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Solvent (Water) Effect on Geometry Properties of Patuletin Dyes for Formation of Metal Complex by DFT Method

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ABSTRACT

For determine the metal complex structure used is the costly and complicated spectrum method but due to DFT method, fast computer we can interested to sketch of metal complex with patuletin ligand in proper solvent over the calculation of geometrical properties by DFT method. The interested result is outcome that, only optimization and charge density properties explain by the probable side attack of metal on ligand.

Keywords : Solvent effect, Geometry, DFT Method, Patuletin dye.

I. INTRODUCTION

Computational chemistry is used in a number of different ways [1]. One particularly important way is to model a molecular system prior to synthesizing the target molecule in the laboratory [2]. Although computational models may not be precisely accurate, but they are often good enough to rule out 90% of possible compounds as being unsuitable for their intended use [3]. This is very useful information because synthesizing a single compound may require months of labour, raw materials cost and also generate toxic waste. A second use of computational chemistry is in understanding a problem more completely [4]. There are some properties of a molecule such as electronic charge distribution, dipoles and vibrations frequency that can be obtained computationally more easily than by experimental means. There are also insights into molecular bonding, which can be obtained from the results of computations, which cannot be obtained from any experimental method. In 2011, Jadhao N.U. and Rathod S.P. were done the quantum mechanical calculation for Schiff bases by DFT method which shows the appropriate result to experimental data and they shows the type of electronic state of UV-Visible spectrum and clear the transition type by the TD-DFT method [5].

For determine the metal complex structure used is the costly and complicated spectrum method but we have been interested to sketch of metal complex with patuletin ligand in proper solvent over the calculation of geometry properties by DFT method. For the above mentioned reasons, optimization in gas phase and water phase will be carried out. Computational calculations will be employed to study charge density properties for patuletin dye.

II. MATERIAL AND METHODS

Computation work was done using the GAUSSIAN 03W program suite. The patuletin studied in C_1 symmetry and molecule was fully optimized with the tight criteria using the DFT (PBE1) level of theory with basis set 3-21G used without solvent and same

parameters are used to optimize the patuletin in water as a solvent with IEFPCM model.

The following is structure of patuletin.

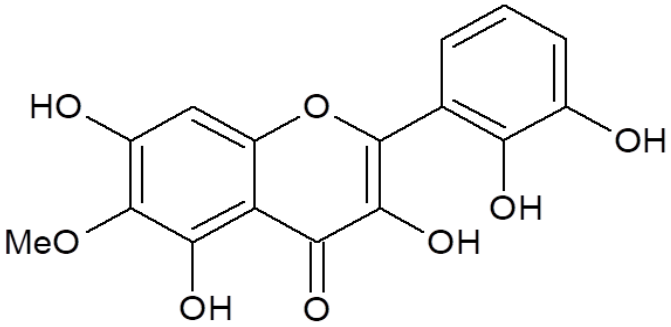

Figure 1.1 Structure of Patuletin

III. RESULT AND DISCUSSION

3.1. MOLECULAR OPTIMIZATION GEOMETRY

We started the geometry optimization of patuletin, without symmetry constraints. Optimized structure converged to C_1 symmetrical species. The geometry was optimized in a singlet ground state by the DFT method with the PBE1function using 3-21G** basis set in gas phase and water phase using with IEFPCM model. The optimized structure in gas phase shown in figure 1.2a and in water phase shown in figure 1.2b.

