

Structure and Vibrational Spectra of *N,N*-Dimethyl-*N'*(2-chlorobenzoyl)thiourea: Hartree-Fock and Density Functional Theory Studies

HAKAN ARSLAN*†, FATİH MEHMET EMEN† and NEVZAT KÜLCÜ†

Department of Chemistry, Faculty of Pharmacy, Mersin University

Mezitli-Çiftlikköyü Kampüsü 33169-Mersin, Turkey

Fax: (90)(324)3413022; Tel: (90)(532)7073122; E-mail: arslanh@mersin.edu.tr

The molecular geometry and vibrational frequencies of *N,N*-dimethyl-*N'*(2-chlorobenzoyl)thiourea in the ground state has been calculated using the Hartree-Fock and density functional using Becke's three-parameter hybrid method with the Lee, Yang and Parr correlation functional (B3LYP) methods with 6-31G(d) and 6-311G(d) basis sets. The computational frequencies are in good agreement with the results of observed and normal coordinate analysis. The comparison of the observed fundamental vibrational frequencies of *N,N*-dimethyl-*N'*(2-chlorobenzoyl)thiourea and calculated density functional B3LYP and Hartree-Fock methods indicate that B3LYP is superior to the scaled Hartree-Fock approach for molecular vibrational problems.

Key Words: *N,N*-Dimethyl-*N'*(2-chlorobenzoyl)thiourea, Density functional theory, Infrared spectrum, Hartree-Fock, Molecular calculations.

INTRODUCTION

Study of the thiourea derivatives has recently attracted interest in view of the potential use of these compounds as highly selective reagents for the concentration and separation of metal cations¹. *N*-Benzoyl-*N',N'*-diheptadecylthiourea and *N*-benzoyl-*N',N'*-diethylthiourea have been successfully used in the extraction of copper and gold ions from acidic media^{2,3}. These derivatives have also been implemented in a solid supported liquid membrane system for the selective transport of palladium and gold ions^{4,5}. In addition, the platinum, palladium and rhodium contents in bimetallic Pt-Re, Pd and Pt catalysts were determined by high performance-TLC after forming their chelates with *N*-benzoyl-*N',N'*-diethylthiourea⁶.

†Department of Chemistry, Faculty of Arts and Science, Mersin University, 33343-Mersin, Turkey.

In previous studies, new thiourea derivatives having such properties were synthesized and examined⁷⁻¹⁴. The crystal structure and vibrational analysis of *N,N*-dimethyl-*N'*(2-chlorobenzoyl)thiourea (DMBT) has been reported by Arslan *et al.*¹⁴. The calculations of the vibrational frequencies have been carried out on the basis of normal coordinate analysis using simple general valence force field in Wilson's GF matrix method.

The purpose of this work is to calculate the molecular geometry and vibrational spectra of *N,N*-dimethyl-*N'*(2-chloro-benzoyl)thiourea by applying the Hartree-Fock and density functional using Becke's three-parameter hybrid method with the Lee, Yang and Parr correlation functional methods with 6-31G(d) and 6-311G(d) basis sets and to compare the performance of Hartree-Fock and density functional theory methods at different basis sets with normal coordinate analysis. The calculated vibrational frequencies were analyzed and compared with the results of experimental and normal coordinate analysis.

EXPERIMENTAL

DMBT was obtained as described in the literature^{10,14}. The solid-state infrared spectrum of the compound studied was recorded using KBr pellet by Bomem MB102 FT-IR instrument in the 4000-200 cm⁻¹ ranges; the resolution was 1 cm⁻¹. The molecular structure of the *N,N*-dimethyl-*N'*(2-chlorobenzoyl)thiourea in the ground state are optimized by Hartree-Fock and density functional using Becke's three-parameter hybrid method with the Lee, Yang and Parr correlation functional methods with the standard 6-31G(d) and 6-311G(d) basis sets. The vibrational frequencies were also calculated with these methods. These calculations were carried out using Gaussian 03W program package on a double Xeon/3.2 GHz processor with 4 GB Ram¹⁵. The frequency values computed at these levels contain known systematic errors¹⁶. The scaling factor values of 0.8929 and 0.9613 for HF and B3LYP methods, respectively have been used in present studies¹⁷. The assignment of the calculated wave numbers is aided by the animation option of GaussView 3.0 graphical interface for gaussian programs, which gives a visual presentation of the shape of the vibrational modes.

