Asian Journal of Chemistry Vol. 20, No. 1 (2008), 452-462

A Quantum Chemical Study on Structure of 1,2-*Bis*(diphenylphosphinoyl)ethane and 4-chlorophenol cocrystal

CENGIZ YENIKAYA*, MEHMET POYRAZ† and SABRI ÇEVIK†
Department of Chemistry, Faculty of Arts and Sciences
Dumlupinar University, Kütahya, Turkey
Fax: (90)(274)2652066; Tel: (90)(274)2652051; E-mail: yenikaya@dumlupinar.edu.tr

The cocrystal of 1,2-*bis*(diphenylphosphinoyl)ethane (DPPEO) with 4-chlorophenol (1:2) were studied theoretically with MINDO/3, MNDO, PM3 and AM1 semi empirical methods to elucidate its structure. The bond lengths and angles from theoretical studies of molecule DPPEO/4-chlorophenol (1:2) were found to be as expected. Theoretical results, concerning with intermolecular van der Waals forces in cocrystal, were compared with the previously obtained experimental data and AM1 results were found to be the best fit for selected C-C, C-P and P-O bond lengths and angles of DPPEO/4-chlorophenol. For the hydrogen bond geometry none of the theoretical methods were found to be comparable with experimental data.

Key Words: Cocrystal, Quantum chemical studies, Hydrogen bonding, Semi-empirical methods, Vander Waals forces.

INTRODUCTION

Phosphine oxides are an excellent hydrogen bond acceptor and can form large, high quality crystals when cocrystallized with a variety of hydrogen bond donors. They can be used to promote the crystallization for compounds that do not crystallize well on their own[1]. There are a few examples of hydrogen bonded complexes for triphenylphosphine oxide (TPPO) and alcohols (diphenylmethanol)[2] or phenols[3-5]. Hydrogen bond geometry is similar in all of the TPPO cocrystals with phenols consisting of a single linear bond except in TPPO/phenol (2:3) complex having two different almost linear bonds[6].

The traditional X-ray diffraction techniques and the theoretical studies allow the determination of the positions of the atoms in the compounds under study for suitable systems[7,8]. We have previously reported theoretical studies on geometries of hydroquinone complexes with phosphine oxides, (+)-(R)-2,2-*bis*(diphenylphosphinoyl)-1,1'-binaphthyl[9], TPPO[10], 1,2-*bis*(diphenylphosphinoyl)ethane (DPPEO)[11] and phenol complex with DPPEO[12]. The phosphine oxide in the present study, DPPEO, produced

---

†Department of Chemistry, Faculty of Science and Arts, Afyon Kocatepe University, Afyonkarahisar, Turkey.

1:2 complex with 4-chlorophenol. The continuous increase in the development of the computer technology and tremendous development in sophistication of software to apply in structure-reactivity relations[13,14], reaction mechanism[15-17], corrosion[18-20] and in some biological processes[21,22]. Thus, it is worthwhile to study the structure of the title compound to find the parallelism of the computed results with the experimental ones. In this respect, for bond lengths and angles as well as hydrogen bonding in the cocrystal of DPPEO and 4-chlorophenol, it is considered appropriate to compare the quantum chemical results in the gas phase to the results of X-ray structural studies[23].

EXPERIMENTAL

Theoretical calculation were carried out at the Restricted Hartree-Fock level using MINDO/3, MNDO, PM3 and AM1 semi empirical SCF-MO methods in the MOPAC 7.0 program[24], implemented on an Intel Pentium Pro. 400 MHz computer. Initial estimates for the geometries of all were obtained by a molecular mechanics program (CS Chemoffice Pro for Windows)[25], followed by full optimization of all geometrical variables (bond lengths, bond angles and dihedral angles), without any symmetry constraint, using the semi empirical MINDO/3, MNDO, PM3, AM1 quantum chemical methods in the MOPAC 7.0 program. The molecular plots for the cocrystal of DPPEO/HQ and the van der Waals contacts in cocrystal were produced by MERCURY program from Cambridge Crystallographic Data Centre (CCDC)[26,27].

RESULTS AND DISCUSSION

Cocrystals of DPPEO/4-chlorophenol, suitable for single crystal X-ray diffraction, were grown as colourless plates from benzene. The compound crystallizes in the centrosymmetric monoclinic space group $P2_1/c$, with two formula units per unit cell. There is a single crystallographically distinct residue in the asymmetric unit with the two halves of the DPPEO being symmetry related. The asymmetric unit contains half of the DPPEO molecule and one 4-chlorophenol molecule. The molecular structure of the 1:2 cocrystal of DPPEO/4-chlorophenol is shown in Fig. 1.

