

SUPPORTING INFORMATION.

Interplay of stereo-electronic, environmental, and dynamical effects in determining the EPR parameters of aromatic spin-probes: INDCO as a test case

Paola Cimino^{a*}, Alfonso Pedone^b, Emiliano Stendardo^c, Vincenzo Barone^b

Dipartimento di Scienze Farmaceutiche, Università di Salerno, via Ponte don Melillo, 84084, Fisciano (Sa), Italy and Scuola Normale Superiore, piazza dei Cavalieri 7, 56126 Pisa, Italy, Dipartimento di Chimica, Università di Napoli "Federico II", Italy.

frmod.INDCO.dat

INDCO parameters update of ff99SB (2009)

MASS

ON 16.00
NN 14.01
CI 12.01
CE 12.01
CF 12.01
LP 9.000

BOND

ON-NN	360.00	1.258
CI-NN	370.00	1.485
CF-NN	428.00	1.390
LP-ON	325.00	0.450
CI-CT	310.00	1.526
CI-CA	317.00	1.510
C-CI	317.00	1.550
C-CE	447.00	1.460
CF-CE	447.00	1.400
CF-CA	469.00	1.400
CE-CA	469.00	1.404

ANGLE

NN-CF-CA	70.00	132.80
C-CE-CA	63.00	134.90
CE-CF-NN	70.00	111.40
NN-CT-CA	63.00	114.00
CF-NN-CT	52.60	120.80
C-CI-CA	63.00	109.40
CE-C-CT	63.00	106.40
C-CE-CF	63.00	108.00
C-CT-NN	70.00	108.70
ON-NN-CF	82.00	121.50
LP-ON-LP	600.00	120.00
LP-ON-NN	600.0	120.00
CT-CI-CA	63.00	112.00
CT-CI-C	63.00	111.10
CT-CI-NN	60.00	107.50
CA-CA-CI	70.00	120.00
HC-CT-CI	50.00	109.50
ON-NN-CI	82.00	118.50
O-C-CI	80.00	120.40
CE-C-CI	63.00	106.40
CF-NN-CI	52.60	110.00
C-CI-NN	70.00	107.00
NN-CI-CA	63.00	109.00
CF-CA-CA	63.00	120.00
CF-CA-HA	50.00	120.00
CF-CE-CA	63.00	116.20
CE-CA-CA	63.00	120.00
CE-CA-HA	50.00	120.00
CE-C-O	80.00	128.80
CE-CF-CA	63.00	122.70

DIHEDRAL

X-CF-NN-X	4	6.000	180	2
X-CI-CT-X	9	1.400	0.0	3
X-CI-CA-X	6	0.000	0.0	2

X-C-CI-X	6	0.000	0.0	3
X-NN-CI-X	6	0.000	0.0	3
X-CA-CE-X	4	14.00	180	2
X-C-CE-X	4	12.00	180	2
X -CA-CF-X	4	14.50	180	2
X -CE-CF-X	4	12.00	180	2
X-NN-ON-LP	1	0.000	180	2
CF-NN-CI-C	1	1.500	180	2
CE-C-CI-NN	1	1.500	180	2
C-CI-NN-ON	1	1.500	180	2
O-C-CI-NN	1	1.500	180	2
NN-CI-CT-HC	1	0.100	0.0	3

