Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Exploring the origin of the anomeric relationships in 2-cyanooxane, 2-cyanothiane, 2-cyanoselenane and their iso-cyano isomers. Correlations between hyper-conjugative anomeric effect, hardness and electrostatic interactions

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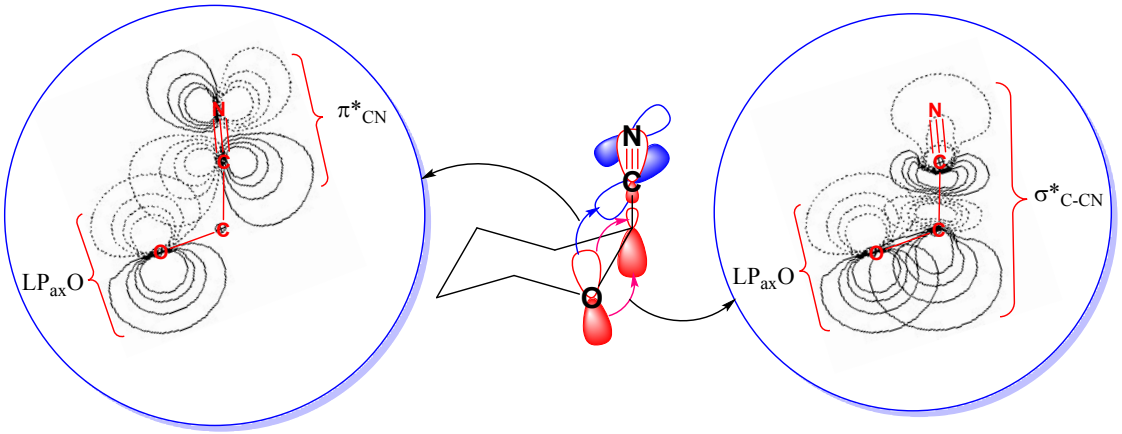

Through-space: $LP_{ax}O_1 \rightarrow \pi^*_{C\equiv N}$ << *Through-bond*: $LP_{ax}O_1 \rightarrow \sigma^*_{C2\text{-}C\equiv N}$

Table SI-1. B3LYP/6-311+G**, LC-ωPBE/6-311+G**[(a)], LC-BLYP/6-311+G**[(b)], M06-2X/6-311+G**[(c)] and MP2/6-311+G**[(d)] calculated structural parameters for the axial and equatorial conformations of compounds **1-6.**

	1		**2**		**3**		**4**		**5**		**6**	
Geometry	*ax*	*eq*	*ax*	*eq*	*ax*	*eq*	*ax*	*eq*	*ax*	*eq*	*ax*	*eq*
Bond lengths (Å)												
$r_{1\text{-}2}$	1.419	1.422	1.851	1.857	2.003	2.009	1.404	1.415	1.843	1.856	1.997	2.007
	(1.403)[a]	(1.406)[a]	(1.812)[a]	(1.817)[a]	(1.949)[a]	(1.954)[a]	(1.391)[a]	(1.401)[a]	(1.806)[a]	(1.817)[a]	(1.944)[a]	(1.954)[a]
	(1.398)[b]	(1.400)[b]	(1.808)[b]	(1.813)[b]	(1.944)[b]	(1.949)[b]	(1.386)[b]	(1.394)[b]	(1.802)[b]	(1.813)[b]	(1.939)[b]	(1.947)[b]
	(1.406)[c]	(1.409)[c]	(1.830)[c]	(1.835)[c]	(1.975)[c]	(1.980)[c]	(1.394)[c]	(1.404)[c]	(1.825)[c]	(1.836)[c]	(1.972)[c]	(1.980)[c]
	(1.417)[d]	(1.419)[d]	(1.824)[d]	(1.828)[d]	(1.977)[d]	(1.980)[d]	(1.401)[d]	(1.410)[d]	(1.815)[d]	(1.826)[d]	(1.971)[d]	(1.978)[d]
			(1.815±1)[e]		(1.953±4)[e]							
$r_{2\text{-}3}$	1.541	1.540	1.544	1.542	1.542	1.540	1.536	1.533	1.538	1.534	1.536	1.532
	(1.527)[a]	(1.525)[a]	(1.530)[a]	(1.529)[a]	(1.530)[a]	(1.528)[a]	(1.523)[a]	(1.520)[a]	(1.526)[a]	(1.522)[a]	(1.525)[a]	(1.521)[a]
	(1.520)[b]	(1.519)[b]	(1.525)[b]	(1.523)[b]	(1.524)[b]	(1.522)[b]	(1.516)[b]	(1.514)[b]	(1.520)[b]	(1.516)[b]	(1.520)[b]	(1.515)[b]
	(1.534)[c]	(1.532)[c]	(1.537)[c]	(1.535)[c]	(1.537)[c]	(1.534)[c]	(1.529)[c]	(1.526)[c]	(1.532)[c]	(1.527)[c]	(1.531)[c]	(1.526)[c]
	(1.533)[d]	(1.532)[d]	(1.538)[d]	(1.536)[d]	(1.538)[d]	(1.535)[d]	(1.529)[d]	(1.526)[d]	(1.533)[d]	(1.528)[d]	(1.533)[d]	(1.528)[d]
			(1.534±2)[e]		(1.536±6)[e]							
$r_{3\text{-}4}$	1.534	1.535	1.534	1.534	1.535	1.535	1.533	1.535	1.534	1.535	1.535	1.535
	(1.522)[a]	(1.523)[a]	(1.523)[a]	(1.523)[a]	(1.524)[a]	(1.523)[a]	(1.522)[a]	(1.523)[a]	(1.523)[a]	(1.523)[a]	(1.523)[a]	(1.524)[a]
	(1.517)[b]	(1.517)[b]	(1.518)[b]	(1.517)[b]	(1.519)[b]	(1.517)[b]	(1.516)[b]	(1.518)[b]	(1.517)[b]	(1.518)[b]	(1.518)[b]	(1.518)[b]
	(1.529)[c]	(1.530)[c]	(1.529)[c]	(1.529)[c]	(1.530)[c]	(1.529)[c]	(1.528)[c]	(1.530)[c]	(1.529)[c]	(1.529)[c]	(1.529)[c]	(1.530)[c]
	(1.530)[d]	(1.531)[d]	(1.531)[d]	(1.531)[d]	(1.531)[d]	(1.532)[d]	(1.530)[d]	(1.531)[d]	(1.530)[d]	(1.531)[d]	(1.531)[d]	(1.532)[d]
			(1.526±2)[e]		(1.522±7)[e]							
$r_{4\text{-}5}$	1.535	1.535	1.536	1.534	1.536	1.535	1.535	1.535	1.535	1.534	1.536	1.535
	(1.523)[a]	(1.523)[a]	(1.524)[a]	(1.523)[a]	(1.525)[a]	(1.524)[a]	(1.523)[a]	(1.523)[a]	(1.524)[a]	(1.523)[a]	(1.524)[a]	(1.524)[a]
	(1.518)[b]	(1.518)[b]	(1.519)[b]	(1.518)[b]	(1.519)[b]	(1.518)[b]	(1.518)[b]	(1.518)[b]	(1.518)[b]	(1.518)[b]	(1.519)[b]	(1.518)[b]
	(1.530)[c]	(1.530)[c]	(1.531)[c]	(1.530)[c]	(1.531)[c]	(1.530)[c]	(1.530)[c]	(1.530)[c]	(1.530)[c]	(1.530)[c]	(1.531)[c]	(1.530)[c]
	(1.532)[d]	(1.531)[d]	(1.532)[d]	(1.530)[d]	(1.533)[d]	(1.531)[d]	(1.531)[d]	(1.531)[d]	(1.531)[d]	(1.530)[d]	(1.532)[d]	(1.531)[d]
			(1.517±2)[e]		(1.530±7)[e]							
$r_{5\text{-}6}$	1.526	1.526	1.529	1.528	1.527	1.526	1.526	1.527	1.528	1.528	1.527	1.526
	(1.516)[a]	(1.516)[a]	(1.520)[a]	(1.519)[a]	(1.519)[a]	(1.518)[a]	(1.516)[a]	(1.517)[a]	(1.519)[a]	(1.519)[a]	(1.519)[a]	(1.518)[a]