The geometries of the DPPEO molecule and 4-chlorophenol molecules are almost identical with those in DPPEO/phenol (1:2)[28]. There are two identical, symmetry related, almost linear, hydrogen bonds from each 4-chlorophenol molecule to the oxygen of a P=O bond.

All these experimental results were confirmed in the present study (Tables 1 and 5). The molecule (DPPEO/4-chlorophenol) in gas phase was studied with MINDO/3, MNDO, PM3 and AM1 semi empirical methods

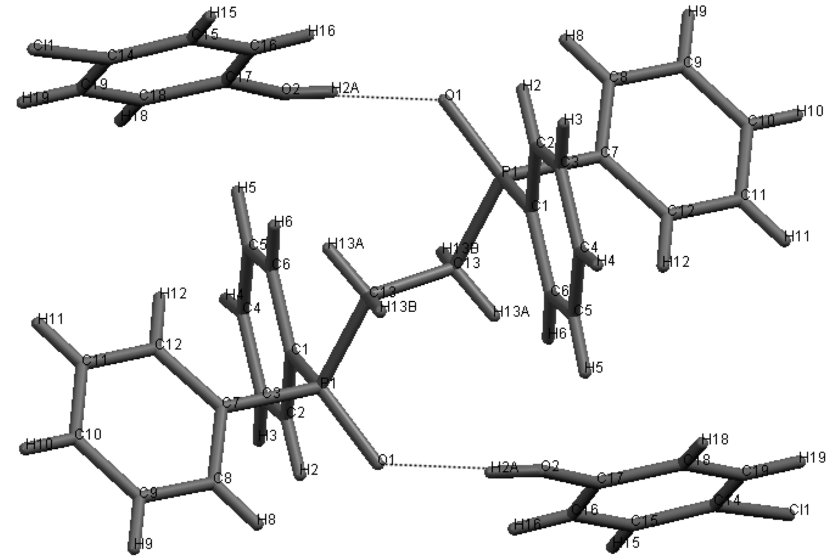

Fig. 1. Structure of DPPEO/4-clorophenol

TABLE-1
MODELS OF COCRYSTAL OF DPPEO/4-CHLOROPHENOL (1:2)
WITH VANDER WAALS INTERACTIONS UP TO 3 Å [Ref. 23]

M1		M2		M3	
H2A···O1	1.826	H2A···O1	1.826	H2A···O1	1.826
O2···O1	2.643	O2···O1	2.643	O2···O1	2.643
		H16···O1	2.812	H16···O1	2.812
		H18···H12	2.819	H18···H12	2.819
				O2···H6	2.573
				H2A···H13A	2.443

M4		M5	
H2A···O1	1.826	H2A···O1	1.826
O2···O1	2.643	O2···O1	2.643
H16···O1	2.812	H16···O1	2.812
H18···H12	2.819	H18···H12	2.819
O2··· H6	2.573	O2··· H6	2.573
H2A···H13A	2.443	H2A···H13A	2.443
O2···H13A	2.577	O2···H13A	2.577
H2A···H6	2.909	H2A···H6	2.909
		H2A···P1	2.991

at 20 °C at which the experimental values were obtained[23]. Tables 2 and 3 listed the gas phase computation results of MINDO/3, MNDO, PM3 and AM1 semi empirical methods for selected C-C, C-P and P-O bond lengths and angles, respectively. There are two different results for each theoretical study in gas phase for the two halves of the molecule although they are symmetric in solid state. In order to find the effects of vander Waals interactions on symmetry, contacts in cocrystal up to 3 Å in addition to hydrogen bonding interaction were used to obtain models. They were abbreviated as M1, M2, M3, M4 and M5 and computed with semi empirical methods (Table 1 and Fig. 2). Deviations from symmetry between the same methods were obtained from the differences between corresponding bond lengths or angles of the two halves of the models and shown in the Tables 2 and 3. Deviations from symmetry for selected bond lengths and angles were presented in Figs. 3 and 4, respectively for each model. Results were indicated that AM1 gives better results accord for symmetry.

