Supplementary material

Molecular complexes of diethyl *N,N′*-1,3-phenyldioxalamate and resorcinols: conformational switching through intramolecular three-centered hydrogen-bonding

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Figures S1, S2, S3, S4, S5, S6 and S7.

Tables S1, S2, S3, S4, S5 and S6.

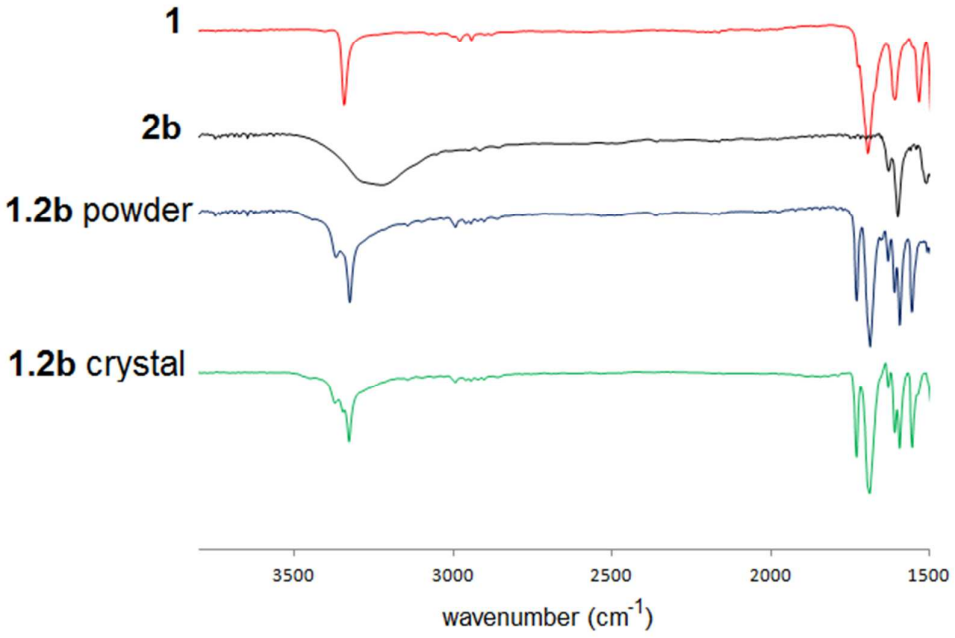

Figure S1. IR spectra of (a) **1**, (b) **2b**, (c) **1·2b**$_{powd}$ and (d) **1·2b** crystals.

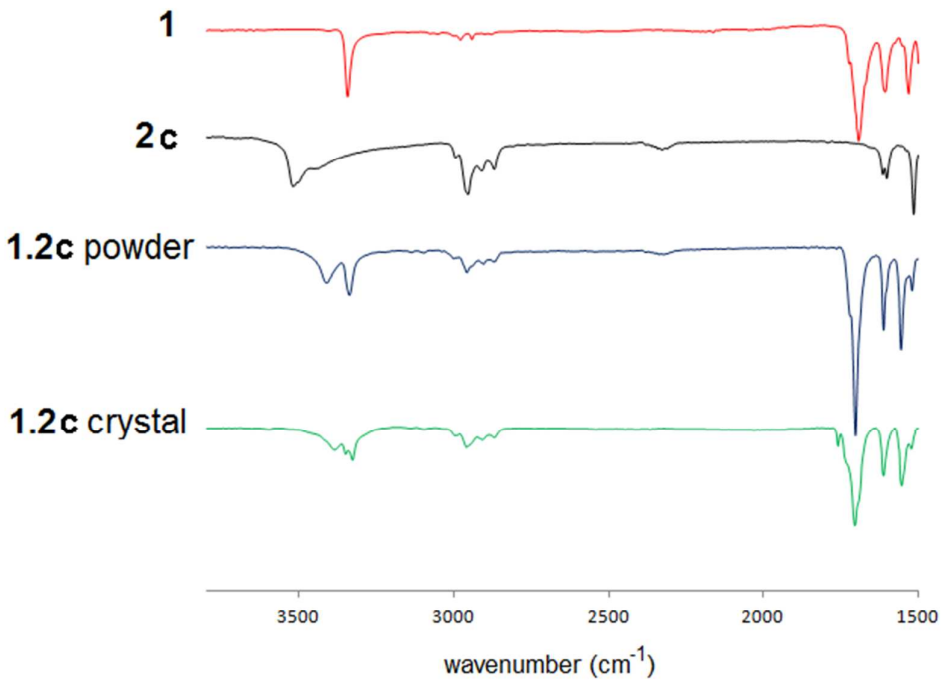

Figure S2. IR spectra of (a) **1**, (b) **2c**, (c) **1·2c**$_{powd}$ and (d) **1·2c** crystals.