Table SI-1 continued…

	(1.510)[b]	(1.510)[b]	(1.514)[b]	(1.513)[b]	(1.513)[b]	(1.513)[b]	(1.510)[b]	(1.510)[b]	(1.514)[b]	(1.513)[b]	(1.513)[b]	(1.512)[b]
	(1.522)[c]	(1.522)[c]	(1.525)[c]	(1.525)[c]	(1.524)[c]	(1.523)[c]	(1.523)[c]	(1.523)[c]	(1.525)[c]	(1.524)[c]	(1.523)[c]	(1.523)[c]
	(1.524)[d]	(1.524)[d]	(1.527)[d]	(1.526)[d]	(1.527)[d]	(1.526)[d]	(1.523)[d]	(1.523)[d]	(1.527)[d]	(1.526)[d]	(1.526)[d]	(1.525)[d]
			(1.519±2)[e]		(1.515±7)[e]							
$r_{6\text{-}1}$	1.437	1.433	1.838	1.837	1.984	1.984	1.440	1.433	1.838	1.838	1.983	1.984
	(1.422)[a]	(1.418)[a]	(1.804)[a]	(1.803)[a]	(1.936)[a]	(1.936)[a]	(1.424)[a]	(1.418)[a]	(1.804)[a]	(1.804)[a]	(1.936)[a]	(1.938)[a]
	(1.416)[b]	(1.412)[b]	(1.800)[b]	(1.799)[b]	(1.931)[b]	(1.931)[b]	(1.418)[b]	(1.412)[b]	(1.800)[b]	(1.800)[b]	(1.931)[b]	(1.933)[b]
	(1.426)[c]	(1.422)[c]	(1.823)[c]	(1.821)[c]	(1.963)[c]	(1.963)[c]	(1.428)[c]	(1.422)[c]	(1.823)[c]	(1.822)[c]	(1.964)[c]	(1.964)[c]
	(1.432)[d]	(1.429)[d]	(1.815)[d]	(1.815)[d]	(1.961)[d]	(1.962)[d]	(1.436)[d]	(1.431)[d]	(1.815)[d]	(1.816)[d]	(1.962)[d]	(1.964)[d]
			(1.8080±15)[e]		(1.937±5)[e]							
$r_{2\text{-}C\equiv N}$	1.484	1.468	1.463	1.458	1.457	1.453	-	-	-	-	-	-
	(1.481)[a]	(1.467)[a]	(1.463)[a]	(1.458)[a]	(1.459)[a]	(1.455)[a]	-	-	-	-	-	-
	(1.475)[b]	(1.460)[b]	(1.457)[b]	(1.452)[b]	(1.453)[b]	1(.449)[b]	-	-	-	-	-	-
	(1.487)[c]	(1.471)[c]	(1.466)[c]	(1.461)[c]	(1.461)[c]	(1.457)[c]	-	-	-	-	-	-
	(1.484)[d]	(1.469)[d]	(1.466)[d]	(1.462)[d]	(1.461)[d]	(1.458)[d]	-	-	-	-	-	-
			(1.477±2)[e]		(1.465±6)[e]							
$r_{C\equiv N}$	1.153	1.152	1.154	1.153	1.155	1.154	-	-	-	-	-	-
	(1.146)[a]	(1.145)[a]	(1.147)[a]	(1.146)[a]	(1.147)[a]	(1.147)[a]	-	-	-	-	-	-
	(1.138)[b]	(1.137)[b]	(1.139)[b]	(1.138)[b]	(1.139)[b]	(1.139)[b]	-	-	-	-	-	-
	(1.149)[c]	(1.148)[c]	(1.149)[c]	(1.149)[c]	(1.150)[c]	(1.149)[c]	-	-	-	-	-	-
	(1.176)[d]	(1.175)[d]	(1.177)[d]	(1.176)[d]	(1.178)[d]	(1.177)[d]	-	-	-	-	-	-
			(1.138±2)[e]		(1.137±6)[e]							
$r_{2\text{-}N=C}$	-	-	-	-	-	-	1.449	1.423	1.430	1.420	1.423	1.416
	-	-	-	-	-	-	(1.442)[a]	(1.420)[a]	(1.428)[a]	(1.419)[a]	(1.423)[a]	(1.417)[a]
	-	-	-	-	-	-	(1.437)[b]	(1.414)[b]	(1.423)[b]	(1.414)[b]	(1.419)[b]	(1.412)[b]
	-	-	-	-	-	-	(1.448)[c]	(1.424)[c]	(1.429)[c]	(1.420)[c]	(1.424)[c]	(1.418)[c]
	-	-	-	-	-	-	(1.444)[d]	(1.422)[d]	(1.430)[d]	(1.421)[d]	(1.424)[d]	(1.419)[d]
$r_{N=C}$	-	-	-	-	-	-	1.171	1.171	1.171	1.172	1.172	1.172
	-	-	-	-	-	-	(1.165)[a]	(1.164)[a]	(1.165)[a]	(1.165)[a]	(1.165)[a]	(1.165)[a]
	-	-	-	-	-	-	(1.157)[b]	(1.156)[b]	(1.157)[b]	(1.157)[b]	(1.157)[b]	(1.157)[b]
	-	-	-	-	-	-	(1.168)[c]	(1.168)[c]	(1.429)[c]	(1.168)[c]	(1.168)[c]	(1.168)[c]