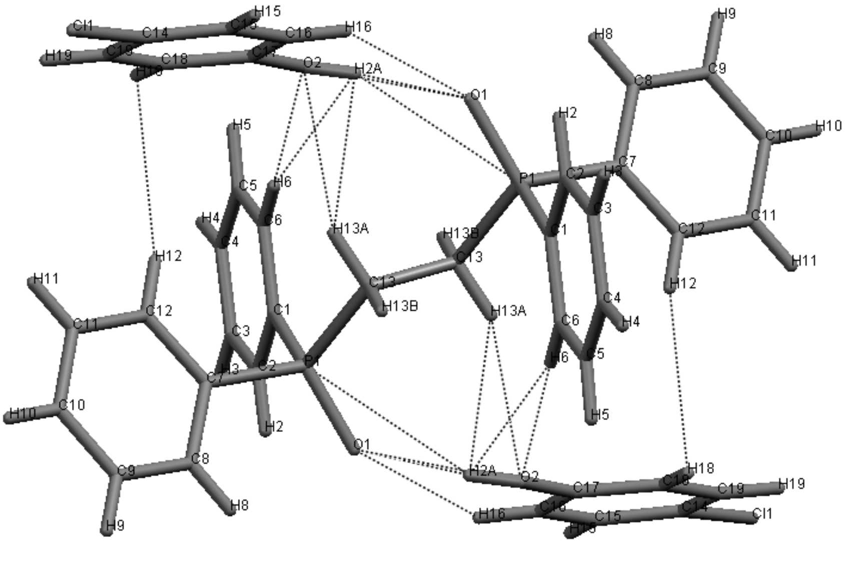

Fig. 2. vander Waals interactions of DPPEO/4-chlorophenol

Table-4 listed the mean values of the same theoretical results and previously obtained experimental results[23]. Theoretical results for each bond lengths and angles were recalculated by taking arithmetic average of the corresponding bond lengths or angles of two halves of the models to compare with experimental ones. Percentage values of the differences were also plotted against models for bond lengths (Fig. 5) and angles (Fig. 6). Among the applied methods, AM1 seems to give better results for both bond lengths and angles of DPPEO/4-chlorophenol.

TABLE-2

PERCENTAGE DEVIATIONS FROM SYMMETRY FOR SELECTED BOND LENGTHS OF TWO HALVES OF THE COCRYSTAL OF 4-CHLOROPHENOL WITH DPPEO

Bond lengths (Å)		M1^{a}	M1^{b}	M2^{a}	M2^{b}	M3^{a}	M3^{b}	M4^{a}	M4^{b}	M5^{a}	M5^{b}	Exp.[23]
P1-O1	AM1	1.594	1.470	1.480	1.836	1.480	1.837	1.480	1.835	1.478	4.873	1.486(3)
P1-C7		1.599	1.678	1.620	1.670	1.670	1.671	1.620	1.670	1.624	1.707	1.793(3)
P1-C1		1.603	1.757	1.622	1.623	1.622	1.622	1.621	1.623	1.623	1.642	1.787(4)
P1-C13		1.645	1.726	1.658	1.650	1.658	1.650	1.658	1.649	1.654	1.676	1.800(3)
O2-H2A		2.095	0.986	0.978	2.206	0.978	2.200	0.978	2.196	0.978	5.100	0.820
		45.202^{C}		*52.678*^{C}		*51.988*^{C}		*52.443*^{C}		*163.240*^{C}		
P1-O1	PM3	1.487	1.741	1.489	1.839	1.489	1.839	1.489	1.840	1.616	9.741	1.486(3)
P1-C7		1.814	1.749	1.818	1.949	1.817	1.949	1.810	1.949	1.753	1.970	1.793(3)
P1-C1		1.828	1.596	1.821	1.827	1.822	1.827	1.822	1.827	1.779	1.798	1.787(4)
P1-C13		1.863	1.832	1.859	1.863	1.859	1.863	1.859	1.862	1.813	1.875	1.800(3)
O2-H2A		0.957	0.972	0.964	0.964	0.964	2.530	0.964	2.540	1.645	8.557	0.820
		14.871^{C}		*16.018*^{C}		*54.214*^{C}		*54.382*^{C}		*325.294*^{C}		
P1-O1	MNDO	6.432	1.683	1.519	4.386	1.519	4.349	1.520	4.510	4.978	5.417	1.486(3)
P1-C7		1.736	1.762	1.772	1.739	1.771	1.740	1.771	1.738	1.737	1.735	1.793(3)
P1-C1		1.736	1.699	1.768	5.648	1.769	5.662	1.770	5.773	1.741	6.612	1.787(4)
P1-C13		1.782	1.821	1.823	1.788	1.826	1.789	1.826	1.789	1.784	1.788	1.800(3)
O2-H2A		5.857	0.967	0.951	0.963	0.949	0.961	0.949	0.961	1.832	0.963	0.820
		198.629^{C}		*90.808*^{C}		*90.380*^{C}		*93.814*^{C}		*184.175*^{C}		
P1-O1	MINDO/3	1.647	2.666	1.535	11.266	1.644	2.742	1.646	2.460	1.661	2.794	1.486(3)
P1-C7		1.851	1.827	1.876	1.830	1.857	1.835	1.855	1.846	1.861	1.844	1.793(3)
P1-C1		1.859	1.879	1.878	10.713	1.858	3.951	1.861	3.689	1.859	4.047	1.787(4)
P1-C13		1.883	1.827	1.893	1.844	1.876	1.852	1.883	1.852	1.885	1.857	1.800(3)
O2-H2A		0.977	0.965	0.949	0.963	0.957	0.971	0.975	0.976	0.971	0.965	0.820
		29.498^{C}		*242.701*^{C}		*53.674*^{C}		*47.746*^{C}		*56.184*^{C}		