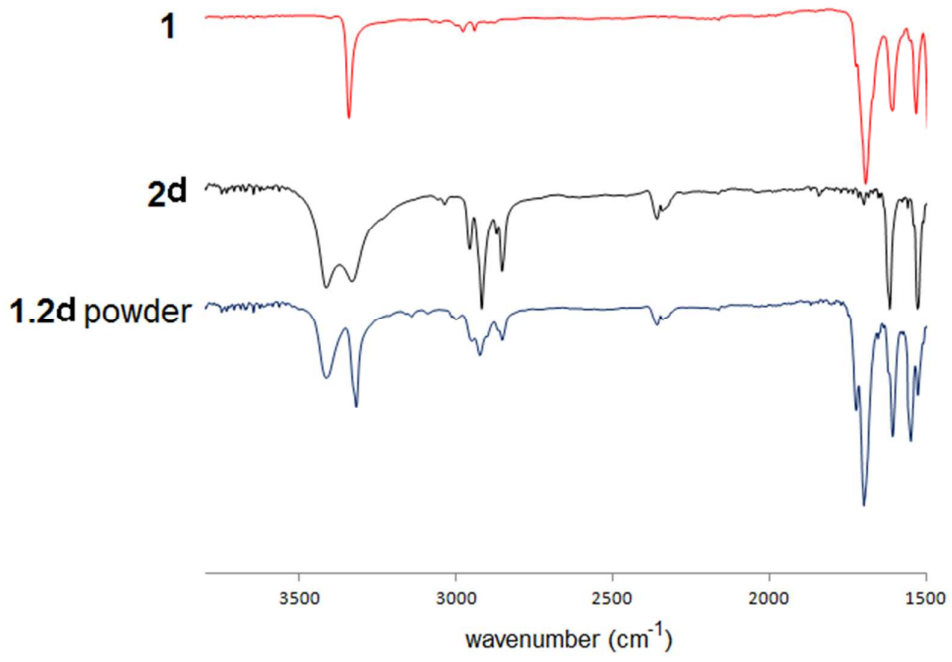

Figure S3. IR spectra of (a) **1**, (b) **2d**, (c) **1·2d**$_{powd}$ and (d) **1·2d** crystals.

Table S1. Bond lengths (Å) and angles (°) of cocrystal $\mathbf{1_4 \cdot 2a_3}$.