Table SI-1 continued…

	-	-	-	-	-	-	(1.188)[d]	(1.187)[d]	(1.188)[d]	(1.188)[d]	(1.189)[d]	(1.188)[d]
$\Delta[r_{1\text{-}2}(\text{eq})\text{-}r_{1\text{-}2}(\text{ax})]$	0.003		0.006		0.006		0.011		0.013		0.01	
	0.003		0.005		0.005		0.010		0.011		0.01	
	0.003		0.006		0.005		0.01		0.011		0.01	
	0.003		0.006		0.005		0.01		0.011		0.01	
	(0.002)[d]		(0.004)[d]		(0.003)[d]		(0.01)[d]		(0.011)[d]		(0.01)[d]	
$\Delta[r_{2\text{-}C\equiv N}(\text{ax})\text{-}r_{2\text{-}C\equiv N}(\text{eq})]$	0.016		0.005		0.004		-		-		-	
	0.014		0.005		0.004		-		-		-	
	0.016		0.005		0.004		-		-		-	
	0.016		0.005		0.004		-		-		-	
	(0.015)[d]		(0.004)[d]		(0.003)[d]		-		-		-	
$\Delta[r_{2\text{-}N=C}(\text{ax})\text{-}r_{2\text{-}N=C}(\text{eq})]$	-		-		-		0.026		0.010		0.007	
	-		-		-		0.022		0.009		0.006	
	-		-		-		0.023		0.009		0.007	
	-		-		-		0.024		0.009		0.006	
	-		-		-		(0.022)[d]		(0.009)[d]		(0.005)[d]	
$\Delta[r_{1\text{-}2}(\text{ax})\text{-}r_{1\text{-}6}(\text{ax})]$	-0.018		0.013		0.019		-0.036		0.005		0.014	
	-0.019		0.008		0.013		-0.033		0.002		0.008	
	-0.02		-0.008		0.012		-0.034		0.002		0.008	
	-0.02		-0.008		0.012		-0.034		0.002		0.008	
	(-0.015)[d]		(0.009)[d]		(0.016)[d]		(-0.035)[d]		(0.004)[d]		(0.009)[d]	
$\Delta[r_{1\text{-}2}(\text{eq})\text{-}r_{1\text{-}6}(\text{eq})]$	-0.011		0.020		0.025		-0.018		0.018		0.023	
	-0.012		0.014		0.018		-0.017		0.013		0.016	
	-0.013		0.014		0.017		-0.018		0.014		0.016	
	-0.013		0.014		0.017		-0.018		0.014		0.016	
	(-0.010)[d]		(0.013)[d]		(0.018)[d]		(-0.021)[d]		0.01)[d]		(0.014)[d]	
Bond angles (°)												
$\theta_{1\text{-}2\text{-}3}$	112.0	111.9	112.0	112.3	111.6	112.0	112.6	111.8	112.4	112.3	111.8	112.0
	(112.1)[a]	(111.9)[a]	(112.1)[a]	(112.4)[a]	(111.8)[a]	(112.1)[a]	(112.6)[a]	(111.8)[a]	(112.4)[a]	(112.4)[a]	(112.0)[a]	(112.1)[a]
	(111.9)[b]	(111.7)[b]	(112.2)[b]	(112.5)[b]	(111.8)[b]	(112.2)[b]	(112.3)[b]	(111.6)[b]	(112.5)[b]	(112.5)[b]	(112.1)[b]	(112.3)[b]