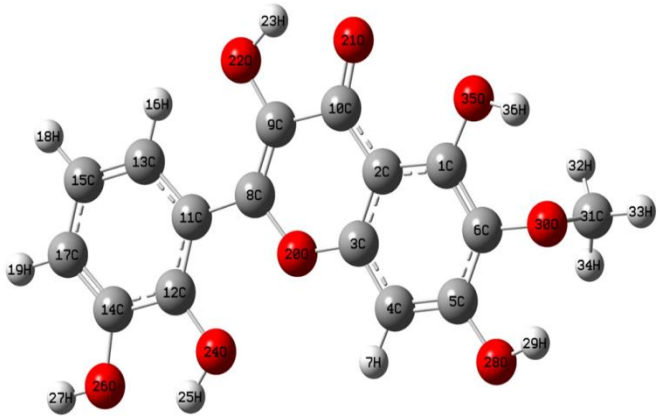

Figure 1.2 a) Optimized structure in gas phase of patuletin.

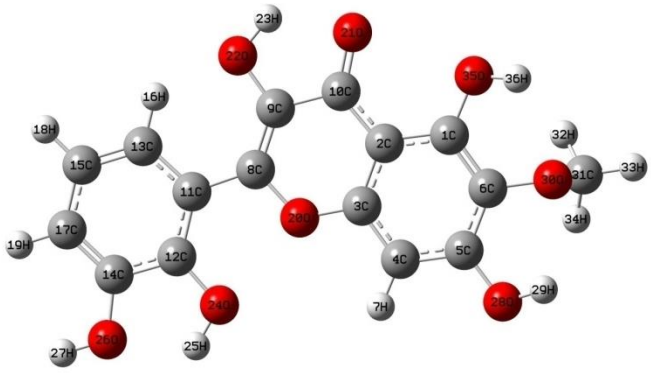

Figure 1.2 b) Optimized structure in water phase of patuletin

In both phases the molecule behaves the planner structure only methyl group is out of plane. The bond length of all O-H bond are higher in water phase as compare to gas phase because in water phase, the H-bonding was occurred due to this bonding all O-H bond length are changed as compare to gas phase moiety are shown in table 1.

The large effect show in 26 – O and 27- H that is in gas phase the bond length between these atoms is 0.984836 Å and in water phase the bond length between these atoms is 1.011795 Å.

So the 27-hydrogen atom in water phase is goes long from 26-oxygen atom and it is good intense towards, breaking of bond with low energy and formation of metal complex.

The optimized geometric all parameters are gathered in following table.

Table 1. Bond length of O-H in Å in water and gas phase

Sr.no.	No. of atom	Bond length of O-H in Å	
		In water phase	In gas phase
1.	22,23	1.023189	1.024274
2.	24,25	1.006361	0.998632
3.	**26,27**	**1.011795**	**0.984836**
4.	28,29	1.009733	0.997015
5.	35,36	1.010088	0.997357

The optimized geometric all parameters are gathered in following table.