^{a} data for first half of the cocrystal, ^{b} data for second half of the cocrystal, ^{c} mean values for the percentage difference between two halves of the cocrystal [(Exp-M^{a}) + (Exp-M^{b})]/[(Exp) × 100]

TABLE-3
PERCENTAGE DEVIATIONS FROM SYMMETRY FOR SELECTED ANGLES OF TWO HALVES OF THE COCRYSTAL OF 4-CHLOROPHENOL WITH DPPEO

Bond lengths (Å)		M1 [a]	M1 [b]	M2 [a]	M2 [b]	M3 [a]	M3 [b]	M4 [a]	M4 [b]	M5 [a]	M5 [b]	Exp. [23]
O1-P1-C1	AM1	113.1	36.3	112.2	85.6	112.2	86.0	112.4	85.7	112.5	67.3	112.1(2)
O1-P1-C13		102.5	140.8	111.1	89.7	110.7	89.4	110.7	89.5	112.4	146.6	112.1(2)
O1-P1-C7		115.6	104.2	111.9	167.0	112.0	166.8	112.0	167.0	111.8	115.2	111.8(2)
C1-P1-C7		110.3	107.2	107.8	96.3	107.7	96.6	107.7	96.1	106.6	91.3	107.6(2)
C1-P1-C13		106.2	110.1	105.2	115.6	105.1	115.6	105.1	115.6	104.0	116.1	107.7(2)
C7-P1-C13		108.3	106.9	108.3	101.0	108.8	101.0	108.7	101.3	109.0	98.2	105.2(2)
		20.656 [c]		*20.225* [c]		*20.287* [c]		*20.391* [c]		*18.664* [c]		
O1-P1-C1	PM3	113.4	112.5	112.7	82.0	112.7	81.9	112.7	81.7	104.7	48.3	112.1(2)
O1-P1-C13		112.8	107.4	113.5	92.1	113.8	92.3	113.5	92.3	112.3	155.5	112.1(2)
O1-P1-C7		112.8	98.4	113.9	171.2	113.8	170.8	114.0	170.8	113.9	107.0	111.8(2)
C1-P1-C7		105.3	114.3	104.4	90.0	104.6	89.8	104.6	89.9	109.4	92.1	107.6(2)
C1-P1-C13		104.8	113.1	105.6	118.0	105.4	118.0	105.3	118.1	107.1	116.5	107.7(2)
C7-P1-C13		107.0	110.1	105.8	94.9	105.7	95.1	105.9	95.1	109.2	91.4	105.2(2)
		6.942 [c]		*23.782* [c]		*23.720* [c]		*23.783* [c]		*25.051* [c]		
O1-P1-C1	MNDO	95.8	109.8	113.0	6.6	112.8	6.4	112.8	6.5	131.3	6.8	112.1(2)
O1-P1-C13		111.0	106.4	110.8	150.1	110.9	148.3	111.0	147.8	98.4	144.3	112.1(2)
O1-P1-C7		125.7	103.4	109.7	101.6	109.5	103.8	109.5	103.9	105.6	107.3	111.8(2)
C1-P1-C7		106.3	111.9	107.1	102.6	107.2	104.2	106.9	104.4	105.8	113.4	107.6(2)
C1-P1-C13		107.2	116.2	104.1	148.5	103.9	147.6	103.8	146.8	103.2	138.9	107.7(2)
C7-P1-C13		108.7	108.3	112.1	108.3	112.5	107.9	112.8	108.3	111.9	107.5	105.2(2)
		10.407 [c]		*32.803* [c]		*31.851* [c]		*31.750* [c]		*35.057* [c]		
O1-P1-C1	MINDO/3	107.4	29.9	111.0	6.4	107.2	10.7	105.3	11.5	105.2	8.2	112.1(2)
O1-P1-C13		99.8	117.5	113.0	67.2	103.0	122.1	110.4	129.6	105.3	130.2	112.1(2)
O1-P1-C7		108.9	111.1	109.2	84.4	107.9	100.0	107.5	100.6	107.6	96.9	111.8(2)
C1-P1-C7		114.7	124.7	107.3	89.5	116.1	100.3	115.4	99.6	117.0	100.7	107.6(2)
C1-P1-C13		108.9	119.4	104.9	68.1	108.7	130.5	107.4	139.3	108.5	134.0	107.7(2)
C7-P1-C13		115.8	114.5	111.2	113.7	113.0	111.0	110.7	107.3	112.4	108.5	105.2(2)
		24.986 [c]		*38.869* [c]		*29.270* [c]		*29.721* [c]		*31.405* [c]		