IMPROPER TORSIONS

LP-LP-ON-NN	10.10	180.	2
CE-CI-C-O	1.100	180	2
CA-CA-CA-CI	1.100	180.	2
CF-CA-CE-C	1.100	180.	2
CA-CE-CF-NN	1.100	180.	2

NONBON

CF	1.9080	0.0860
CE	1.9080	0.0860
CI	1.9080	0.0860
NN	1.90	0.2627
ON	1.6750	0.2445
LP	0.00	0.0000

INDCO09.lib

```
!!index array str
"IND"
!entry.IND.unit.atoms table str name str type int typex int resx int flags int seq
int elmnt dbl chg
"C1" "CF" 0 1 131074 1 6 0.069100
"C2" "CE" 0 1 131074 2 6 -0.002200
"C3" "CA" 0 1 131072 3 6 -0.147100
"C4" "CA" 0 1 131072 4 6 -0.119700
"C5" "CA" 0 1 131072 5 6 -0.154500
"C6" "CA" 0 1 131072 6 6 -0.101600
"C7" "CI" 0 1 131072 7 6 0.150700
"C8" "C" 0 1 131072 8 6 0.400900
"H1" "HA" 0 1 131072 9 1 0.151900
"H2" "HA" 0 1 131072 10 1 0.137300
"H3" "HA" 0 1 131072 11 1 0.145900
"H4" "HA" 0 1 131072 12 1 0.142100
"O1" "O" 0 1 131072 13 8 -0.467400
"O2" "ON" 0 1 131072 14 8 -0.127800
"N1" "NN" 0 1 131072 15 7 0.091200
"C9" "CA" 0 1 131072 16 6 -0.015600
"C10" "CA" 0 1 131072 17 6 -0.131600
"C11" "CA" 0 1 131072 18 6 -0.131600
"C12" "CA" 0 1 131072 19 6 -0.156700
"H5" "HA" 0 1 131072 20 1 0.148700
"C13" "CA" 0 1 131072 21 6 -0.156700
"H6" "HA" 0 1 131072 22 1 0.148700
"C14" "CA" 0 1 131072 23 6 -0.123900
"H7" "HA" 0 1 131072 24 1 0.140200
"H8" "HA" 0 1 131072 25 1 0.140200
"H9" "HA" 0 1 131072 26 1 0.136500
"C15" "CT" 0 1 131072 27 6 -0.081800
"H10" "HC" 0 1 131072 28 1 0.044800
"H11" "HC" 0 1 131072 29 1 0.044800
"H12" "HC" 0 1 131072 30 1 0.044800
"Lp1" "LP" 0 1 131072 31 -1 -0.109800
"Lp2" "LP" 0 1 131072 32 -1 -0.109800
!entry.IND.unit.atoms pertinfo table str pname str ptype int ptypex int pelmnt dbl
pchg
"C1" "CN" 0 -1 0.0
"C2" "CB" 0 -1 0.0
"C3" "CA" 0 -1 0.0
"C4" "CA" 0 -1 0.0
"C5" "CA" 0 -1 0.0
"C6" "CA" 0 -1 0.0
"C7" "CI" 0 -1 0.0
"C8" "C" 0 -1 0.0
"H1" "HA" 0 -1 0.0
"H2" "HA" 0 -1 0.0
"H3" "HA" 0 -1 0.0
"H4" "HA" 0 -1 0.0
"O1" "O" 0 -1 0.0
"O2" "ON" 0 -1 0.0
"N1" "NN" 0 -1 0.0
"C9" "CA" 0 -1 0.0
"C10" "CA" 0 -1 0.0
"C11" "CA" 0 -1 0.0
"C12" "CA" 0 -1 0.0
"H5" "HA" 0 -1 0.0
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"C13" "CA" 0 -1 0.0
"H6" "HA" 0 -1 0.0
"C14" "CA" 0 -1 0.0
"H7" "HA" 0 -1 0.0
"H8" "HA" 0 -1 0.0
"H9" "HA" 0 -1 0.0
"C15" "CT" 0 -1 0.0
"H10" "HC" 0 -1 0.0
"H11" "HC" 0 -1 0.0
"H12" "HC" 0 -1 0.0
"Lp1" "LP" 0 -1 0.0
"Lp2" "LP" 0 -1 0.0
!entry.IND.unit.boundbox array dbl
-1.000000
0.0
0.0
0.0
0.0
!entry.IND.unit.childsequence single int
2
!entry.IND.unit.connect array int
0
0
!entry.IND.unit.connectivity table int atom1x int atom2x int flags
1 6 1
1 2 1
1 15 1
2 3 1
2 8 1
3 4 1
3 9 1
4 5 1
4 10 1
5 6 1
5 11 1
6 12 1
7 8 1
7 15 1
7 27 1
7 16 1
8 13 1
14 15 1
14 32 1
14 31 1
16 17 1
16 18 1
17 19 1
17 20 1
18 21 1
18 22 1
19 23 1
19 24 1
21 23 1
21 25 1
23 26 1
27 30 1
27 28 1
27 29 1
!entry.IND.unit.hierarchy table str abovetype int abovex str belowtype int belowx
"U" 0 "R" 1
"R" 1 "A" 1
"R" 1 "A" 2
"R" 1 "A" 3

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"R" 1 "A" 4
"R" 1 "A" 5
"R" 1 "A" 6
"R" 1 "A" 7
"R" 1 "A" 8
"R" 1 "A" 9
"R" 1 "A" 10
"R" 1 "A" 11
"R" 1 "A" 12
"R" 1 "A" 13
"R" 1 "A" 14
"R" 1 "A" 15
"R" 1 "A" 16
"R" 1 "A" 17
"R" 1 "A" 18
"R" 1 "A" 19
"R" 1 "A" 20
"R" 1 "A" 21
"R" 1 "A" 22
"R" 1 "A" 23
"R" 1 "A" 24
"R" 1 "A" 25
"R" 1 "A" 26
"R" 1 "A" 27
"R" 1 "A" 28
"R" 1 "A" 29
"R" 1 "A" 30
"R" 1 "A" 31
"R" 1 "A" 32

!entry.IND.unit.name single str
""

!entry.IND.unit.positions table db1 x db1 y db1 z
0.0 0.0 0.0
0.0 0.0 1.402000
1.199000 0.0 2.109000
2.388000 0.007000 1.386000
2.371000 0.001000 -0.020000
1.183000 -0.006000 -0.741000
-2.295000 0.037000 0.608000
-1.392000 -0.047000 1.866000
1.189000 -0.006000 3.196000
3.341000 0.012000 1.908000
3.316000 0.001000 -0.559000
1.157000 -0.017000 -1.826000
-1.800000 -0.156000 2.998000
-1.604000 -0.120000 -1.700000
-1.296000 -0.015000 -0.486000
-3.054000 1.361000 0.607000
-3.931000 1.634000 1.663000
-2.904000 2.305000 -0.412000
-4.646000 2.827000 1.696000
-4.034000 0.920000 2.476000
-3.624000 3.498000 -0.375000
-2.242000 2.107000 -1.249000
-4.497000 3.764000 0.676000
-5.320000 3.025000 2.527000
-3.500000 4.221000 -1.178000
-5.057000 4.696000 0.701000
-3.223000 -1.170000 0.511000
-3.908000 -1.170000 1.362000
-3.795000 -1.116000 -0.419000
-2.649000 -2.103000 0.524000
-1.281000 -0.157000 -2.011000