Full optimized parameter in gas phase

#	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	C							-2.988753	0.700149	-0.180053
2	C	1			1.408478			-1.581500	0.731382	-0.130326
3	C	2	1		1.408482	117.639461		-0.900294	-0.501406	-0.126732
4	C	3	2	1	1.393131	122.945613	0.898173	-1.555550	-1.729284	-0.188136
5	C	4	3	2	1.382931	118.364344	-0.993369	-2.937693	-1.734807	-0.234482
6	C	1	2	3	1.379311	118.964411	0.092546	-3.628755	-0.521022	-0.220523
7	H	4	3	2	1.079072	119.621492	178.921737	-0.979147	-2.641438	-0.199629
8	C	3	2	1	2.416493	92.245163	-179.888473	1.257083	0.582830	-0.028789
9	C	8	3	2	1.357606	89.633500	-0.157193	0.639895	1.792022	-0.034172
10	C	2	1	6	1.435028	123.514503	-179.900709	-0.817050	1.944944	-0.083537
11	C	8	3	2	1.454500	142.860368	179.700343	2.686371	0.318334	0.023642
12	C	11	8	3	1.403555	122.530631	-0.216167	3.213412	-0.982482	0.032192
13	C	11	8	3	1.414672	119.228100	179.861856	3.589028	1.406630	0.069687
14	C	12	11	8	1.407575	119.120192	-179.899032	4.609242	-1.155677	0.086327
15	C	13	11	8	1.382304	121.455434	179.913342	4.956017	1.208259	0.122180
16	H	13	11	8	1.080951	117.495327	-0.043442	3.170110	2.403083	0.063059
17	C	14	12	11	1.377223	122.184513	-0.016640	5.479577	-0.089253	0.131046
18	H	15	13	11	1.083330	119.928619	179.991533	5.624819	2.059801	0.156579
19	H	17	14	12	1.085499	120.683223	179.996189	6.552160	-0.250995	0.172439
20	O	3	2	1	1.365196	121.123522	-179.796374	0.462929	-0.554193	-0.075767
21	O	10	2	1	1.260671	128.153898	0.101221	-1.240481	3.132359	-0.076967
22	O	9	8	3	1.365325	125.842044	-179.981564	1.261361	3.007006	0.007134
23	H	22	9	8	1.024274	101.380116	-179.836063	0.459965	3.644644	-0.010736
24	O	12	11	8	1.369395	124.542780	0.052026	2.460485	-2.125606	-0.007946
25	H	24	12	11	0.998632	105.404110	179.950117	3.117958	-2.877053	0.009987
26	O	14	12	11	1.394731	111.871634	179.967089	4.965805	-2.504059	0.088348
27	H	26	14	12	0.984836	111.615236	179.777908	5.943088	-2.620833	0.122739
28	O	5	4	3	1.367428	122.018135	179.906781	-3.656336	-2.896447	-0.297760
29	H	28	5	4	0.997015	106.384094	-169.939801	-4.599217	-2.633849	-0.487648
30	O	6	1	2	1.415223	118.968375	178.093274	-5.043580	-0.553430	-0.229306
31	C	30	6	1	1.487317	110.478362	-88.882434	-5.572083	-0.580310	1.160685
32	H	31	30	6	1.094601	109.966538	60.254643	-5.248431	0.314932	1.701003
33	H	31	30	6	1.091157	105.816795	179.800416	-6.658874	-0.600606	1.065305
34	H	31	30	6	1.094714	110.004241	-60.635167	-5.213203	-1.474364	1.680561
35	O	1	6	5	1.362768	119.139350	178.920002	-3.734360	1.840798	-0.191284
36	H	35	1	6	0.997357	106.374600	-10.227444	-4.669500	1.563401	-0.399336