RESULTS AND DISCUSSION

The features of molecular geometry and vibration spectra of DMBT have been characterized¹⁴. DMBT geometric structure is monoclinic, space group P2₁/c, with the cell dimensions $a = 5.6601(13)$ Å, $b = 10.748(2)$ Å, $c = 17.778(4)$ Å, $\beta = 94.266(5)^\circ$ and $V = 1078.5(4)$ Å³¹⁴. The optimized structure parameters (bond lengths and angles) of *N,N*-dimethyl-*N'*(2-chlorobenzoyl)thiourea calculated at *ab initio* HF and density functional theory-B3LYP levels with the standard 6-31G(d) and 6-311G(d) basis sets are listed in Table-1 in accordance with the atom numbering scheme given in Fig. 1.

TABLE-1
OPTIMIZED GEOMETRIES OF THE *N,N*-DIMETHYL-*N'*(2-CHLORO-
BENZOYL)THIOUREA IN THE GROUND STATE

	Exp. ^a	HF		B3LYP	
		6-31G(d)	6-311G(d)	6-31G(d)	6-311G(d)
Bond lengths (Å)					
Cl(1)-C(1)	1.716(3)	1.737	1.737	1.752	1.752
S(1)-C(8)	1.669(3)	1.678	1.676	1.679	1.678
O(1)-C(7)	1.199(3)	1.188	1.182	1.215	1.209
N(1)-C(7)	1.383(3)	1.388	1.389	1.403	1.401
N(1)-C(8)	1.398(3)	1.400	1.401	1.415	1.414
N(2)-C(8)	1.314(3)	1.320	1.318	1.345	1.342
N(2)-C(9)	1.450(3)	1.458	1.458	1.464	1.463
N(2)-C(10)	1.452(3)	1.458	1.457	1.461	1.460
C(1)-C(2)	1.381(4)	1.384	1.383	1.395	1.392
C(1)-C(6)	1.383(4)	1.392	1.391	1.406	1.402
C(2)-C(3)	1.361(4)	1.384	1.383	1.394	1.391
C(3)-C(4)	1.365(4)	1.383	1.383	1.395	1.392
C(4)-C(5)	1.371(4)	1.383	1.382	1.393	1.390
C(5)-C(6)	1.390(4)	1.392	1.391	1.404	1.402
C(6)-C(7)	1.500(4)	1.505	1.506	1.506	1.507
<i>r</i>		0.9984	0.9982	0.9974	0.9976
Bond Angles (°)					
C(7)-N(1)-C(8)	125.6(2)	125.0	124.4	125.4	125.0
C(8)-N(2)-C(9)	124.6(2)	124.6	124.5	124.3	124.1
C(8)-N(2)-C(10)	121.2(2)	120.1	120.1	119.7	119.7
C(9)-N(2)-C(10)	114.0(2)	114.7	114.7	115.3	115.5
C(2)-C(1)-C(6)	122.0(3)	120.5	120.5	120.7	120.7
C(2)-C(1)-Cl(1)	117.3(3)	117.6	117.7	117.4	117.5
C(6)-C(1)-Cl(1)	120.6(2)	121.9	121.8	121.8	121.7
C(3)-C(2)-C(1)	117.8(3)	120.1	120.1	120.1	120.1
C(2)-C(3)-C(4)	122.6(3)	120.2	120.2	120.1	120.1
C(3)-C(4)-C(5)	118.7(3)	119.5	119.4	119.5	119.5
C(4)-C(5)-C(6)	121.4(4)	121.2	121.3	121.5	121.5
C(1)-C(6)-C(5)	117.4(3)	118.5	118.5	118.1	118.1
C(1)-C(6)-C(7)	123.3(3)	122.6	122.6	122.6	122.6
C(5)-C(6)-C(7)	119.2(3)	118.8	118.8	119.3	119.3
O(1)-C(7)-N(1)	123.5(3)	123.8	123.9	123.6	123.8
O(1)-C(7)-C(6)	124.2(3)	123.3	123.2	123.6	123.5
N(1)-C(7)-C(6)	112.3(3)	112.9	112.8	112.8	112.7
N(2)-C(8)-N(1)	116.9(2)	117.7	117.6	116.8	116.7
N(2)-C(8)-S(1)	124.5(2)	125.0	125.0	125.1	125.1
N(1)-C(8)-S(1)	118.6(2)	117.3	117.4	118.0	118.2
<i>r</i>		0.9540	0.9538	0.9576	0.9567

^aTaken from Ref(14).

