JA012700P-3-a-335

SUPPLEMENTARY MATERIAL

Table 7. Atomic electric charges derived from a Mulliken Population Analysis, and, in parentheses, Natural Population Analysis) at the MPW1K/6-311G** level on the sulfoxide precursor of a variety of compounds (see first entry for details).

Obtained compound	O	S	C_α	C_β	H_β
Ethylene	-0.63	+0.68	-0.44	-0.36	+0.17
	(-0.98)	(+1.18)	(-0.54)	(-0.59)	(+0.22)
α-CN-ethylene[a]	-0.61	+0.74	-0.45	-0.31	+0.18
	(-0.96)	(+1.22)	(-0.47)	(-0.58)	(+0.23)
β-CN-ethylene[a]	-0.62	+0.69	-0.44	-0.24	+0.19
	(-0.98)	(+1.19)	(-0.53)	(-0.51)	(+0.24)
α-Cl-ethylene[a]	-0.62	+0.73	-0.48	-0.30	+0.18
	(-0.97)	(+1.20)	(-0.34)	(-0.62)	(+0.24)
β-Cl-ethylene[a]	-0.62	+0.69	-0.43	-0.34	+0.20
	(-0.98)	(+1.19)	(-0.57)	(-0.35)	(+0.20)
α-Methoxy-ethylene[a]	-0.61	+0.65	-0.20	-0.29	+0.18
	(-0.97)	(+1.15)	(+0.01)	(-0.62)	(+0.24)
β-Methoxy-ethylene[a]	-0.63	+0.68	-0.45	-0.02	+0.12
	(-0.98)	(+1.19)	(-0.56)	(-0.03)	(+0.16)
α-Phenyl-ethylene[a]	-0.62	+0.70	-0.45	-0.28	+0.17
	(-0.98)	(+1.20)	(-0.37)	(-0.59)	(+0.23)
β-Phenyl-ethylene[a]	-0.61	+0.65	-0.41	-0.26	+0.15
	(-0.98)	(+1.19)	(-0.54)	(-0.42)	(+0.23)
Trans-stilbene	-0.62	+0.71	-0.41	-0.21	+0.18
	(-0.98)	(+1.20)	(-0.36)	(-0.42)	(+0.24)
Cis-stilbene	-0.62	+0.71	-0.41	-0.21	+0.18
	(-0.98)	(+1.20)	(-0.36)	(-0.42)	(+0.24)
Tetracyano (2,2',5,5') stilbene	-0.60	+0.72	-0.51	-0.24	+0.21
	(-0.98)	(+1.27)	(-0.47)	(-0.43)	(+0.25)
Tetramethoxy (2,2',5,5') stilbene	-0.62	+0.71	-0.42	-0.20	+0.19
	(-1.00)	(+1.26)	(-0.42)	(-0.47)	(+0.27)
Biisothianaphthene	-0.63	+0.78	-0.53	-0.35	+0.24
	(-1.00)	(+1.22)	(-0.31)	(-0.35)	(+0.25)

[a] α or β refer to the location of the substituent in the precursor.

SUPPLEMENTARY MATERIAL

Table 8. Atomic electric charges derived from a Mulliken Population Analysis, and, in parentheses, Natural Population Analysis) at the MPW1K/6-311G** level on the sulfoxide transition state leading to the compounds listed in the first entry of the table.

Obtained compound	O	S	C_α	C_β	H_β
Ethylene	-0.54	+0.46	-0.39	-0.45	+0.29
	(-0.87)	(+0.82)	(-0.37)	(-0.70)	(+0.39)
α-CN-ethylene[a]	-0.52	+0.52	-0.39	-0.37	+0.29
	(-0.85)	(+0.87)	(-0.33)	(-0.64)	(+0.38)
β-CN-ethylene[a]	-0.50	+0.55	-0.37	-0.44	+0.33
	(-0.86)	(+0.93)	(-0.39)	(-0.65)	(+0.44)
α-Cl-ethylene[a]	-0.53	+0.51	-0.41	-0.39	+0.29
	(-0.86)	(+0.85)	(-0.23)	(-0.72)	(+0.39)
β-Cl-ethylene[a]	-0.52	+0.49	-0.36	-0.45	+0.33
	(-0.86)	(+0.85)	(-0.41)	(-0.49)	(+0.40)
α-Methoxy-ethylene[a]	-0.57	+0.40	-0.08	-0.43	+0.30
	(-0.89)	(+0.74)	(+0.21)	(-0.73)	(+0.37)
β-Methoxy-ethylene[a]	-0.55	+0.46	-0.41	-0.11	+0.29
	(-0.87)	(+0.82)	(-0.40)	(-0.14)	(+0.36)
α-Phenyl-ethylene[a]	-0.55	+0.47	-0.36	-0.38	+0.29
	(-0.87)	(+0.82)	(-0.17)	(-0.68)	(+0.38)
β-Phenyl-ethylene[a]	-0.53	+0.51	-0.39	-0.39	+0.32
	(-0.87)	(+0.88)	(-0.38)	(-0.52)	(+0.41)
Trans-stilbene	-0.54	+0.52	-0.41	-0.26	+0.32
	(-0.87)	(+0.88)	(-0.19)	(-0.51)	(+0.40)
Cis-stilbene	-0.56	+0.47	-0.33	-0.25	+0.33
	(-0.88)	(+0.82)	(-0.15)	(-0.50)	(+0.39)
Tetracyano (2,2',5,5') stilbene	-0.51	+0.58	-0.54	-0.32	+0.32
	(-0.90)	(+0.98)	(-0.28)	(-0.56)	(+0.45)
Tetramethoxy (2,2',5,5') stilbene	-0.54	+0.52	-0.42	-0.26	+0.32
	(-0.91)	(+0.91)	(-0.24)	(-0.56)	(+0.45)
Biisothianaphthene	-0.57	+0.46	-0.38	-0.41	+0.38
	(-0.88)	(+0.80)	(-0.12)	(-0.45)	(+0.39)

[a] α or β refer to the location of the substituent in the precursor.