Full optimized parameter in water phase

#	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	C							-3.003452	0.701015	-0.185644
2	C	1			1.413264			-1.591124	0.731355	-0.144109
3	C	2	1		1.407281	117.702158		-0.909910	-0.500055	-0.148076
4	C	3	2	1	1.388718	122.702305	1.381827	-1.567603	-1.721107	-0.218863
5	C	4	3	2	1.388235	118.798839	-1.408448	-2.955220	-1.731973	-0.258829
6	C	1	2	3	1.383830	119.334543	-0.040751	-3.654362	-0.519408	-0.228883
7	H	4	3	2	1.083011	120.042092	178.799368	-0.999207	-2.642763	-0.238575
8	C	3	2	1	2.419824	92.312924	-179.515244	1.251233	0.583546	-0.044073
9	C	8	3	2	1.360446	89.453219	-0.380904	0.630003	1.793866	-0.047467
10	C	2	1	6	1.435377	123.506141	-179.858467	-0.825749	1.944644	-0.094737
11	C	8	3	2	1.458122	142.946310	179.017748	2.683871	0.319083	0.016986
12	C	11	8	3	1.406104	122.593502	-0.011777	3.213804	-0.983271	0.030151
13	C	11	8	3	1.417790	119.273664	-179.701417	3.588409	1.409452	0.072077
14	C	12	11	8	1.413067	119.444000	-179.558676	4.613668	-1.162917	0.099917
15	C	13	11	8	1.382554	121.389472	179.587857	4.954687	1.208966	0.139487
16	H	13	11	8	1.080584	117.697869	-0.265403	3.173569	2.407184	0.062077
17	C	14	12	11	1.379719	121.616237	-0.054642	5.478800	-0.089521	0.154621
18	H	15	13	11	1.086626	119.915737	-179.951535	5.626202	2.062227	0.181558
19	H	17	14	12	1.088028	120.045896	179.969903	6.552460	-0.257370	0.208331
20	O	3	2	1	1.369856	121.135416	-179.477268	0.458035	-0.552930	-0.098727
21	O	10	2	1	1.262415	127.778058	-0.194040	-1.256894	3.131105	-0.083960
22	O	9	8	3	1.367092	124.845825	-179.939315	1.270543	3.000771	-0.002406
23	H	22	9	8	1.023189	103.673240	-179.605120	0.506146	3.680838	-0.013424
24	O	12	11	8	1.367126	124.092475	0.337316	2.455430	-2.119714	-0.018826
25	H	24	12	11	1.006361	106.992711	-179.629300	3.091313	-2.899151	0.011074
26	O	14	12	11	1.378803	112.170304	179.924419	4.967594	-2.495510	0.105430
27	H	26	14	12	1.011795	112.824177	-179.437891	5.967899	-2.635683	0.164333
28	O	5	4	3	1.360398	119.713615	-179.108634	-3.619061	-2.918307	-0.309906
29	H	28	5	4	1.009733	110.690317	-162.773260	-4.572257	-2.780957	-0.613408
30	O	6	1	2	1.405386	118.911030	176.234483	-5.059005	-0.542058	-0.189198
31	C	30	6	1	1.490613	110.075221	-88.961073	-5.530136	-0.596134	1.223968
32	H	31	30	6	1.094460	109.898615	59.605102	-5.167411	0.279466	1.771323
33	H	31	30	6	1.091189	105.719625	178.975509	-6.620107	-0.592188	1.172575
34	H	31	30	6	1.094475	109.841620	-61.729088	-5.171231	-1.513805	1.700354
35	O	1	6	5	1.358005	120.340657	179.402218	-3.714814	1.857687	-0.169742
36	H	35	1	6	1.010088	109.727449	-16.772299	-4.663510	1.678613	-0.466705

3.2. Charge Density:

The atomic charge density gives the information about the oxidation state of atoms and oxidation state is very important to formation of metal complexes.

The figure 1.3 and 1.4 shows the charge density of all atoms present in the patuletin dye in gas phase and water phase respectively.

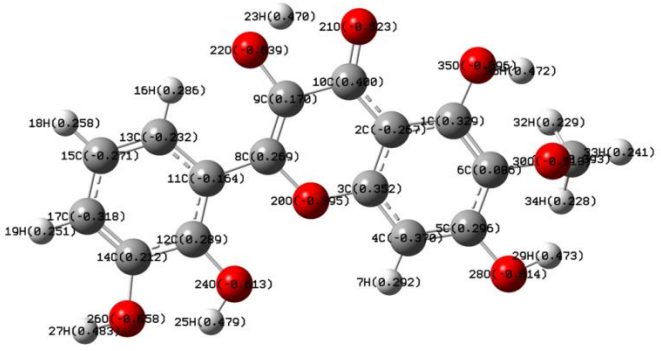

Figure 1.3. Charge density of patuletin in gas phase.

Table 2. Charge density of O-H atom in water and gas phase

Sr. no.	No. of atom	Charge density in water phase		Charge density in gas phase	
		Oxygen	Hydrogen	Oxygen	Hydrogen

1.	22,23	-0.652	0.490	-0.639	0.470
2.	24,25	-0.633	0.502	-0.613	0.479
3.	**26,27**	**-0.680**	**0.544**	**-0.658**	**0.483**
4.	28,29	-0.641	0.520	-0.614	0.473
5.	35,36	-0.630	0.517	-0.596	0.472

