Supporting Information

Crystal Morphology as an Evidence of Supramolecular Organization in Adducts of 1,2-bis(chloromercurio)tetrafluorobenzene with Organic Esters

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Table 1S. Comparison of ethyl acetate (1) structural parameters determined by different methods

Parametr	**X-ray**		**Electron diffraction**	**Quantum chemistry**		
	Uncoord. A/B	in complex **II·1**	Trans/Gauche ref[1S]	HF/6-31G*ref[2S] Trans/Gauche	B3LYP/6-311++G**	MP2/6-31G**
O(1)-C(1)	1.206(2)/1.194(2)	1.21(1)	1.203(2)	1.188/1.189	1.207	1.219
O(2)-C(1)	1.348(2)/1.347(2)	1.323(9)	1.345(3)	1.326/1.326	1.351	1.358
O(2)-C(3)	1.455(2)/1.462(2)	1.474(9)	1.448(3)	1.424/1.426	1.450	1.447
C(1)-C(2)	1.493(2)/1.501(2)	1.49(1)	1.508(2)	1.505/1.505	1.508	1.505
C(3)-C(4)	1.511(2)/1.501(3)	1.51(1)	1.515	1.514/1.517	1.515	1.510
C(1)-O(2)-C(3)	116.2(1)/115.7(1)	116.7(6)	115.7(5)	117.4/118.4	116.6	114.5
O(1)-C(1)-O(2)	122.8(2)/122.9(1)	124.1(8)	124.0(3)		123.4	123.6
O(1)-C(1)-C(2)	125.7(2)/125.6(2)	124.6(8)	124.1(10)	125.0/124.9	125.5	125.9
O(2)-C(1)-C(2)	111.5(1)/111.5(1)	111.3(7)	119.0	111.4/111.4	111.0	110.5
O(2)-C(3)-C(4)	106.8(1)/106.9(1)	107.9(7)	108.2(11)	107.4/107.4	107.6	106.7
C(1)-O(2)-C(3)-C(4)	178.8(2)/177.0(2)	165.1(7)	180/79(62(7)%)	180/83.8	180	180

Table 2S. Comparison of diethylcarbonate (2) structural parameters determined by different methods

Parametr	**X-ray**		**Quantum chemistry**		
	Uncoord. A/B/C/D	in complex **2(II)·2**	HF/6-31G*ref[2S] gg/tt	B3LYP/6-311++G**	MP2/6-31G**
O(1)-C(1)	1.201(2)/1.201(2)/1.203(2)/1.198(2)	1.21(1)	1.190/1.185	1.208	1.218
O(2)-C(1)	1.329(2)/1.333(2)/1.332(2)/1.334(2)	1.32(1)	1.313/1.321	1.338	1.346
O(2)-C(2)	1.449(2)/1.455(2)/1.458(2)/1.450(2)	1.51(1)	1.425/1.427	1.450	1.447
O(3)-C(1)	1.335(2)/1.333(2)/1.334(2)/1.338(2)	1.31(1)	1.313/1.315	1.338	1.346
O(3)-C(4)	1.451(2)/1.447(2)/1.457(2)/1.451(2)	1.46(1)	1.425/1.424	1.450	1.447
C(2)-C(3)	1.501(3)/1.498(3)/1.500(2)/1.497(3)	1.51(2)		1.514	1.509
C(4)-C(5)	1.498(3)/1.502(2)/1.499(2)/1.503(2)	1.49(1)		1.514	1.509
C(1)-O(2)-C(2)	114.8(2)/115.4(1)/115.3(1)/115.7(1)	113.0(8)	116.9/116.8	115.7	113.7
C(1)-O(3)-C(4)	114.8(1)/115.3(1)/115.3(1)/115.5(1)	117.3(8)	116.9/121.7	115.7	133.7
O(1)-C(1)-O(2)	126.6(2)/126.2(2)/126.3(1)/126.6(2)	126.5(9)	125.4/124.7	125.9	126.3
O(1)-C(1)-O(3)	125.6(1)/125.9(2)/126.6(2)/126.0(2)	125.1(9)	125.4/122.6	125.9	126.3
O(2)-C(1)-O(3)	107.5(2)/107.9(1)/107.1(2)/107.4(1)	108.4(8)	109.2/112.7	108.1	107.5
O(2)-C(2)-C(3)	106.9(2)/107.3(1)/106.8(1)/106.7(1)	106.0(8)		107.3	106.5
O(3)-C(4)-C(5)	107.2(1)/106.7(1)/107.0(2)/106.4(1)	110.1(8)		107.3	106.5
C(1)-O(2)-C(2)-C(3)	178.7(1)/176.3(1)/175.4(1)/174.9(1)	179.6(9)		180.0	180.0
C(1)-O(3)-C(4)-C(5)	177.2(1)/179.5(1)/173.5(1)/177.3(1)	160.2(9)		180.0	180.0
O(1)-C(1)-O(2)-C(3)	2.1(2)/4.0(2)/3.1(2)/1.0(2)	3(1)	0.0/0.0	0.0	0.0

O(1)-C(1)-O(3)-C(5)	3.9(2)/1.3(2)/4.5(2)/4.4(2)	-2(1)	0.0/180.0	0.0	0.0

Table 3S. Comparison of methyl benzoate (3) structural parameters determined by different methods