[a] data for first half of the cocrystal, [b] data for second half of the cocrystal, [c] mean values for the percentage difference between two halves of the cocrystal $[(\text{Exp-M}^a) + (\text{Exp-M}^b)]/[(\text{Exp}) \times 100]$

TABLE-4

MEAN VALUES OF SELECTED BOND LENGTHS AND ANGLES OBTAINED FROM PERCENTAGE DIFFERENCES BETWEEN QUANTUM CHEMICAL CALCULATIONS AND PREVIOUSLY OBTAINED EXPERIMENTAL DATA FOR DPPEO/4-CHLOROPHENOL

	Exp. [23]	M1[a]	M2[a]	M3[a]	M4[a]	M5[a]	M1[a]	M2[a]	M3[a]	M4[a]	M5[a]
Lengths(Å)		AM1					PM3				
P1-O1	1.486(3)	1.532	1.658	1.659	1.658	3.176	1.614	1.664	1.664	1.665	5.679
P1-C7	1.793(3)	1.639	1.645	1.671	1.645	1.666	1.782	1.884	1.883	1.880	1.862
P1-C1	1.787(4)	1.680	1.623	1.622	1.622	1.633	1.712	1.824	1.825	1.825	1.789
P1-C13	1.800(3)	1.686	1.654	1.654	1.654	1.665	1.848	1.861	1.861	1.861	1.844
O2-H2A	0.820	1.541	1.592	1.589	1.587	3.039	0.965	0.964	1.747	1.752	5.101
Angles(°)		*22.385*[b]	*26.258*[b]	*25.913*[b]	*26.141*[b]	*81.512*[b]	*6.743*[b]	*8.009*[b]	*27.107*[b]	*27.191*[b]	*162.111*[b]
O1-P1-C1	112.1(2)	74.700	98.900	99.100	99.050	89.900	112.950	97.350	97.300	97.200	76.500
O1-P1-C13	112.1(2)	121.650	100.400	100.050	100.100	129.500	110.100	102.800	103.050	102.900	133.900
O1-P1-C7	111.8(2)	109.900	139.450	139.400	139.500	113.500	105.600	142.550	142.300	142.400	110.450
C1-P1-C7	107.6(2)	108.750	102.050	102.150	101.900	98.950	109.800	97.200	97.200	97.250	100.750
C1-P1-C13	107.7(2)	108.150	110.400	110.350	110.350	110.050	108.950	111.800	111.700	111.700	111.800
C7-P1-C13	105.2(2)	107.600	104.650	104.900	105.000	103.600	108.550	100.350	100.400	100.500	100.300
		7.892[c]	*9.189*[c]	*9.141*[c]	*9.178*[c]	*8.098*[c]	*2.413*[c]	*11.174*[c]	*11.083*[c]	*11.112*[c]	*11.207*[c]
Lengths(Å)		MNDO					MINDO/3				
P1-O1	1.486(3)	4.058	2.953	2.934	3.015	5.198	2.157	6.401	2.193	2.053	2.228
P1-C7	1.793(3)	1.749	1.756	1.756	1.755	1.736	1.839	1.853	1.846	1.851	1.853
P1-C1	1.787(4)	1.718	3.708	3.716	3.772	4.177	1.869	6.296	2.905	2.775	2.953
P1-C13	1.800(3)	1.802	1.806	1.808	1.808	1.786	1.855	1.869	1.864	1.868	1.871
O2-H2A	0.820	3.412	0.957	0.955	0.955	1.398	0.971	0.956	0.964	0.976	0.968
Angles(°)		*99.115*[b]	*45.058*[b]	*44.867*[b]	*46.595*[b]	*91.573*[b]	*14.749*[b]	*121.350*[b]	*26.837*[b]	*23.873*[b]	*28.092*[b]
O1-P1-C1	112.1(2)	102.800	59.800	59.600	59.650	69.050	68.650	58.700	58.950	58.400	56.700
O1-P1-C13	112.1(2)	108.700	130.450	129.600	129.400	121.350	108.650	90.100	112.550	120.000	117.750
O1-P1-C7	111.8(2)	114.550	105.650	106.650	106.700	106.450	110.000	96.800	103.950	104.050	102.250
C1-P1-C7	107.6(2)	109.100	104.850	105.700	105.650	109.600	119.700	98.400	108.200	107.500	108.850
C1-P1-C13	107.7(2)	111.700	126.300	125.750	125.300	121.050	114.150	86.500	119.600	123.350	121.250
C7-P1-C13	105.2(2)	108.500	110.200	110.200	110.550	109.700	115.150	112.450	112.000	109.000	110.450
		3.672[c]	*15.517*[c]	*15.055*[c]	*15.004*[c]	*11.662*[c]	*11.690*[c]	*19.301*[c]	*12.151*[c]	*13.353*[c]	*13.623*[c]