Table SI-1 continued…

	(112.0)[c]	(111.9[c]	(112.0)[c]	(112.4)[c]	(111.7)[c]	(112.1)[c]	(112.5)[c]	(111.8)[c]	(112.4)[c]	(112.4)[c]	(111.1)[c]	(112.1)[c]
	(111.9)[d]	(111.9[d]	(112.0)[d]	(112.4)[d]	(111.5)[d]	(112.0)[d]	(112.8)[d]	(112.1)[d]	(112.7)[d]	(112.6)[d]	(112.1)[d]	(112.3)[d]
			(112.73±9)[e]		(112.4±3)[e]							
$\theta_{2\text{-}3\text{-}4}$	111.0	109.6	113.5	112.3	114.3	113.3	111.2	109.7	113.8	112.4	114.7	113.2
	(110.5)[a]	(109.2)[a]	(112.8)[a]	(111.8)[a]	(113.6)[a]	(112.6)[a]	(110.8)[a]	(109.3)[a]	(113.1)[a]	(111.9)[a]	(113.9)[a]	(112.6)[a]
	(110.6)[b]	(109.4)[b]	(112.9)[b]	(112.0)[b]	(113.7)[b]	(112.8)[b]	(110.8)[b]	(109.4)[b]	(113.2)[b]	(112.1)[b]	(113.9)[b]	(112.8)[b]
	(110.3)[c]	(109.1)[c]	(112.7)[c]	(111.7)[c]	(113.5)[c]	(112.5)[c]	(110.5)[c]	(109.2)[c]	(112.9)[c]	(111.8)[c]	(113.7)[c]	(112.6)[c]
	(110.2)[d]	(109.2)[d]	(112.4)[d]	(111.6)[d]	(113.2)[d]	(112.5)[d]	(110.3)[d]	(109.1)[d]	(112.5)[d]	(111.6)[d]	(113.3)[d]	(112.5)[d]
			(112.50±11)[e]		(113.1±4)[e]							
$\theta_{3\text{-}4\text{-}5}$	110.1	110.5	113.4	113.6	114.3	114.7	110.0	110.4	113.4	113.6	114.4	114.6
	(109.7)[a]	(110.1)[a]	(113.0)[a]	(113.1)[a]	(114.0)[a]	(114.1)[a]	(109.6)[a]	(110.1)[a]	(112.9)[a]	(113.1)[a]	(113.9)[a]	(114.0)[a]
	(109.8)[b]	(110.1)[b]	(113.1)[b]	(113.2)[b]	(114.0)[b]	(114.1)[b]	(109.7)[b]	(110.1)[b]	(113.0)[b]	(113.1)[b]	(114.0)[b]	(114.1)[b]
	(109.6)[c]	(109.9)[c]	(113.0)[c]	(113.1)[c]	(114.0)[c]	(114.1)[c]	(109.4)[c]	(109.9)[c]	(112.1)[c]	(113.0)[c]	(113.9)[c]	(114.0)[c]
	(109.4)[d]	(109.7)[d]	(112.9)[d]	(112.9)[d]	(114.0)[d]	(114.0)[d]	(109.3)[d]	(109.7)[d]	(112.8)[d]	(112.8)[d]	(114.0)[d]	(113.9)[d]
			(113.27±12)[e]		(114.1±4)[e]							
$\theta_{4\text{-}5\text{-}6}$	110.5	110.3	113.0	112.8	113.7	113.7	110.3	110.2	112.8	112.7	113.7	113.6
	(110.1)[a]	(110.0)[a]	(112.5)[a]	(112.3)[a]	(113.2)[a]	(113.1)[a]	(110.0)[a]	(109.9)[a]	(112.3)[a]	(112.2)[a]	(113.1)[a]	(113.0)[a]
	(110.2)[b]	(110.1)[b]	(112.5)[b]	(112.3)[b]	(113.3)[b]	(113.1)[b]	(110.1)[b]	(109.9)[b]	(112.4)[b]	(112.2)[b]	(113.1)[b]	(113.0)[b]
	(110.0)[c]	(109.9)[c]	(112.5)[c]	(112.2)[c]	(113.3)[c]	(113.0)[c]	(109.9)[c]	(109.7)[c]	(112.4)[c]	(112.1)[c]	(113.1)[c]	(112.9)[c]
	(110.2)[d]	(109.9)[d]	(112.5)[d]	(112.0)[d]	(113.3)[d]	(112.9)[d]	(110.2)[d]	(109.7)[d]	(112.4)[d]	(111.9)[d]	(113.3)[d]	(112.9)[d]
			(112.51±12)[e]		(113.6±3)[e]							
$\theta_{5\text{-}6\text{-}1}$	111.7	111.6	112.9	113.1	112.6	112.8	111.7	111.6	112.9	113.0	112.7	112.8
	(111.6)[a]	(111.5)[a]	(112.6)[a]	(112.8)[a]	(112.4)[a]	(112.6)[a]	(111.6)[a]	(111.4)[a]	(112.6)[a]	(112.8)[a]	(112.4)[a]	(112.6)[a]
	(111.4)[b]	(111.3)[b]	(112.7)[b]	(112.9)[b]	(112.5)[b]	(112.8)[b]	(111.4)[b]	(111.2)[b]	(112.7)[b]	(112.9)[b]	(112.5)[b]	(112.7)[b]
	(111.5[c]	(111.4)[c]	(112.5)[c]	(112.7)[c]	(112.2)[c]	(112.5)[c]	(111.5)[c]	(111.3)[c]	(112.5)[c]	(112.7)[c]	(112.3)[c]	(112.4)[c]
	(111.6)[d]	(111.4)[d]	(112.4)[d]	(112.6)[d]	(112.2)[d]	(112.4)[d]	(111.6)[d]	(111.3)[d]	(112.5)[d]	(112.6)[d]	(112.2)[d]	(112.5)[d]
			(112.93±10)[e]		(113.1±3)[e]							
$\theta_{6\text{-}1\text{-}2}$	113.9	112.0	98.1	97.0	94.8	94.1	114.6	112.0	98.3	97.0	94.9	94.1
	(113.3)[a]	(111.5)[a]	(97.8)[a]	(96.9)[a]	(94.5)[a]	(94.0)[a]	(114.1)[a]	(111.5)[a]	(98.0)[a]	(96.7)[a]	(94.7)[a]	(94.1)[a]
	(113.9)[b]	(112.2)[b]	(97.8)[b]	(96.9)[b]	(94.6)[b]	(94.1)[b]	(114.6)[b]	(112.2)[b]	(98.0)[b]	(96.8)[b]	(94.7)[b]	(94.2)[b]
	(113.5)[c]	(111.7)[c]	(97.1)[c]	(96.3)[c]	(93.5)[c]	(93.4)[c]	(114.1)[c]	(111.7)[c]	(97.2)[c]	(96.2)[c]	(93.8)[c]	(93.5)[c]

