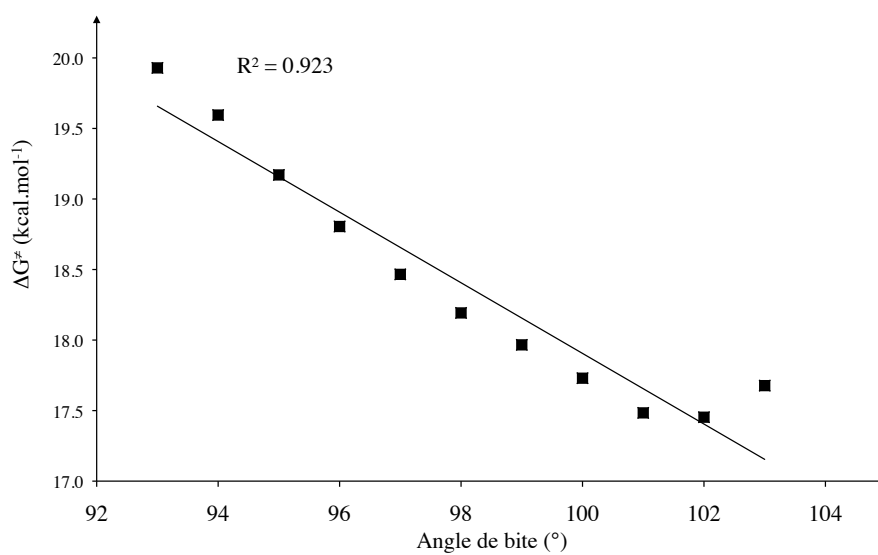


Figure 6 – Influence de l'angle de bite sur la barrière d'activation de la première étape du cycle catalytique pour les réactifs HCu[BiEt-Ph] et Me₂CO.

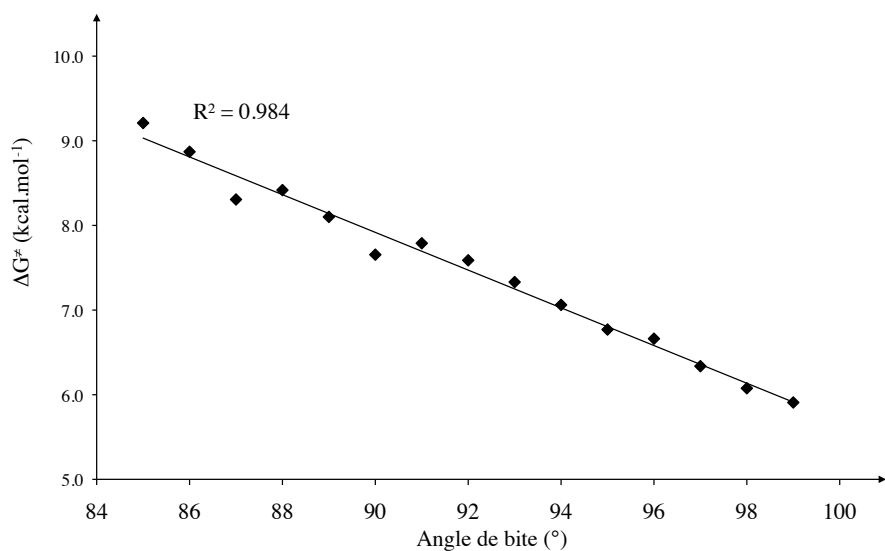


Figure 7 – Influence de l'angle de bite sur la barrière d'activation de la première étape du cycle catalytique pour les réactifs $\text{HCu}[\text{BiEt-H}]$ et H_2CO .

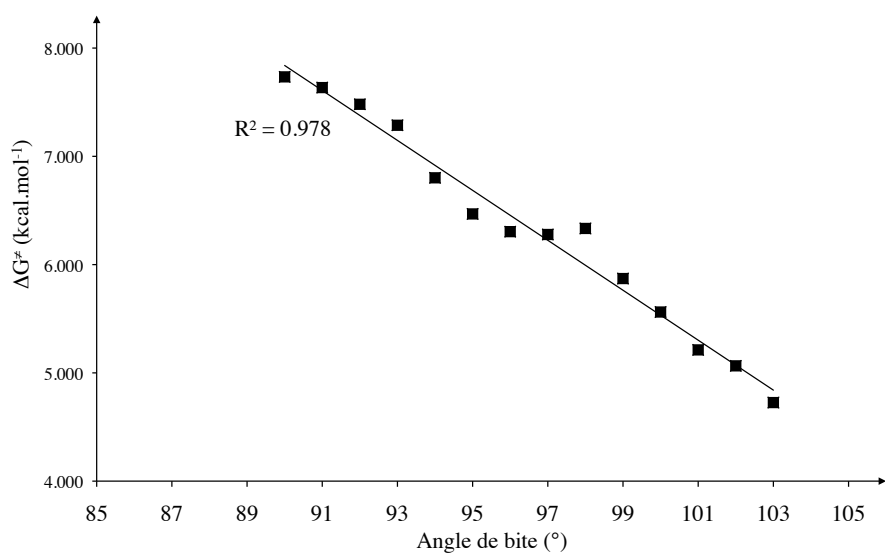


Figure 8 – Influence de l'angle de bite sur la barrière d'activation de la première étape du cycle catalytique pour les réactifs $\text{HCu}[\text{BiEt-Me}]$ et H_2CO .

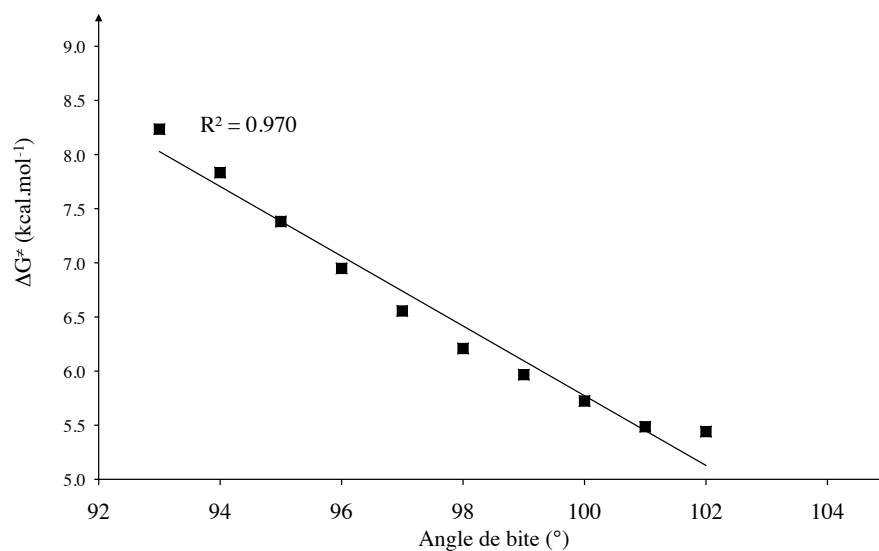


Figure 9 – Influence de l'angle de bite sur la barrière d'activation de la première étape du cycle catalytique pour les réactifs $\text{HCu}[\text{BiEt-Ph}]$ et H_2CO .