[a] mean values for two halves of the molecule, [b] mean values for the percentage difference of theoretical and experimental results of bond lengths $[(M^a\text{-}M^b)/\text{Exp} \times 100]$, [c] mean values for the percentage difference of theoretical and experimental results of angles $[(M^a\text{-}M^b)/\text{Exp} \times 100]$

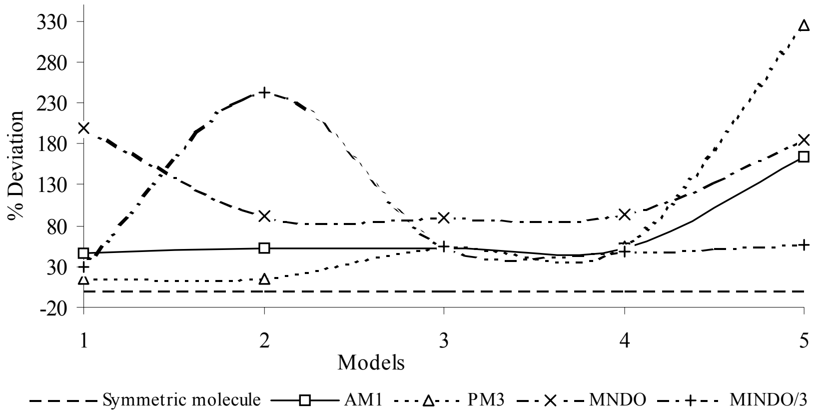

Fig. 3. Deviations from symmetry between the two halves of the molecule for the selected bond lengths

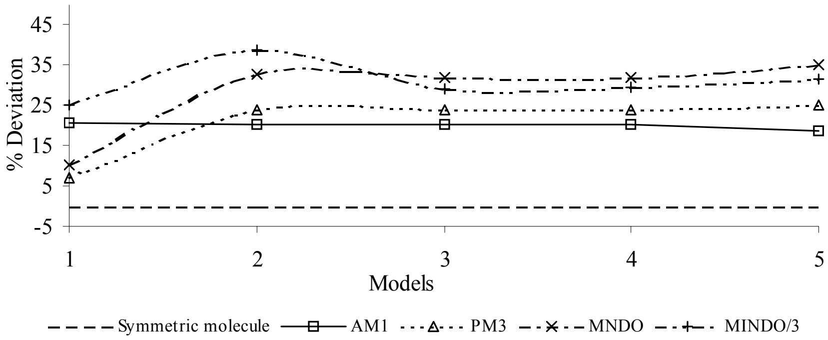

Fig. 4. Deviations from symmetry between the two halves of the molecule for the selected angles