Bond lengths					
Atoms	Lengths	Atoms	Lengths	Atoms	Lengths
O(8)-C(8)	1.213(5)	O(9) -C(9)	1.190(5)	O(10)-C(9)	1.306(4)
O(18)-C(18)	1.209(4)	O(19)-C(19)	1.192(4)	O(20)-C(19)	1.305(5)
N(7)-C(1)	1.413(4)	N(7)-C(8)	1.327(5)	N(17)-C(3)	1.424(5)
C(1)-C(2)	1.392(5)	C(1)-C(6)	1.401(5)	C(2)-C(3)	1.384(4)
C(4)-C(5)	1.380(5)	C(5)-C(6)	1.367(4)	C(8)-C(9)	1.553(5)
C(18)-C(19)	1.552(5)	C(21)-C(22)	1.439(9)	N(17)-C(18)	1.330(5)
O(10)-C(11)	1.464(4)	O(20)-C(21)	1.466(6)	C(11)-C(12)	1.473(7)
C(3)-C(4)	1.379(5)	O(40)-C(41)	1.465(6)	O(50)-C(51)	1.457(5)
O(38)-C(38)	1.213(5)	O(39)-C(39)	1.195(4)	O(40)-C(39)	1.306(5)
O(48)-C(48)	1.210(5)	O(49)-C(49)	1.196(5)	O(50)-C(49)	1.304(5)
N(37)-C(31)	1.407(5)	N(37)-C(38)	1.339(5)	N(47)-C(33)	1.411(4)
C(31)-C(32)	1.391(4)	C(31)-C(36)	1.390(5)	C(32)-C(33)	1.394(5)
C(34)-C(35)	1.380(5)	C(35)-C(36)	1.383(5)	C(38)-C(39)	1.534(5)
C(48)-C(49)	1.541(4)	C(51)-C(52)	1.475(10)	N(47)-C(48)	1.340(4)
C(33)-C(34)	1.381(5)	C(41)-C(42)	1.474(8)	O(70)-C(71)	1.468(4)
O(68)-C(68)	1.221(5)	O(69)-C(69)	1.194(5)	O(70)-C(69)	1.311(4)
O(78)-C(78)	1.223(4)	O(79)-C(79)	1.202(4)	O(80)-C(79)	1.294(4)
N(67)-C(61)	1.414(4)	N(67)-C(68)	1.332(4)	N(77)-C(63)	1.422(4)
C(61)-C(62)	1.391(5)	C(61)-C(66)	1.394(5)	C(62)-C(63)	1.393(4)
C(64)-C(65)	1.383(5)	C(65)-C(66)	1.377(5)	C(68)-C(69)	1.542(5)
C(78)-C(79)	1.550(5)	C(81)-C(82)	1.477(7)	O(80)-C(81)	1.472(5)
N(77) - C(78)	1.326(5)	C(63)-C(64)	1.384(5)	C(71)-C(72)	1.491(7)
O(98)-C(98)	1.201(5)	O(99)-C(99)	1.194(5)	O(100)-C(99)	1.304(5)
O(108)-C(108)	1.204(5)	O(109)-C(109)	1.189(5)	O(110)-C(109)	1.310(5)
N(97)-C(91)	1.417(4)	N(97)-C(98)	1.340(5)	N(107)-C(93)	1.415(5)
C(91)-C(92)	1.391(5)	C(91)-C(96)	1.393(5)	C(92)-C(93)	1.398(4)
C(94)-C(95)	1.379(5)	C(95)-C(96)	1.387(5)	C(98)-C(99)	1.542(5)
C(108)-C(109)	1.549(5)	C(111)-C(112)	1.489(8)	O(100)-C(101)	1.460(6)
O(110)-C(111)	1.461(5)	N(107)-(108)	1.330(5)	C(93)-C(94)	1.390(5)
C(101)-C(102)	1.440(9)	C(23)-C(28)	1.384(8)	C(27)-C(28)	1.387(8)
O(23)-C(23)	1.371(7)	O(25)-C(25)	1.361(6)	C(23)-C(24)	1.377(6)
C(24)-C(25)	1.385(7)	C(25)-C(26)	1.396(8)	C(26)-C(27)	1.376(6)
O(53)-C(53)	1.365(5)	O(55)-C(55)	1.361(6)	C(53)-C(54)	1.384(6)
C(54)-C(55)	1.379(6)	C(55)-C(56)	1.348(7)	C(56)-C(57)	1.388(7)
O(83)-C(83)	1.350(8)	O(85)-C(85)	1.366(9)	C(83)-C(84)	1.357(8)
C(84)-C(85)	1.340(8)	C(85)-C(86)	1.359(8)	C(86)-C(87)	1.354(9)
C(53)-C(58)	1.377(7)	C(57)-C(58)	1.384(8)	C(83)-C(88)	1.449(7)
C(87)-C(88)	1.379(8)				
Bond Angles					