Table SI-1 continued…

	(112.2)[d]	(110.5)[d]	(96.7)[d]	(96.2)[d]	(93.0)[d]	(93.1)[d]	(113.0)[d]	(110.5)[d]	(96.8)[d]	(95.9)[d]	(93.0)[d]	(93.0)[d]
			(98.93±7)[e]		(95.7±2)[e]							
$\theta_{1\text{-}2\text{-}C\equiv N}$	111.1	107.7	110.8	108.1	110.2	107.7	-	-	-	-	-	-
	(110.9)[a]	(107.8)[a]	(110.7)[a]	(108.3)[a]	(110.3)[a]	(108.1)[a]	-	-	-	-	-	-
	(110.8)[b]	(107.8)[b]	(110.8)[b]	(108.4)[b]	(110.4)[b]	(108.2)[b]	-	-	-	-	-	-
	(110.8)[c]	(107.6)[c]	(110.1)[c]	(107.9)[c]	(109.5)[c]	(107.70)[c]	-	-	-	-	-	-
	(110.8)[d]	(107.3)[d]	(110.5)[d]	(108.0)[d]	(109.7)[d]	(107.7)[d]	-	-	-	-	-	-
			(109.55±10)[e]		(110.1±3)[e]							
$\theta_{1\text{-}2\text{-}N=C}$	-	-	-	-	-	-	110.7	107.1	111.5	107.7	111.3	107.7
	-	-	-	-	-	-	(110.5)[a]	(107.2)[a]	(111.3)[a]	(107.8)[a]	(111.1)[a]	(107.9)[a]
	-	-	-	-	-	-	(110.3)[b]	(107.3)[b]	(111.3)[b]	(107.8)[b]	(111.0)[b]	(107.9)[b]
	-	-	-	-	-	-	(110.3)[c]	(107.1)[c]	(110.8)[c]	(107.6)[c]	(110.5)[c]	(107.7)[c]
	-	-	-	-	-	-	(110.2)[d]	(106.6)[d]	(110.9)[d]	(107.5)[d]	(110.4)[d]	(107.5)[d]
$\Delta[\theta_{6\text{-}1\text{-}2}(ax)\text{-}\theta_{6\text{-}1\text{-}2}(eq)]$	1.8		1.1		0.71		2.5		1.4		0.8	
	(1.8)[a]		(0.9)[a]		(0.5)[a]		(2.6)[a]		(1.3)[a]		(0.6)[a]	
	(1.8)[b]		(0.8)[b]		(0.1)[b]		(2.4)[b]		(1.3)[b]		(0.3)[b]	
	(1.8)[c]		(0.8)[c]		(0.1)[c]		(2.4)[c]		(1.3)[c]		(0.3)[c]	
	(1.7)[d]		(0.5)[d]		(0.1)[d]		(2.5)[d]		(0.9)[d]		(0.0)[d]	
Torsion angles (°)												
$\phi_{1\text{-}2\text{-}3\text{-}4}$	53.2	55.9	59.5	61.0	60.6	61.5	52.2	56.3	58.9	61.2	60.2	61.7
	(54.3)[a]	(57.0)[a]	(60.5)[a]	(61.9)[a]	(61.7)[a]	(62.5)[a]	(53.3)[a]	(57.3)[a]	(59.9)[a]	(62.2)[a]	(61.1)[a]	(62.7)[a]
	(54.0)[b]	(56.5[b]	(60.4)[b]	(61.6)[b]	(61.5)[b]	(62.2)[b]	(53.1)[b]	(56.8)[b]	(59.9)[b]	(61.8)[b]	(61.0)[b]	(62.4)[b]
	(54.6)[c]	(56.9[c]	(61.3)[c]	(62.2)[c]	(62.4)[c]	(62.9)[c]	(53.7)[c]	(57.3)[c]	(60.7)[c]	(62.5)[c]	(62.0)[c]	(63.0)[c]
	(55.9)[d]	(57.8)[d]	(62.0)[d]	(62.4)[d]	(63.3)[d]	(63.2)[d]	(54.9)[d]	(58.0)[d]	(61.4)[d]	(62.8)[d]	(62.8)[d]	(63.4)[d]
$\phi_{2\text{-}3\text{-}4\text{-}5}$	-51.4	-51.6	-59.1	-59.6	-62.8	-63.0	-51.1	-51.7	-58.8	-59.8	-62.2	-63.4
	(-52.2)[a]	(-52.4)[a]	(-59.0)[a]	(-59.6)[a]	(-61.8)[a]	(-62.6)[a]	(-52.0)[a]	(-52.4)[a]	(-58.8)[a]	(-59.7)[a]	(-61.6)[a]	(-63.0)[a]
	(-52.3)[b]	(52.4)[b]	(-59.0)[b]	(-59.5)[b]	(-61.8)[b]	(-62.6)[b]	(-52.1)[b]	(-52.4)[b]	(-58.9)[b]	(-59.6)[b]	(-61.6)[b]	(-62.9)[b]
	(-52.7)[c]	(-52.7)[c]	(-59.2)[c]	(-60.0)[c]	(-61.8)[c]	(-63.2)[c]	(-52.4)[c]	(-52.8)[c]	(-59.1)[c]	(-60.1)[c]	(-62.2)[c]	(-63.6)[c]
	(-52.7)[d]	(52.8)[d]	(-58.9)[d]	(-59.8)[d]	(-61.7)[d]	(-63.0)[d]	(-52.5)[d]	(-52.8)[d]	(-58.7)[d]	(-59.8)[d]	(-61.3)[d]	(-63.1)[d]
$\phi_{3\text{-}4\text{-}5\text{-}6}$	52.5	51.9	59.2	59.4	63.0	62.8	52.7	51.7	59.3	59.4	62.3	63.0
	(53.29)[a]	(52.6)[a]	(59.3)[a]	(59.5)[a]	(61.9)[a]	(62.5)[a]	(53.6)[a]	(52.3)[a]	(59.4)[a]	(59.3)[a]	(62.0)[a]	(62.6)[a]