Parametr	**X-ray**		**Quantum chemistry**		
	Uncoord.	in complex **II·3**	HF/6-311+G** ref[3S]	B3LYP/6-311++G**	MP2/6-31G**
O(1)-C(1)	1.208(2)	1.210(10)	1.187	1.210	1.222
O(2)-C(1)	1.336(2)	1.291(12)	1.321	1.352	1.357
O(2)-C(3)	1.446(2)	1.467(11)	1.417	1.438	1.439
C(1)-C(2)	1.494(2)	1.556(13)	1.492	1.491	1.488
C(2)-C(4)	1.385(2)	1.381(13)	1.390	1.400	1.400
C(2)-C(8)	1.395(2)	1.389(13)	1.386	1.400	1.400
C(4)-C(5)	1.390(2)	1.328(15)	1.383	1.392	1.394
C(5)-C(6)	1.386(2)	1.346(15)	1.387	1.395	1.397
C(6)-C(7)	1.389(2)	1.377(15)	1.386	1.395	1.397
C(7)-C(8)	1.389(2)	1.436(16)	1.385	1.391	1.393
C(1)-O(2)-C(3)	115.9(1)	113.0(7)	117.4	115.8	113.8
O(1)-C(1)-O(2)	123.6(1)	127.4(10)	123.1	122.9	123.2
O(1)-C(1)-C(2)	124.2(2)	122.1(10)	123.9	124.6	124.7
O(2)-C(1)-C(2)	112.1(1)	110.5(7)	113.1	112.5	112.1
C(4)-C(2)-C(8)	120.4(1)	121.7(9)	119.9	119.8	120.3
C(4)-C(2)-C(1)	118.9(1)	116.8(8)	118.0	117.9	117.6
C(8)-C(2)-C(1)	120.8(1)	121.5(9)	122.0	122.3	122.1
C(2)-C(4)-C(5)	119.9(1)	119.6(11)	120.1	119.9	119.5
C(6)-C(5)-C(4)	120.0(2)	120.9(10)	119.9	120.1	120.4
C(5)-C(6)-C(7)	120.1(1)	123.0(10)	120.2	120.0	119.9

C(8)-C(7)-C(6)	120.2(1)	117.2(10)	120.0	120.0	120.1
C(7)-C(8)-C(2)	119.4(2)	117.6(9)	119.9	120.1	119.8
φ(Ph/COOMe)	23.4(4)	12(1)	0	0	0

Table 4S. Comparison of phenyl acetate (4) structural parameters determined by different methods

Parametr	**X-ray**		**Quantum chemistry**		
	Uncoord.	in complex **II·4** A/B	HF/6-31G* ref[4S]	B3LYP/6-311++G**	MP2/6-31G**
O(1)-C(1)	1.196(2)	1.20(6)/1.15(6)	1.208	1.200	1.213
O(2)-C(1)	1.363(2)	1.32(6)/1.37(4)	1.375	1.372	1.378
O(2)-C(3)	1.413(2)	1.40(4)/1.43(6)	1.404	1.400	1.402
C(1)-C(2)	1.500(2)	1.61(6)/1.42(8)	1.501	1.506	1.503
C(3)-C(8)	1.371(3)	1.39(2)/1.39(2)	1.392	1.390	1.392
C(3)-C(4)	1.382(2)	1.39(2)/1.39(2)	1.395	1.391	1.393
C(4)-C(5)	1.398(2)	1.39(2)/1.39(2)	1.394	1.393	1.395
C(5)-C(6)	1.377(3)	1.39(2)/1.39(2)	1.396	1.395	1.397
C(6)-C(7)	1.388(3)	1.39(2)/1.39(2)	1.395	1.394	1.396
C(7)-C(8)	1.398(2)	1.39(2)/1.39(2)	1.395	1.394	1.395
C(1)-O(2)-C(3)	117.3(1)	116(3)/122(4)	119.3	120.0	117.0
O(1)-C(1)-O(2)	123.2(1)	125(5)/117(5)	124.3	124.0	124.2
O(1)-C(1)-C(2)	126.1(3)	127(5)/133(5)	126.4	126.2	126.6
O(2)-C(1)-C(2)	110.7(1)	107(4)/110(5)	109.3	109.8	109.2
C(8)-C(3)-C(4)	122.4(1)	120(1)/120(1)	121.4	121.4	121.7
C(8)-C(3)-O(2)	118.1(2)	119(2)/118(2)	117.1	117.1	117.0
C(4)-C(3)-O(2)	119.3(2)	121(2)/122(2)	121.2	121.4	121.1
C(3)-C(4)-C(5)	118.2(2)	120(1)/120(1)	118.5	118.9	118.6
C(6)-C(5)-C(4)	120.5(2)	120(1)/120(1)	120.6	120.5	120.5
C(5)-C(6)-C(7)	120.2(1)	120(1)/120(1)	119.7	119.8	119.9

C(6)-C(7)-C(8)	119.9(2)	120(1)/120(1)	120.2	120.2	120.2
C(3)-C(8)-C(7)	118.8(2)	120(1)/120(1)	119.1	119.2	119.0
C(3)-O(2)-C(1)-O(1)	2.2(3)	0(7)/13(7)	0.5	0.3	0.7
φ(MeCOO/Ph)	72.7(5)	86(1)/84(2)	58.4	59.0	60.2

References

(1S) Sugino, M.; Takeuchi, H.; Egava, T; Konaka, S. *J. Mol. Struct.* **1991**, *245*, 357.

(2S) Labrenz, D.; Schroer, W. *J. Mol. Struct.* **1991**, *249*, 327.

(3S) Sundaraganesan, N.; Dominic Joshua, B. *Spectrochimica Acta Part A*, **2007**, *68*, 771.

(4S) Neuvonen, H.; Neuvonen, K.; Koch, A.; Kleinpeter, E. *J.Phys.Chem.A* **2005**, *109*, 6279