Atoms	Angles	Atoms	Angles
C(9)-O(10)-C(11)	116.8(3)	C(19)-O(20)-C(21)	117.3(3)
C(3)-N(17)-C(18)	127.7(3)	N(7)-C(1)-C(2)	122.6(3)
C(2)-C(1)-C(6)	120.3(3)	C(1)-C(2)-C(3)	118.5(3)
N(17)-C(3)-C(4)	116.6(3)	C(2)-C(3)-C(4)	121.3(3)
C(4)-C(5)-C(6)	120.9(3)	C(1)-C(6)-C(5)	119.5(3)
O(8)-C(8)-C(9)	120.8(3)	N(7)-C(8)-C(9)	111.8(3)
O(9)-C(9)-C(8)	123.2(3)	O(10)-C(9)-C(8)	110.0(3)
O(18)-C(18)-N(17)	127.7(3)	O(18)-C(18)-C(19)	120.7(3)
O(19)-C(19)-O(20)	127.0(3)	O(19)-C(19)-C(18)	123.6(3)
O(20)-C(21)-C(22)	106.6(5)	C(1)-N(7)-C(8)	127.9(3)
N(7)-C(1)-C(6)	117.0(3)	N(17)-C(3)-C(2)	122.1(3)
C(3)-C(4)- C(5)	119.4(3)	O(8)-C(8)-N(7)	127.4(3)
O(9)-C(9)- O(10)	126.8(3)	O(10)-C(11)-C(12)	106.8(4)
N(17)-C(18)- C(19)	111.6(3)	O(20)-C(19)- C(18)	109.4(3)
C(39)-O(40)-C(41)	117.7(3)	C(49)-O(50)-C(51)	118.4(3)
C(33)-N(47)-C(48)	128.3(3)	N(37)-C(31)-(32)	122.7(3)
C(32)-C(31)-C(36)	120.9(3)	C(31)-C(32)-C(33)	118.3(3)
N(47)-C(33)-C(34)	116.4(3)	C(32)-C(33)-C(34)	121.3(3)
C(34)- C(35)-C(36)	120.7(3)	C(31)-(36)- (35)	119.5(3)
O(38)-C(38)-C(39)	121.4(3)	N(37)-C(38)-C(39)	112.0(3)
O(39)-C(39)-C(38)	123.8(3)	O(40)-C(39)-C(38)	110.3(3)
O(48)-C(48)-N(47)	127.2(3)	O(48)- (48)-C(49)	121.2(3)
O(49)-C(49)-O(50)	126.4(3)	O(49)-C(49)-C(48)	124.0(3)
O(50)-C(51)-C(52)	106.2(5)	N(47)-C(33)-C(32)	122.2(3)
C(31)-N(37)-C(38)	128.6(3)	N(37)-C(31)-C(36)	116.5(3)
C(33)-C(34)-C(35)	119.4(3)	O(38)-C(38)-N(37)	126.6(4)
O(39)-C(39)-O(40)	125.9(4)	O(40)-C(41)-C(42)	106.3(4)
N(47)-C(48)-C(49)	111.6(3)	O(50)-C(49)-C(48)	109.6(3)
C(69)-O(70)-C(71)	117.3(3)	C(79)-O(80)-C(81)	117.8(3)
C(63)-N(77)-C(78)	128.3(3)	N(67)-C(61)-C(62)	122.6(3)
C(62)-C(61)-C(66)	120.5(3)	C(61)-C(62)-C(63)	118.6(3)
N(77)-C(63)-C(64)	117.2(3)	C(62)-C(63)-C(64)	121.0(3)
C(64)-C(65)-C(66)	120.4(3)	C(61)-C(66)-C(65)	119.9(3)
O(68)-C(68)-C(69)	121.3(3)	N(67)-C(68)-C(69)	111.5(3)
O(69)-C(69)-C(68)	123.4(3)	O(70)-C(69)-C(68)	110.3(3)
O(78)-C(78)-N(77)	127.4(3)	O(78)-C(78)-C(79)	120.7(3)
O(79)-C(79)-O(80)	126.7(3)	O(79)-C(79)-C(78)	122.7(3)
O(80)-C(81)-C(82)	107.5(4)	C(61)-N(67)-C(68)	127.7(3)
N(67)-C(61)-C(66)	116.9(3)	N(77)-C(63)-C(62)	121.8(3)
C(63)-C(64)-C(65)	119.7(3)	O(68)-C(68)-N(67)	127.2(3)
O(69)-C(69)-O(70)	126.4(3)	O(70)-C(71)-C(72)	106.4(4)

N(77)-C(78)-C(79)	111.8(3)	O(80)-C(79)-C(78)	110.6(3)
C(99)-O(100)-C(101)	118.2(4)	C(109)-O(110)-C(111)	116.9(3)
C(93)-N(107)-C(108)	127.6(3)	N(97)-C(91)-C(92)	121.9(3)
C(92)-C(91)-C(96)	120.9(3)	C(91)-C(92)-C(93)	118.5(3)
N(107)-C(93)-C(94)	117.7(3)	C(92)-C(93)-C(94)	120.9(3)
C(94)-C(95)-C(96)	120.8(3)	C(91)-C(96)-C(95)	119.3(3)
O(98)-C(98)-C(99)	121.3(3)	N(97)-C(98)-C(99)	111.3(3)
O(99)-C(99)-C(98)	123.6(3)	O(100)-C(99)-C(98)	110.2(3)
O(108)-C(108)-N(107)	127.4(4)	O(108)-C(108)-C(109)	121.2(4)
O(109)-C(109)-O(110)	126.5(4)	O(109)-C(109)-C(108)	123.4(3)
O(110)-C(111)-C(112)	105.8(4)	C(91)-N(97)-C(98)	127.4(3)
N(97)-C(91)-C(96)	117.1(3)	N(107)-C(93)-C(92)	121.5(3)
C(93)-C(94)-C(95)	119.6(3)	O(98)-C(98)-N(97)	127.4(3)
O(99)-C(99)-O(100)	126.3(4)	O(100)-C(101)-C(102)	108.4(5)
N(107)-C(108)-C(109)	111.4(3)	O(110)-C(109)-C(108)	110.1(3)
O(23)-C(23)-C(24)	120.8(5)	O(23)-C(23)-C(28)	117.6(4)
C(23)-C(24)-C(25)	119.5(4)	O(25)-C(25)-C(24)	122.2(5)
C(24)-C(25)-C(26)	120.2(4)	C(25)- C(26)-C(27)	118.8(5)
C(23)-C(28)-C(27)	117.9(4)	C(24)-C(23)-C(28)	121.6(5)
O(25)-C(25)-C(26)	117.6(5)	C(26)-C(27)-C(28)	122.0(5)
O(53)-C(53)-C(54)	122.3(4)	O(53)-C(53)-C(58)	117.2(4)
C(53)-C(54)-C(55)	119.5(4)	O(55)-C(55)-C(54)	117.5(4)
C(54)-C(55)-C(56)	120.9(4)	C(55)-C(56)-C(57)	119.8(5)
C(53)-C(58)-C(57)	118.8(4)	C(56)-C(57)-C(58)	120.6(5)
O(83)-C(83)-C(84)	124.3(5)	O(83)-C(83)-C(88)	115.4(5)
C(83)-C(84)-C(85)	119.7(5)	O(85)-C(85)-C(84)	120.7(5)
C(84)-C(85)-C(86)	121.3(6)	C(85)-C(86)-C(87)	121.7(6)
C(83)-C(88)-C(87)	117.4(5)	C(54)-C(53)-C(58)	120.5(4)
O(55)-C(55)-C(56)	121.7(4)	C(84)-C(83)-C(88)	120.2(5)
O(85)-C(85)-C(86)	118.0(6)	C(86)-C(87)-C(88)	119.7(5)