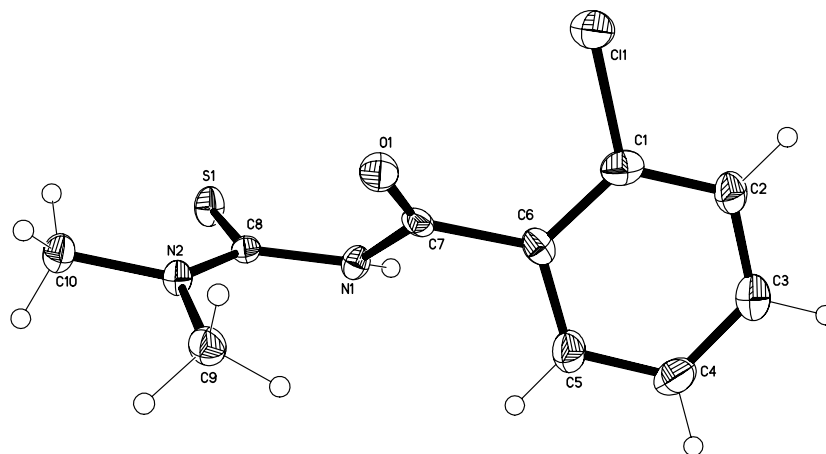


Fig. 1. Molecular structure of *N,N*-dimethyl-*N'*-(2-chloro-benzoyl)thiourea. Thermal ellipsoids are shown at the 50% probability level¹⁴

The correlation between the experimental and calculated geometric parameters obtained by *ab initio* HF and density functional theory-B3LYP methods is given in Table-1. On the basis of present calculations, HF methods correlates well for the bond length compare with the DFT methods. The largest difference between experimental and calculated HF bond length is about 0.023 Å. The bond angles provided by DFT method is much closer to experimental values. The largest difference between experimental and calculated DFT bond angles is about 2.5°. As a result, the optimized bond lengths obtained by *ab initio* HF method (6-31G(d)) and bond angles by DFT (6-31G(d)) method show the best agreement with the experimental values.

FT-IR spectrum of DMBT is given in Fig. 2. Table-2 listed the vibrational frequencies obtained using *ab initio* HF/6-31G(d), HF/6-311G(d), DFT-B3LYP/6-31G(d) and -B3LYP/6-311G(d) calculations together with the experimental frequencies and the approximate description of each normal modes. The calculated vibrational frequencies¹⁴ which have been carried out on the basis of normal coordinate analysis (NCA) using simple general valence force field in Wilson's GF matrix method with the SPSIM computer program¹⁸ are also given in Table-2.

The vibrational bands' assignments have been made by using GausView molecular visualization program. A linear regression correlation test was performed to investigate correlations between experimental and calculated frequencies. The values of the correlations coefficients are given in Table-3. It is clear from Table-3 that the experimental and NCA fundamentals are in better agreement with the scaled fundamentals and are found to have a good correlation for DFT-B3LYP (6-31G(d)) than HF.