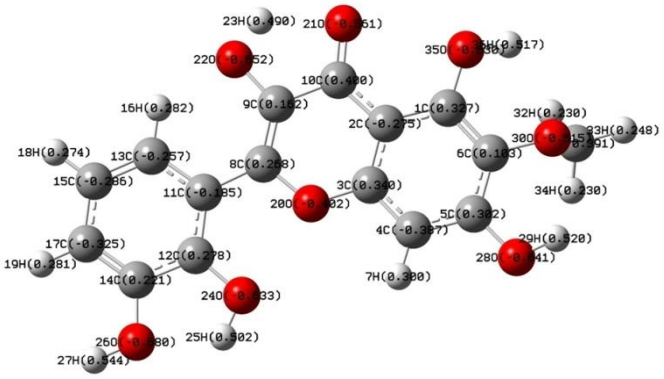

Figure 1.4. Charge density of patuletin in water phase.

In table 2 show the charge density on Oxygen and Hydrogen atom which is involve in O-H bond. From the table 2 , charge density in water phase are higher than gas phase moiety. The large effect show on 26-O and 27-H in water phase that are -0.680 and 0.544 respectively. Due to large negative charge on 26-Oxygen atom, it attract the metal towards itself.

The charge density presented in 26-O and 27-H atoms showing the good intense towards metal complex formation. So the charge density is very much important to study in the metal complex formation.

IV. CONCLUSION

From the present work, we concluded that, the quantum mechanical calculation is very much helpful to sketch the probable metal complex structure with patuletin ligand in water solvent for this only use the optimization and charge density properties by DFT method instead of complicated and costly spectrum method.

V. ACKNOWLEDGEMENTS

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VI. REFERENCES

[1]. Koch Wolfram and Holthausen Max C., "A Chemist's Guide to Density Functional Theory". Second Edition, Copyright © (2001) Wiley-VCH Verlag GmbH.ISBNs: 3-527-30372-3 (Softcover); 3-527-60004-3 (Electronic).

[2]. Kohn W., Sham L., J. Phys. Rev. A 140 (1965) 1133.

[3]. Frisch M.J. et al., GAUSSIAN 03, Revision B04, Gaussian Inc., Wallingford, CT,(2004).

[4]. Legault C.Y., CYLVIEW, 1.0b , Université de Sherbrooke, (2009).

[5]. Jadhao N.U. and Rathod S.P., The ecosphere, 2 (1&2):103-106, (2011), ISSN: 0976-1578.

[6]. Dennington R., Keith T., Millam J., Eppinnett K., Hovell W.L., Gilliland R., Gaussview, Version 3.09, Semichem, INC., Shawnee Mission, KS, (2003).

[7]. Zhdankin V.V., Crittell C.M., Stang P.J., Tetrahedron Lett. 31 (1990) 4821.

[8]. H. Chermette, Coord. Chem. Rev. 178–180 (1998) 699.

[9]. M.C. Aragoni, M. Arca, T. Cassano, C. Denotti, F.A. Devillanova, F. Isaia, V. Lippolis, D. Natali, L. Niti, M. Sampietro, R. Tommasi, G. Verani, Inorg. Chem. Commun. 5 (2002) 869.

[10]. P. Romaniello, F. Lelj, Chem. Phys. Lett. 372 (2003) 51.

[11]. A. Voigt, U. Abram, R. Bo¨ ttcher, U. Richter, J. Reinhold, R. Kirmse, Chem. Phys. 253 (2000) 171.

[12]. B. Machura, R. Kruszynski, Polyhedron 25 (2006) 1985.

[13]. J. Gancheff, C. Kremer, E. Kremer, O.N. Ventura, J. Mol. Struct. (Theochem) 580 (2002) 107.
[14]. M.J. Frisch et al., GAUSSIAN 03, Revision B04, Gaussian Inc., Wallingford, CT, (2004).
[15]. A. D. Becke, J. Chem. Phys. 98 (1993) 5648.