Table S2. Bond lengths (Å) and angles (º) of cocrystal **1·2b**.

Bond lengths					
Atoms	Lengths	Atoms	Lengths	Atoms	Lengths
O(8)-C(8)	1.2142(18)	O(9)-C(9)	1.197(2)	O(10)-C(9)	1.316(2)
N(7)-(1)	1.4164(19)	N(7)-C(8)	1.340(2)	C(1)-C(2)	1.3876(18)
C(4)-C(5)	1.377(2)	C(8)-C(9)	1.537(2)	C(11)-C(12)	1.474(3)
O(10)-C(11)	1.453(2)	C(1)-C(4)	1.385(2)		

Bond angles			
Atoms	Angles	Atoms	Angles
C(9)-O(10)-C(11)	117.51(14)	C(1)-N(7)-C(8)	127.99(13)

N(7)-C(1)-C(4)	117.26(13)	C(2)-C(1)-C(4)	120.86(15)
N(7)-C(1)-C(2)	121.77(15)	C(1)-C(2)-C(1)a	118.51(19)
C(1)-C(4)-C(5)	119.63(16)	C(4)-C(5)-C(4)a	120.5(2)
O(8)-C(8)-C(9)	121.42(14)	N(7)-C(8)-C(9)	111.57(13)
O(9)-C(9)-C(8)	123.70(15)	O(10)-C(9)-C(8)	109.87(13)
O(8)-C(8)-N(7)	127.01(14)	O(9)-C(9)-O(10)	126.43(15)
O(10)-C(11)-C(12)	110.24(18)		

Table S3. Bond lengths (Å) and angles (º) of cocrystal **1·2c**.

Bond lengths					
Atoms	Lengths	Atoms	Lengths	Atoms	Lengths
O(8)-C(8)	1.206(4)	O(9)-C(9)	1.180(4)	O(10)-C(9)	1.313(5)
O(18)-C(18)	1.201(4)	O(19)-C(19)	1.192(4)	O(20)-C(19)	1.310(4)
O(10)-C(11)	1.461(5)	O(20)-C(21)	1.460(4)	N(17)-C(18)	1.343(5)
N(7)-C(1)	1.418(4)	N(7)-C(8)	1.343(5)	N(17)-C(5)	1.418(4)
C(1)-C(2)	1.386(5)	C(1)-C(6)	1.387(4)	C(2)-C(3)	1.374(5)
C(4)-C(5)	1.386(5)	C(5)-C(6)	1.391(4)	C(8)-C(9)	1.541(4)
C(18)-C(19)	1.542(4)	C(21)-C(22)	1.490(6)	C(3)-C(4)	1.377(5)
C(11)-C(12)	1.431(9)				
Bond angles					
Atoms		Angles	Atoms		Angles
C(9)-O(10)-C(11)		116.7(3)	C(19)-O(20)-C(21)		116.9(3)
C(5)-N(17)-C(18)		128.7(3)	N(7)-C(1)-C(2)		116.3(3)
C(1)-N(7)-C(8)		128.2(3)	N(7)-C(1)-C(6)		122.5(3)
C(2)-C(1)-C(6)		121.1(3)	C(1)-C(2)-C(3)		119.7(3)
C(3)-C(4)-C(5)		119.3(3)	N(17)-C(5)-C(4)		116.3(3)
C(2)-C(3)-C(4)		120.6(4)	N(17)-C(5)-C(6)		122.3(3)
C(4)-C(5)-C(6)		121.5(3)	C(1)-C(6)-C(5)		117.8(3)
O(8)-C(8)-C(9)		122.5(3)	N(7)-C(8)-C(9)		110.4(3)
O(8)-C(8)-N(7)		127.1(3)	O(9)-C(9)-O(10)		125.7(3)
O(9)-C(9)-C(8)		123.9(3)	O(10)-C(9)-C(8)		110.4(3)
O(18)-C(18)-N(17)		126.7(3)	O(18)-C(18)-C(19)		123.0(3)
O(19)-C(19)-O(20)		126.7(3)	O(19)-C(19)-C(18)		122.7(3)
O(20)-C(21)-C(22)		106.7(3)	O(10)-C(11)-C(12)		109.1(4)
N(17)-C(18)-C(19)		110.3(3)	O(20)-C(19)-C(18)		110.6(3)

Table S4. Intramolecular and intracomplexes hydrogen bonding interactions.