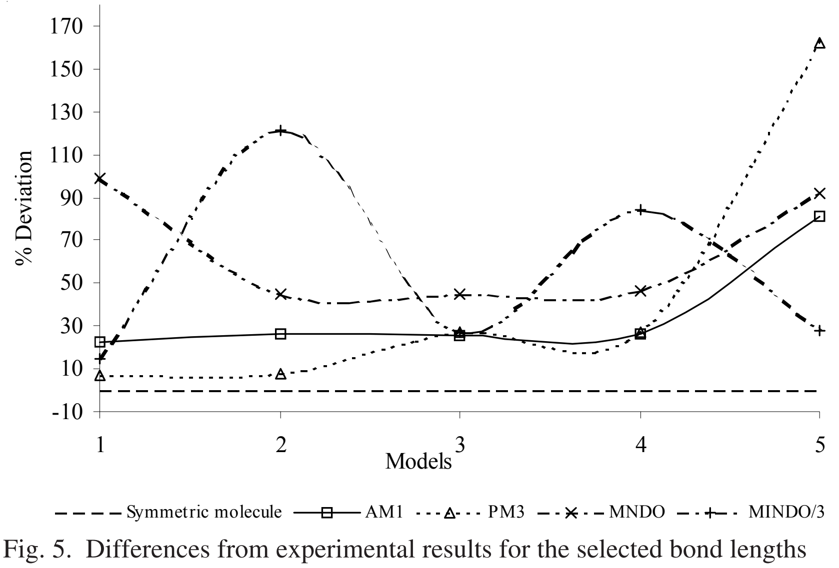

Fig. 5. Differences from experimental results for the selected bond lengths

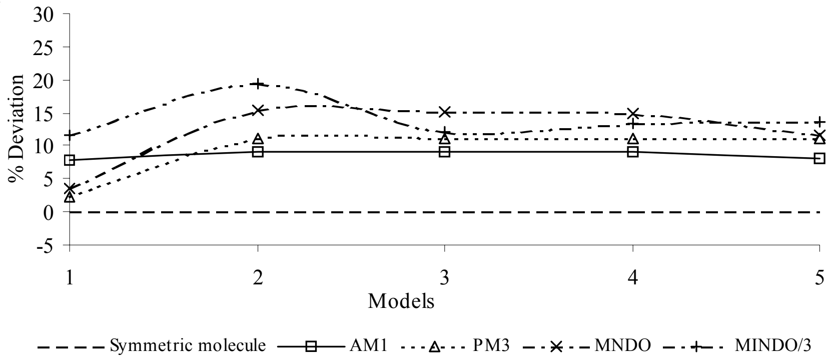

Fig. 6. Differences from experimental results for the selected angles

For hydrogen bond geometry, none of the theoretical methods for all models are fit for experimental hydrogen bond geometry (Table-5). This might be due to the difference between gas phase where the cocrystal being as isolated molecule and solid state connected to the neighbour molecules. In present study, only the vander Waals contacts in cocrystal up to 3 Å could be established. For theoretical methods used in this study, the limit of allowed number of atoms is 100, inter-molecular contacts between the neighbour cocrystals could not established. This probably caused significant elongation of hydrogen bond length (H2A···O1) and related bond lengths of O2···O1 and O2-H2A as well as hydrogen bond angle (O2-H2A···O1) in all calculations.

TABLE-5
MEAN VALUES FOR TWO HALVES OF THE MOLECULE FOR HYDROGEN BONDING

	Exp.[23]	M1	M2	M3	M4	M5
AM1						
H2A···O1 (Å)	1.826	1.775	2.044	2.040	2.046	3.295
O2···O1 (Å)	2.643	1.285	2.139	2.137	2.139	2.055
O2-H2A···O1 (°)	173	35.600	101.150	101.600	101.400	90.550
PM3						
H2A···O1 (Å)	1.826	1.811	2.012	2.013	2.012	5.235
O2···O1 (Å)	2.643	2.087	2.129	2.127	2.126	1.885
O2-H2A···O1 (°)	173	105.300	106.100	106.050	105.350	82.289
MNDO						
H2A···O1 (Å)	1.826	3.695	2.490	2.425	2.488	1.398
O2···O1 (Å)	2.643	1.204	2.656	2.587	2.653	1.300
O2-H2A···O1 (°)	173	25.750	96.750	96.400	96.750	42.700
MINDO/3						
H2A···O1 (Å)	1.826	1.884	4.484	1.873	1.897	1.889
O2···O1 (Å)	2.643	1.395	4.125	1.399	1.412	1.395
O2-H2A···O1 (°)	173	45.900	59.150	58.700	46.300	45.550

Conclusion

All available hydrogen bond donors and acceptors are involved forming hydrogen bonds in the cocrystal. This is according with the Etter rules that in the solid state all available acidic hydrogen atoms participate in hydrogen bonds[29]. The crystal structure of the cocrystal DPPEO/4-chlorophenol has been thoroughly examined previously and it revealed that out there are no apparent holes in the packing diagram due to dense packing behaviour in the lattice[23]. With and without vander Waals interactions in cocrystal for computing, AM1 gave comparable results between experimental and theoretical studies for the selected bond lengths and angles. In previous study, AM1 was also seemed to be the best fit for the C-C, C-P and P-O bond lengths and angles as well as for hydrogen bond geometry for the cocrystal of DPPEO/HQ[11]. The effects of vander Waals interactions on geometries of molecules will need to be checked out in future studies.

ACKNOWLEDGEMENT

The authors like to express sincere thanks and gratitude to Prof. Dr. Cemil Ögretir for his support in this study.