Table SI-1 continued…

	(53.3)[b]	(52.6)[b]	(59.2)[b]	(59.5)[b]	(61.8)[b]	(62.5)[b]	(53.6)[b]	(52.4)[b]	(59.4)[b]	(59.4)[b]	(62.0)[b]	(62.6)[b]
	(53.7)[c]	(53.1)[c]	(59.5)[c]	(60.1)[c]	(62.1)[c]	(63.3)[c]	(54.0)[c]	(52.9)[c]	(59.6)[c]	(60.0)[c]	(62.6)[c]	(63.4)[c]
	(53.3)[d]	(-53.1)[d]	(58.9)[d]	(60.0)[d]	(61.5)[d]	(63.0)[d]	(53.8)[d]	(53.0)[d]	(59.2)[d]	(59.9)[d]	(61.6)[d]	(63.1)[d]
$\phi_{4\text{-}5\text{-}6\text{-}1}$	-55.2	-55.6	-60.6	-60.9	-61.9	-61.6	-54.9	-55.3	-60.6	-60.9	-61.4	-61.4
	(-56.1)[a]	(-56.3)[a]	(-61.5)[a]	(-61.8)[a]	(-62.5)[a]	(-62.5)[a]	(-55.8)[a]	(-56.2)[a]	(-61.6)[a]	(-61.8)[a]	(-62.6)[a]	(-62.3)[a]
	(-55.7)[b]	(56.0)[b]	(-61.4)[b]	(-61.6)[b]	(-62.3)[b]	(-62.3)[b]	(-55.5)[b]	(-55.8)[b]	(-61.4)[b]	(-61.6)[b]	(-62.4)[b]	(-62.1)[b]
	(-56.2)[c]	(-56.7)[c]	(-62.0)[c]	(-62.4)[c]	(-63.3)[c]	(-63.1)[c]	(-56.0)[c]	(-56.5)[c]	(-62.1)[c]	(-62.4)[c]	(-63.2)[c]	(-62.9)[c]
	(-56.5)[d]	(57.5)[d]	(-62.2)[d]	(-62.8)[d]	(-63.4)[d]	(-63.4)[d]	(-56.2)[d]	(-57.4)[d]	(-62.3)[d]	(-62.9)[d]	(-63.5)[d]	(-63.4)[d]
$\phi_{5\text{-}6\text{-}1\text{-}2}$	58.1	60.2	53.9	54.6	51.8	52.0	57.2	60.4	53.7	54.6	51.6	51.6
	(58.8)[a]	(60.9)[a]	(55.6)[a]	(56.0)[a]	(53.9)[a]	(53.6)[a]	(57.8)[a]	(61.2)[a]	(55.2)[a]	(56.1)[a]	(53.6)[a]	(53.4)[a]
	(58.6)[b]	(-60.6)[b]	(55.3)[b]	(55.7)[b]	(53.6)[b]	(53.3)[b]	(57.6)[b]	(60.9)[b]	(55.0)[b]	(55.7)[b]	(53.3)[b]	(53.0)[b]
	(58.8)[c]	(60.9)[c]	(56.0 [c]	(56.2)[c]	(54.0)[c]	(53.7)[c]	(58.0)[c]	(61.2)[c]	(55.8)[c]	(56.3)[c]	(54.0)[c]	(53.5)[c]
	(59.5)[d]	(-61.7)[d]	(56.8)[d]	(56.9)[d]	(55.4)[d]	(54.4)[d]	(58.2) [d]	(61.8)[d]	(56.3)[d]	(57.0)[d]	(55.1)[d]	(54.2)[d]
$\phi_{6\text{-}1\text{-}2\text{-}3}$	-56.8	-60.5	-53.0	-54.5	-50.7	-51.9	-55.4	-61.0	-52.3	-54.7	-50.5	-51.8
	(-57.7)[a]	(-61.4)[a]	(-54.8)[a]	(-56.1)[a]	(-53.2)[a]	(-53.6)[a]	(-56.3)[a]	(-61.9)[a]	(-54.0)[a]	(-56.3)[a]	(-52.5)[a]	(-53.6)[a]
	(-57.5)[b]	(-61.0)[b]	(-54.5)[b]	(-55.6)[b]	(-52.9)[b]	(-53.2)[b]	(-56.2)[b]	(-61.5)[b]	(-53.9)[b]	(-55.8)[b]	(-52.3)[b]	(-53.1)[b]
	(-57.9)[c]	(-61.3)[c]	(-55.4)[c]	(-56.2)[c]	(-54.0)[c]	(-53.7)[c]	(-56.7)[c]	(-61.8)[c]	(-54.8)[c]	(-56.4)[c]	(-53.1)[c]	(-53.6)[c]
	(-59.1)[d]	(-62.1)[d]	(-56.6)[d]	(-56.8)[d]	(-55.1)[d]	(-54.3)[d]	(-57.5)[d]	(-62.4)[d]	(-55.9)[d]	(-57.1)[d]	(-54.7)[d]	(-54.4)[d]
$\Delta[\phi_{6\text{-}1\text{-}2\text{-}3}(\text{ax})\text{-}\phi_{6\text{-}1\text{-}2\text{-}3}(\text{eq})]$	3.7		1.5		1.2		5.6		2.4		1.3	
	3.7		1.3		0.4		5.6		2.3		1.1	
	3.5		1.1		0.3		5.3		1.9		0.8	
	3.7		1.5		1.2		5.6		2.4		1.3	
	(3.0)[d]		(0.2)[d]		(0.8)[d]		(4.9)[d]		(1.2)[d]		(0.3)[d]	

[e] From X-ray crystallography, Ref. 20.

Table SI-2. LC-ωPBE/6-311+G**, LC-BLYP/6-311+G**[(a)] and MP2/6-311+G**[(b)] calculated zero-point energies (ZPE), corrected electronic energies (E_o), thermodynamic functions (*H, G* in hartree, *S* in: cal mol^{-1}K^{-1}) and parameters [ΔZPE, ΔE_o, ΔH, ΔG (in: kcal mol^{-1})] and ΔS (in: cal mol^{-1}K^{-1})] at 25 ºC and 1 atm pressure for the axial and equatorial conformations of compounds **1-6**.

	H	*S*	*G*	*ZPE*	E_o	ΔH	ΔS	ΔG	ΔZPE	ΔE_o
1-*ax*	-363.714233	82.483	-363.753423	0.147672	-363.722205	0.00	0.000	0.00	0.18	0.00
	(-362.957805)[a]	(82.053)[a]	(-362.996791)[a]	(0.148758)[a]	(-362.965675)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	(0.18)[a]	(0.00)[a]
	(-362.914739)[b]	(82.928)[b]	(-362.954141)[b]	(0.146110)[b]	(-362.922814)[b]	(0.00)[b]	(0.000)[b]	(0.00)[b]	(0.18)[b]	(0.00)[b]
1-*eq*	-363.712609	82.754	-363.751928	0.147378	-363.720626	1.02	0.271	0.94	0.00	0.99
	(-362.956454)[a]	(82.311)[a]	(-362.995563)[a]	(0.148475)[a]	(-362.964366)[a]	(0.85)[a]	(0.258)[a]	(0.77)[a]	(0.00)[a]	(0.82)[a]
	(-362.912804)[b]	(83.209)[b]	(-362.952340)[b]	(0.145826)[b]	(-362.920925)[b]	(1.21)[b]	(0.281)[b]	(1.13)[b]	(0.00)[b])[b]	(1.18)[b]
2-*ax*	-686.613462	85.571	-686.654120	0.144436	-686.621945	0.00	0.000	0.00	0.10	0.00
	(-685.811575)[a]	(85.124)[a]	(-685.852020)[a]	(0.145439)[a]	(-685.819954)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	(0.11)[a]	(0.00[(a)]
	(-685.525245)[b]	(86.056)[b]	(-685.566133)[b]	(0.142747)[b]	(-685.533848)[b]	(0.00)[b]	(0.000)[b]	(0.00)[b]	(0.13)[b]	(0.00)[b]
2-*eq*	-686.611058	86.005	-686.651922	0.144272	-686.619609	1.52	0.434	1.38	0.00	1.47
	(-685.809330)[a]	(85.554)[a]	(-685.849979)[a]	(0.145265)[a]	(-685.817778)[a]	(1.41)[a]	(0.43)[a]	(1.28)[a]	(0.00)[a]	(1.37)[a]
	(-685.522452)[b]	(86.563)[b]	(-685.563581)[b]	(0.142544)[b]	(-685.531129)[b]	(1.75)[b]	(0.510)[b]	(1.60)[b]	(0.00)[b]	(1.71)[b]
3-*ax*	-2689.714633	88.809	-2689.756831	0.143163	-2689.723471	0.00	0.000	0.00	0.10	0.00
	(-2689.001582)[a]	(88.338)[a]	(-2689.043554)[a]	(0.144173)[a]	(-2689.010313)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	(0.10)[a]	(0.00)[a]
	(-2687.775548)[b]	(89.343)[b]	(- 2687.817997)[b]	(0.141270)[b]	(-2687.784525)[b]	(0.00)[b]	(0.000)[b]	(0.00)[b]	(0.14)[b]	(0.00)[b]
3-*eq*	-2689.712719	89.255	-2689.755130	0.142983	-2689.721629	1.18	0.446	1.05	0.00	1.14
	(-2688.999797)[a]	(88.766)[a]	(-2689.041972)[a]	(0.144009)[a]	(-2689.008596)[a]	(1.12)[a]	(0.428)[a]	(0.99)[a]	(0.00)[a]	(1.08)[a]
	(-2687.773076)[b]	(89.957)[b]	(-2687.815817)[b]	(0.141048)[b]	(-2687.782142)[b]	(1.55)[b]	(0.614)[b]	(1.37)[b]	(0.00)[b]	(1.49)[b]
4-*ax*	-363.686485	82.957	-363.725904	0.147332	-363.694590	0.00	0.000	0.00	0.24	0.00
	(-362.932410)[a]	(82.501)[a]	(-362.971609)[a]	(0.148404)[a]	(-362.940409)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	(0.23)[a]	(0.00)[a]
	(-362.881703)[b]	(83.433)[b]	(-362.921345)[b]	(0.146182)[b]	(-362.889897)[b]	(0.00)[b]	(0.000)[b]	(0.00)[b]	(0.26)[b]	(0.00)[b]
4-*eq*	-363.683530	83.299	-363.723113	0.146942	-363.691699	1.87	0.342	1.77	0.00	1.83
	(-362.929546)[a]	(82.810)[a]	(-362.968892)[a]	(0.148036)[a]	(-362.937602)[a]	(1.80[(a)]	(0.309)[a]	(1.70)[a]	(0.00)[a]	(1.76)[a]
	(-362.878130)[b]	(83.781)[b]	(-362.917937)[b]	(0.145772)[b]	(-362.886388)[b]	(2.24)[b]	(0.348)[b]	(2.14)[b]	(0.00)[b]	(2.20)[b]
5-*ax*	-686.579949	86.007	-686.620814	0.143995	-686.588564	0.00	0.000	0.00	0.13	0.00
	(-685.780602)[a]	(85.537)[a]	(-685.821244)[a]	(0.144982)[a]	(-685.789111)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	(0.14)[a]	(0.00)[a]