Comp.	D—H···A	D—H/Å	H···A/Å	D···A/Å	D—H···A/º	Motif

1_4·2a_3	N7—H7···O9	0.86	2.29	2.708(4)	110	*S(5)*
Subunit	N17—H17···O19	0.86	2.30	2.713(4)	110	*S(5)*
1_2·2a	C2—H2···O8	0.93	2.29	2.880(4)	121	*S(6)*
	C2—H2···O18	0.93	2.26	2.868(5)	123	*S(6)*
	O23—H23···O8	0.82	2.00	2.820(5)	180	$R^4_3(10)$
	O25—H25···O18	0.82	2.13	2.947(5)	177	
	N17—H17···O109^i	0.86	2.35	3.176(4)	162	$R^2_2(10)$
	N107—H107···O19^i	0.86	2.34	3.157(4)	158	
	N97—H97···O99	0.86	2.30	2.709(4)	109	*S(5)*
	N107—H107···O109	0.86	2.29	2.701(4)	110	*S(5)*
	C92—H92···O98	0.93	2.26	2.860(4)	122	*S(6)*
	C92—H92···O108	0.93	2.23	2.843(5)	123	*S(6)*
1_4·2a_3	N37—H37···O39	0.86	2.30	2.713(4)	110	*S(5)*
Subunit	N47—H47···O49	0.86	2.32	2.731(4)	109	*S(5)*
1_2·2a_2	C32—H32···O38	0.93	2.28	2.880(5)	122	*S(6)*
	C32—H32···O48	0.93	2.28	2.881(4)	122	*S(6)*
	N67—H67···O69	0.86	2.29	2.704(4)	109	*S(5)*
	N77—H77···O79	0.86	2.30	2.713(4)	110	*S(5)*
	C62—H62···O68	0.93	2.30	2.886(4)	120	*S(6)*
	C62—H62···O78	0.93	2.34	2.914(4)	120	*S(6)*
	O55—H55···O48	0.82	2.06	2.877(5)	173	
	O53—H53···O78^{ii}	0.82	2.10	2.894(5)	161	$R^4_4(20)$
	O83—H83···O68^{iii}	0.82	2.10	2.886(5)	161	
	O85—H85···O38^{vi}	0.82	2.08	2.894(8)	172	
1·2b	N7—H7···O9	0.86	2.30	2.7073(18)	109	*S(5)*
	C2—H2···O8	0.93	2.32	2.907(2)	121	*S(6)*
	O23—H23···O8^v	0.82	2.04	2.8630(18)	176	$R^4_3(10$
1·2c	N7—H7···O9	0.86	2.26	2.681(3)	110	*S(6)*
	N17—H17···O19	0.86	2.25	2.673(3)	110	*S(6)*

C2—H2···O8	0.93	2.29	2.891(4)	122	*S(6)*
C2—H2···O18	0.93	2.29	2.890(4)	122	*S(6)*
O23—H23···O8^{v}	0.82	2.06	2.883(4)	179	$R^4_3(10)$
O25—H25···O18^{vi}	0.82	2.04	2.864(4)	177	

Symmetry codes: *i* (1-x, 1-y, 1-z), *ii* (x, -1+y, z), *iii* (-x, 1-y, 1-z), *iv* (-x, -y, 1-z), *v* (-1+x, y, z), *vi* (x, y, 1+z).

Table S5. Intercomplexes hydrogen bonding interactions.

Complex	D—H···A	D—H (Å)	H···A (Å)	D···A (Å)	D—H···A (º)
1_4·2a_3	N7—H7···O99^{vii}	0.86	2.33	3.162(5)	162
	N37—H37···O79^{i}	0.86	2.35	3.182(4)	163
	N47—H47···O69^{viii}	0.86	2.30	3.133(4)	163
	N67—H67···O49^{viii}	0.86	2.35	3.162(4)	157
	N77—H77···O39^{ix}	0.86	2.34	3.123(4)	152
	N97—H97···O9^{vii}	0.86	2.30	3.121(4)	161
	C4—H4···O109^{i}	0.93	2.53	3.352(5)	147
	C6—H6···O99^{vii}	0.93	2.53	3.344(5)	146
	C64—H64···O39^{ix}	0.93	2.45	3.278(4)	148
	C36—H36···O79^{i}	0.93	2.51	3.334(4)	148
	C94—H94···O19^{vii}	0.93	2.49	3.305(5)	146
	C96—H96···O9^{vii}	0.93	2.50	3.314(4)	147
	C34—H34···O69^{viii}	0.93	2.48	3.302(5)	148
	C66—H66···O49^{viii}	0.93	2.50	3.325(4	148
	C82—H82C···O55^{iii}	0.96	2.58	3.362(7)	139
	C65—H65···O83^{viii}	0.93	2.55	3.412(7)	155
1·2b	N7—H7···O9^{x}	0.86	2.37	3.1969(19)	162
	C4—H4···O9^{x}	0.93	2.60	3.379(2)	142
1·2c	N7—H7··· O19^{xi}	0.86	2.36	3.182(4)	161