REFERENCES

1. M.C. Etter and P.W. Baures, *J. Am. Chem. Soc.*, **110**, 689 (1988).
2. C. Lariucci, R.H. De A. Santos and J.R. Lechat, *Acta. Cryst.*, **C42**, 1824 (1986).
3. R.M. Fuquen and J.R. Lechat, *Acta. Cryst.*, **C48**, 1690 (1992).
4. T. Gramstad, S. Husebye and K. Maartmann-Moe, *Acta Chem. Scand.*, **B40**, 26 (1986).
5. R.M. Harrison, P.A. Chaloner and P.B. Hitchcock, *Acta. Cryst.,* **C49**, 1072 (1993).
6. D.C. Apperley, P.A. Chaloner, L.A. Crowe, R.K. Harris, R.M. Harrison, P.B. Hitchcock and C.M. Lagier, *Phys. Chem. Chem. Phys.*, **2**, 3511 (2000).
7. Z. Dega-Szafran, G. Dutkiewicz, Z. Kosturkiewicz and M. Szafran, *J. Mol. Struct.*, **641**, 251 (2002).
8. Z. Dega-Szafran, E. Tykarska, E. Dulewicz and M. Szafran, *J. Mol. Struct.*, **605**, 319 (2002).
9. C. Yenikaya, C. Ögretir and H. Berber, *J. Mol. Struct. (Theochem.)*, **713**, 171 (2005).
10. C. Yenikaya and C. Ögretir, *J. Mol. Struct. (Theochem)*, **731**, 1 (2005).
11. C. Yenikaya, C. Ögretir and H. Berber, *J. Mol. Struct. (Theochem.)*, **725**, 207 (2005).
12. C. Yenikaya, C. Ögretir and H. Berber, *J. Mol. Struct. (Theochem.)*, **686**, 153 (2004).
13. C. Ögretir and N.F. (Kaypak) Tay, *J. Mol. Struct. (Theochem.)*, **588**, 145 (2002).
14. N. Tokay, and C. Ögretir, *J. Mol. Struct. (Theochem.)*, **594**, 185 (2002).
15. N. Tokay, and C. Ögretir, *J. Mol. Struct. (Theochem.)*, **629**, 51 (2003).
16. N. Tokay and C. Ögretir, *J. Mol. Struct. (Theochem.)*, **626**, 113 (2003).
17. C. Ögretir, S. Çalis, G. Bereket and H. Berber, *J. Mol. Struct. (Theochem.)*, **626**, 179 (2003).
18. G. Bereket, C. Ögretir and Ç. Özsahin, *J. Mol. Struct. (Theochem.)*, **663**, 39 (2003).
19. C. Ögretir, S. Çalis and G. Bereket, *J. Mol. Struct. (Theochem.)*, **635**, 229 (2003).
20. G. Bereket, C. Ögretir, M. Yaman and E. Hür, *J. Mol. Struct. (Theochem.)*, **625**, 31 (2003).

21. S. Yarligan, A.K. Füzery, C. Ögretir and I.G. Csizmadia, *J. Mol. Struct. (Theochem.)*, **666-667**, 269 (2003).
22. C. Ögretir, S. Yarligan, S. Demirayak and T. Arslan, *J. Mol. Struct. (Theochem.)*, **666-667**, 609 (2003).
23. P.A. Chaloner, C. Yenikaya, P.B. Hitchcock, Private Communication to the Cambridge Structural Database, Deposition number CCDC-231230. CCDC, 12 Union Road, Cambridge, UK (2004).
24. J.J.P. Stewart, MOPAC 7.0 QCPE, University of Indiana, Bloomington IN, USA.
25. CS Chemoffice Pro for Microsoft Windows, Cambridge Scientific Computing Inc., 875 Massachusetts Avenue, Suite 61, Cambridge MA 2139, USA.
26. I.J. Bruno, J.C. Cole, P.R. Edgington, M.K. Kessler, C.F. Macrae, P. McCabe, J. Pearson and R. Taylor, *Acta Crystallogr.*, **B58**, 389 (2002).
27. R. Taylor and C.F. Macrae, *Acta Crystallogr.*, **B57**, 815 (2001).
28. P.A. Chaloner, C. Yenikaya, P.B. Hitchcock, Private Communication to the Cambridge Structural Database, deposition number CCDC-231228. CCDC, 12 Union Road, Cambridge, UK (2004).
29. M.C. Etter, *J. Phys. Chem.*, **95**, 4601 (1991).

(*Received*: 15 November 2006; *Accepted*: 14 September 2007) AJC-5845