Table SI-2 continued…

	(-685.486519)[b]	(86.337)[b]	(-685.527540)[b]	(0.142716)[b]	(-685.495214)[b]	(0.00)[b]	(0.000)[b]	(0.00)[b]	(0.19)[b]	(0.00)[b]
5-*eq*	-686.576874	86.503	-686.617975	0.143781	-686.585575	1.930	0.496	1.78	0.00	1.88
	(-685.777704)[a]	(86.024)[a]	(-685.818577)[a]	(0.144764)[a]	(-685.786297)[a]	(1.82)[a]	(0.487)[a]	(1.67)[a]	(0.00)[a]	(1.77)[a]
	(-685.482587)[b]	(87.103)[b]	(-685.523972)[b]	(0.142407)[b]	(-685.491404)[b]	(2.47)[b]	(0.766)[b]	(2.24)[b]	(0.00)[b]	(2.39)[b]
6-*ax*	-2689.679948	89.235	-2689.722351	0.142728	-2689.688920	0.00	0.000	0.00	0.14	0.00
	(-2688.969475)[a]	(88.753)[a]	(-2689.011644)[a]	(0.143713)[a]	(-2688.978339)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	(0.13)[a]	(0.00)[a]
	(-2687.735645)[b]	(89.650)[b]	(-2687.778240)[b]	(0.141206)[b]	(-2687.744723)[b]	(0.00)[b]	(0.000)[b]	(0.00)[b]	(0.20)[b]	(0.00)[b]
6-*eq*	-2689.677757	89.737	-2689.720399	0.142499	-2689.686817	1.37	0.502	1.22	0.00	1.31
	(-2688.967409)[a]	(89.217[(a)]	(-2689.009799)[a]	(0.143499)[a]	(-2688.976355)[a]	(1.30)[a]	(0.464)[a]	(1.16)[a]	(0.00)[a]	(1.24)[a]
	(-2687.732451)[b)]	(90.497)[b]	(-2687.775449)[b]	(0.140879)[b]	(-2687.741660)[b]	(2.00)[b]	(0.847)[b]	(1.75)[b]	(0.00)[b]	(1.92)[b]

Table SI-3. B3LYP/6-311+G** and M06-2X/6-311+G**[(a)] calculated thermodynamic functions and parameters [*H, G* (in hartree), Δ*H*, Δ*G* (in kcal mol^{-1}), *S* and Δ*S* (in cal mol^{-1}K^{-1})] at 25 ºC and 1 atm pressure for the axial and equatorial conformations of compounds **1-3** and **4-6**.

	H	*S*	*G*	*ZPE*	E_o	Δ*H*	Δ*S*	Δ*G*	Δ*ZPE*	ΔE_o
1-*ax*	-363.957505	83.104	-363.996990	0.144451	-363.965624	0.00	0.000	0.00	0.19	0.00
	(-363.801060)[a]	(82.53)[a]	(-363.840274)[a]	(0.146295)[a]	(-363.809052)[a]	(0.00)[a]	0.00[a]	(0.00)[a]	(0.17)[a]	(0.00)[a]
1-*eq*	-363.956694	83.278	-363.996262	0.144143	-363.964841	0.51	0.174	0.46	0.00	0.49
	(-363.798576)[a]	(82.803)[a]	(-363.837919)[a]	(0.146030)[a]	(-363.806614)[a]	(1.56)[a]	0.27[a]	(1.48)[a]	(0.00)[a]	(1.53)[a]
2-*ax*	-686.944965	86.451	-686.986041	0.141116	-686.953653	0.00	0.000	0.00	0.09	0.00
	(-686.783607)[a]	(85.724) [a]	(-686.824337)[a]	(0.142581)[a]	(-686.792157)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	0.03 [a]	(0.00)[a]
2-*eq*	-686.943457	86.737	-686.984669	0.140977	-686.952193	0.95	0.286	0.86	0.00	0.92
	(-686.780431)[a]	(86.222) [a]	(-686.821398)[a]	(0.142541)[a]	(-686.789051)[a]	(1.99)[a]	(0.498)[a]	(1.84)[a]	0.00	(1.95)[a]
3-*ax*	-2690.278766	89.826	-2690.321445	0.139848	-0.287834269	0.00	0.000	0.00	0.07	0.00
	(-2690.150407)[a]	(88.915)[a]	(-2690.192654)[a]	(0.141381)[a]	(-2690.159306)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	(0.05)[a]	(0.00)[a]
3-*eq*	-2690.277820	90.080	-2690.320620	0.139739	-2690.286931	0.59	0.254	0.52	0.00	0.57
	(-2690.147626)[a]	(89.379)[a]	(-2690.190092)[a]	(0.141457)[a]	(-2690.156584)[a]	(0.00)[a]	(0.464)[a]	(1.61)[a]	(0.00)[a]	(1.71)[a]
4-*ax*	-363.929465	83.774	-363.969268	0.144093	-363.937745	0.00	0.000	0.00	0.24	0.00
	(-363.776149)[a]	(82.939)[a]	(-363.815555)[a]	(0.145990)[a]	(-363.784257)[a]	(0.00)[a]	(0.000)[a]	(0.00)a	(0.19)[a]	(0.00)[a]
4-*eq*	-363.927349	83.963	-363.967243	0.143709	-363.935667	1.33	0.189	1.27	0.00	1.30
	(-363.772272)[a]	(83.176)[a]	(-363.811792)[a]	(0.145679)[a]	(-363.780427)[a]	(2.43)[a]	(0.237)[a]	(2.36)[a]	(0.00)[a]	(2.40)[a]
5-*ax*	-686.911635	87.084	-686.953011	0.140614	-686.920484	0.00	0.000	0.00	0.09	0.00
	(-686.752970)[a]	86.085)[a]	-686.793872)[a]	0.142247)[a]	-686.761631)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	(0.08)[a]	(0.00)[a]
5-*eq*	-686.909684	87.334	-686.951179	0.140472	-686.918583	1.22	0.250	1.15	0.00	1.19
	(-686.749345)[a]	86.590)[a]	-686.790486)[a]	0.142121)[a]	-686.758087)[a]	(2.27)[a]	(0.500)[a]	(2.12)[a]	(0.00)[a]	(2.22)[a]