N17—H17···O9^{xi}	0.86	2.45	3.248(4)	155
O23—H23···O8^{vi}	0.82	2.06	2.883(4)	179
O25—H25···O18^{vi}	0.82	2.04	2.864(4)	177
C4—H4···O9^{xii}	0.93	2.47	3.297(4)	149
C6—H6···O19^{xi}	0.93	2.43	3.269(4)	150
C50—H50···O23^{xii}	0.98	2.54	3.485(9)	160

Symmetry codes: *i* (1-x, 1-y, 1-z), *iii* (-x, 1-y, 1-z), *vi* (x, y, 1+z), *vii* (1-x, -y, -z), *viii* (x, y, z), *ix* (x, 1+y, 1+z), *x* (-x, -y, 2-z), *xi* (-x, -1/2+y, 1/2-z), *xii* (x, 1/2-y, -1/2+z).

Table S6. Intercomplex π interactions.

Complex	Y—X···*Cg(n)*	Y···*Cg(n)* (Å)	X···*Cg(n)* (Å)	Y—X···*Cg(n)* (º)	Atoms in *Cg(n)*
1_4·2a_3	C18=O18···*Cg(1)*^{i}	3.853(3)	3.527(4)	65.5(2)	C1-C6
	C19=O19···*Cg(1)*^{i}	3.712(4)	3.452(4)	68.2(2)	C1-C6
	C9=O9···*Cg(4)*^{viii}	3.577(4)	3.818(4)	92.4(2)	C91-C96
	C111—H110···*Cg(5)*^{viii}	2.78	3.607(5)	144	C23-C28
	C82—H82B···*Cg(7)*^{xiii}	2.86	3.813(6)	172	C83-C88
	C102—H102···*Cg(6)*^{vii}	2.92	3.855(8)	165	C53-C58
1·2b	C29—H29B···*Cg(2)*^{xiv}	2.73	3.512(3)	139	C23-C28
	C29—H29B···*Cg(2)*^{xv}	2.73	3.512(3)	139	C23-C28
1·2c	C21—H21B···*Cg(1)*^{xii}	2.95	3.780(4)	145	C1-C6
	C21—H21A···*Cg(2)*^{xii}	2.70	3.627(4)	159	C23-C28

Symmetry codes: *i* (1-x, 1-y, 1-z), *vii* (1-x, -y, -z), *viii* (x, y, z), *xii* (x, 1/2-y, -1/2+z), *xiii* (x, 1+y, z), *xiv* (1+x, y, z), *xv* (1+x, 1/2-y, z).

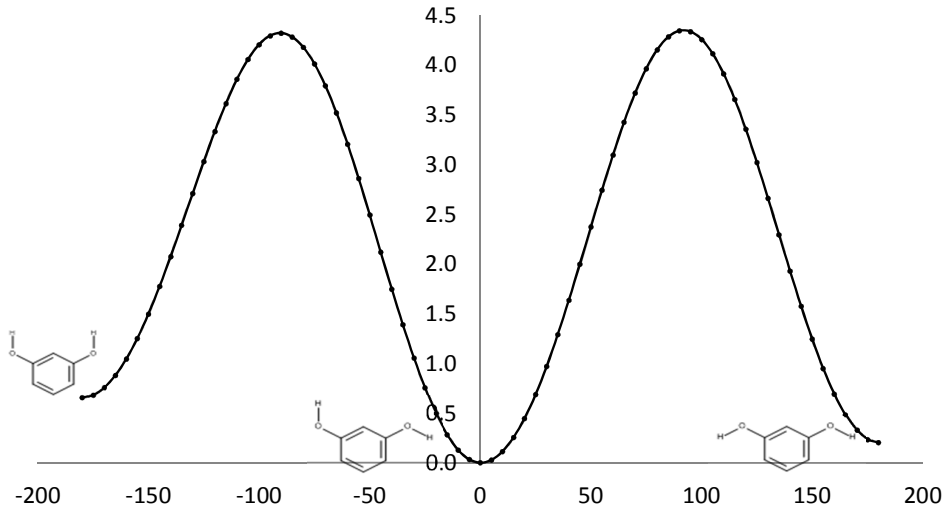

Figure S4. Energy profile of the OH group rotation calculated at the B3LYP/6-31G (*d*, *p*) level of theory between **A**, **B** and **C** conformations of **2a**.

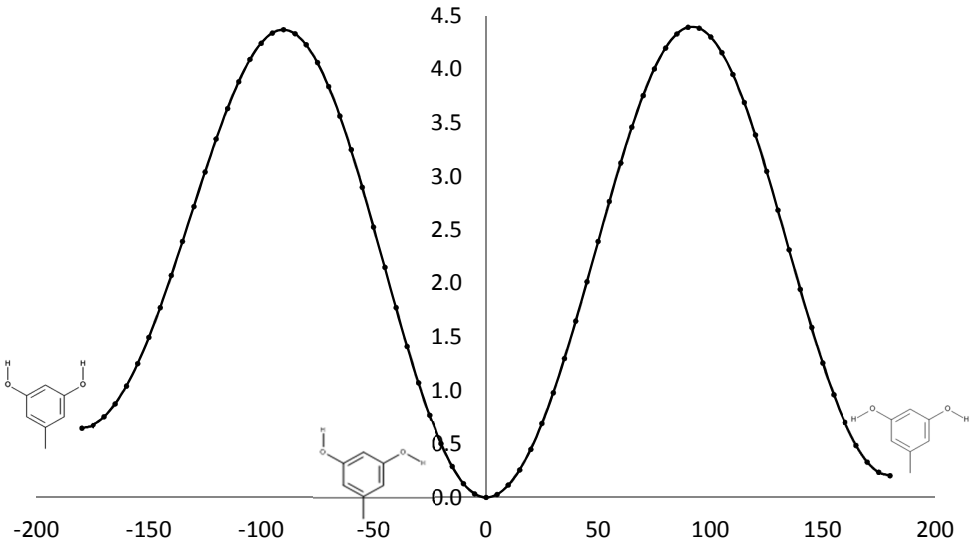

Figure S5. Energy profile of the OH group rotation calculated at the B3LYP/6-31G (*d*, *p*) level of theory between **A**, **B** and **C** conformations of **2b**.

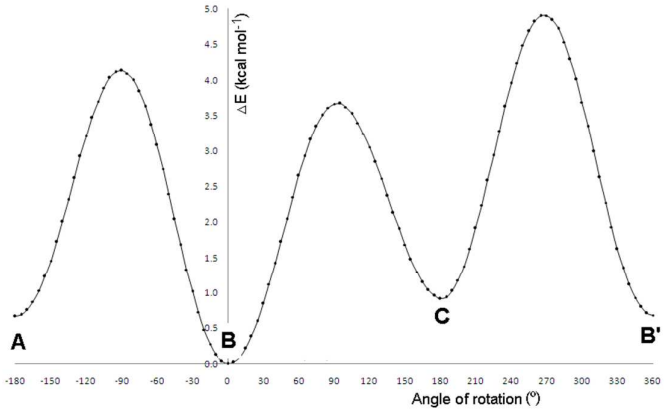

Figure S6. Energy profile of the OH group rotation calculated at the B3LYP/6-31G (*d*, *p*) level of theory between **A**, **B**, **B'** and **C** conformations of 4-hexyl-1,3-benzenediol (**2d**).

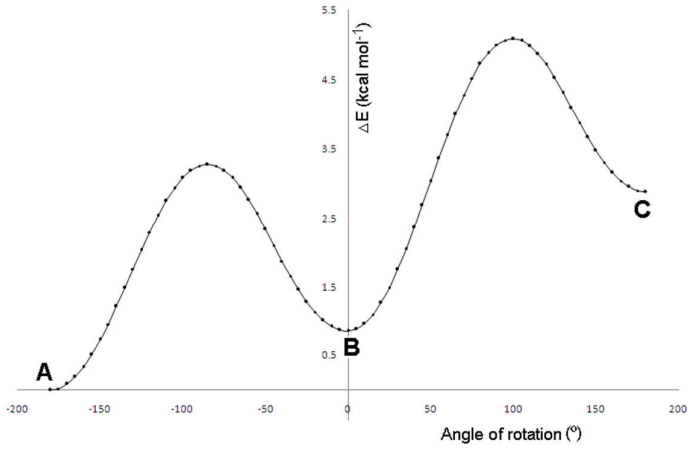

Figure S7. Energy profile of the OH group rotation calculated at the B3LYP/6-31G (*d*, *p*) level of theory between **A**, **B** and **C** conformations of 4,6-di-*tert*butyl-1,3-benzenediol (**2c**).