Table SI-3 continued…

6-*ax*	-2690.244385	90.315	-2690.287297	0.139427	-2690.253592	0.00	0.000	0.00	0.12	0.00
	(-2690.118720)[a]	(89.583)[a]	(-2690.161283)[a]	0.140910)[a]	(-2690.127776)[a]	(0.00)[a]	(0.000)[a]	(0.00)[a]	(0.09)[a]	(0.00)[a]
6-*eq*	-2690.243304	90.640	-2690.286370	0.139229	-2690.25258	0.68	0.325	0.58	0.00	0.64
	(-2690.115761)[a]	(89.741)[a]	(-2690.158400)[a]	0.141044)[a]	(-2690.124841)[a]	(1.86)[a]	(0.160)[a]	(1.81)[a]	(0.00)[a]	(1.84)[a]

Table SI-4. B3LYP/6-311+G** and M06-2X/6-311+G**[(a)] calculated energies (in hartree) of HOMO (ε_{HOMO}), LUMO (ε_{LUMO}), ε_{LUMO}-ε_{HOMO} and global hardness (η) for the axial and equatorial conformations of compounds **1-6**.

	ε_{HOMO}	ε_{LUMO}	ε_{LUMO}-ε_{HOMO}	I	A	η	$\Delta\eta$
1-*ax*	-0.28735	-0.01081	0.27654	0.28735	0.01081	0.13827	0.00192(1.20)[b]
	(-0.35042)[a]	(0.00446)[a]	(0.35488)[a]	(0.35042)[a]	(-0.00446)[a]	(0.17744)[a]	(0.00218)[a](1.37)[b]
1-*eq*	-0.28437	-0.01166	0.27271	0.28437	0.01166	0.13636	0.00000
	(-0.34768)[a]	(0.00284)[a]	(0.35052)[a]	(0.34768)[a]	(-0.00284)[a]	(0.17526)[a]	(0.00000)[a]
2-*ax*	-0.24717	-0.01661	0.23056	0.24717	0.01661	0.11528	0.00122(0.77)[b]
	(-0.29847)[a]	0.00377)[a]	(0.30224)[a]	(0.29847)[a]	(-0.00377)[a]	(0.15112)[a]	(0.00189)[a](1.19)[b]
2-*eq*	-0.24655	-0.01356	0.23299	0.24655	0.01356	0.116495	0.00000
	(-0.29830)[a]	0.00015)[a]	(0.29845)[a]	(0.29830)[a]	(-0.00015)[a]	(0.14923)[a]	(0.00000)[a]
3-*ax*	-0.23519	-0.03593	0.19926	0.23519	0.03593	0.09963	0.00108(0.68)[b]
	-0.28414)[a]	-0.00329)[a]	0.28085[a]	0.28414[a]	0.00329[a]	0.140425[a]	-0.00020[a](-0.131)[b]
3-*eq*	-0.23514	-0.03373	0.20141	0.23514	0.03373	0.100705	0.00000
	-0.28462)[a]	-0.00373)[a]	0.28089[a]	0.28462[a]	0.00373[a]	0.140445[a]	0.00000[a]
4-*ax*	-0.28930	-0.01047	0.27883	0.28930	0.01047	0.139415	0.00324(2.03)[b]
	-0.35128[a]	0.00480[a]	0.35608[a]	0.35128[a]	-0.0048[a]	0.17804[a]	0.00313[a](1.96)[b]
4-*eq*	-0.28288	-0.01053	0.27235	0.28288	0.01053	0.136175	0.00000
	-0.34568[a]	0.00413[a]	0.34981[a]	0.34568[a]	-0.00413[a]	0.17491[a]	0.00000[a]
5-*ax*	-0.24711	-0.0136	0.23351	0.24711	0.0136	0.11676	0.00166(1.04)[b]
	-0.29845[a]	0.00391[a]	0.30236[a]	0.29845[a]	-0.00391[a]	0.15118[a]	0.00236[a](1.48)[b]
5-*eq*	-0.24461	-0.01441	0.23020	0.24461	0.01441	0.11510	0.00000
	-0.29619[a]	0.00144[a]	0.29763[a]	0.29619[a]	-0.00144[a]	0.14882[a]	0.00000[a]
6-*ax*	-0.23419	-0.03193	0.20226	0.23419	0.03193	0.10113	0.00106(0.67)[b]
	-0.28326[a]	-0.00107[a]	0.28219[a]	0.28326[a]	0.00107[a]	0.14110[a]	0.00162[a](1.02)[b]
6-*eq*	-0.2329	-0.03279	0.20011	0.2329	0.03279	0.100055	0.00000
	-0.28224[a]	-0.00329[a]	0.27895[a]	0.28224[a]	0.00329[a]	0.13948[a]	0.00000[a]

[b] Values in kcal mol^{-1}.