TABLE-2
EXPERIMENTAL AND CALCULATED VIBRATIONAL
FREQUENCIES (cm⁻¹) OF DMBT

Exp. ^a	NCA ^b	HF				B3LYP				Assignments ^c
		6-31G(d)		6-311G(d)		6-31G(d)		6-311G(d)		
		Corr.	Inten.	Corr.	Inten.	Corr.	Inten.	Corr.	Inten.	
3166	3166	3458	56.88	3478	47.33	3444	29.98	3459	26.56	v _{N-H}
3091	3095	3064	6.70	3044	8.93	3104	5.55	3084	7.80	v _{C-H} , Ar
3091	3093	3054	14.38	3034	17.99	3093	13.15	3073	15.76	v _{C-H} , Ar
3091	3091	3042	12.27	3023	15.4	3081	9.37	3061	11.18	v _{C-H} , Ar
3091	3090	3033	0.14	3012	0.26	3072	0.20	3052	0.21	v _{C-H} , Ar
3019	3028	3030	15.08	3007	19.33	3062	8.92	3041	11.42	v _{C-H} , asym, CH ₃
3019	3025	3022	5.27	2997	9.35	3055	3.59	3033	7.01	v _{C-H} , asym, CH ₃
3019	3015	2982	18.8	2957	21.63	3016	12.60	2997	14.12	v _{C-H} , asym, CH ₃
3019	3015	2970	29.38	2949	38.59	3005	21.68	2989	27.23	v _{C-H} , asym, CH ₃
2924	2920	2915	63.21	2894	70.38	2948	48.36	2933	52.21	v _{C-H} , sym, CH ₃
2924	2920	2905	18.65	2884	20.95	2935	23.20	2919	24.63	v _{C-H} , sym, CH ₃
1710	1705	1805	315.55	1793	331.98	1730	189.68	1718	203.48	v _{C-O}
1663	1657	1617	26.2	1608	27.51	1584	20.79	1573	21.04	v _{C-C}
1637	1641	1591	21.03	1581	28.68	1561	9.16	1550	9.50	v _{C-N}
1591	1600	1570	438.65	1564	471.14	1537	248.78	1529	282.32	v _{C-N} v _{C-C}
1563	1556	1499	384.53	1494	390.82	1470	24.43	1463	62.58	δ _{C-C-H}
1509	1507	1489	15.76	1482	9.38	1466	68.62	1458	87.68	δ _{C-C-H}
1484	1487	1484	40.7	1475	31.42	1459	74.86	1453	52.21	δ _{H-C-H}
1471	1468	1479	27.52	1473	20.62	1455	24.19	1447	23.08	δ _{C-C-H}
1457	1457	1471	12.2	1464	12.72	1448	16.34	1440	18.47	δ _{H-C-H}
1432	1438	1466	32.89	1460	23.87	1434	215.46	1431	170.38	δ _{H-C-H}
1430	1429	1440	24.46	1431	25.12	1420	23.69	1412	24.14	δ _{C-C-H}
1390	1384	1437	8.16	1429	9.53	1411	2.89	1405	3.21	δ _{H-C-H}
1375	1380	1411	295.29	1403	271.32	1375	269.19	1367	221.78	δ _{H-C-H} , δ _{C-N-H}
1292	1291	1285	87.74	1282	106.83	1290	6.75	1272	9.48	v _{C-C}
1270	1271	1266	55.93	1261	50.46	1254	39.46	1249	47.14	v _{C-C} , δ _{C-C} , δ _{C-}
1240	1238	1244	352.4	1234	340.32	1248	34.79	1244	39.15	N-C δ _{H-C-C}
1201	1199	1201	89.62	1195	99.79	1207	309.21	1197	301.78	δ _{N-C-H} , v _{C-N}
1160	1159	1187	10.95	1181	8.18	1176	103.39	1167	106.28	v _{C-N} , δ _{N-C-H}
1130	1132	1149	29.73	1147	23.69	1153	2.33	1147	2.07	δ _{C-C-H}
1093	1086	1128	135.24	1122	226.34	1129	49.05	1123	48.10	δ _{N-C-H}
1043	1033	1124	98.47	1117	64.18	1119	26.61	1113	29.78	δ _{C-C-H} , v _{C-C}
1037	1033	1106	4.95	1103	3.75	1111	125.54	1105	179.19	δ _{N-C-H}
1009	1009	1086	11.47	1078	23.29	1087	5.56	1082	5.05	δ _{C-C-H}
972	978	1084	22.54	1068	6.31	1070	14.83	1063	14.48	v _{C-C} , δ _{C-C-H}
962	960	1055	26.4	1052	33.18	1045	16.4	1041	19.13	δ _{C-C-H}
952	955	1028	46.64	1022	59	1029	6.63	1022	8.89	v _{C-C} , δ _{C-C-H}

Exp. ^a	NCA ^b	HF				B3LYP				Assignments ^c
		6-31G(d)		6-311G(d)		6-31G(d)		6-311G(d)		
		Corr.	Inten.	Corr.	Inten.	Corr.	Inten.	Corr.	Inten.	
909	910	1026	12.71	1018	7.9	1014	52.53	1014	59.73	δ_{C-C-C}
887	885	1016	0.47	1003	0.29	959	3.69	956	5.09	γ_{CH}
869	869	985	4.4	977	6.09	956	2.23	952	1.11	γ_{CH}
815	823	970	2.96	967	1.89	925	2.21	920	2.34	γ_{CH}
782	779	899	1.07	889	0.84	855	7.12	853	33.15	γ_{CH}
752	749	858	44.31	858	48.37	852	27.14	849	3.33	$\delta_{C-C-C}, \gamma_{CH}$
721	723	795	19.05	794	17.55	762	13.95	764	11.40	γ_{CH}
694	696	763	63.8	756	67.51	741	11.16	740	15.99	γ_{CH}, τ_{C-N}
684	682	745	6.74	743	11.48	732	44.08	728	55.58	$\gamma_{CH}, \delta_{C-C-H}$
647	647	724	41.64	725	40.66	695	29.77	702	28.33	$\gamma_{CH}, \delta_{C-C-C}$
613	611	684	16.34	684	21.71	674	3.46	674	0.95	$\delta_{C-C-C}, \gamma_{NH}$
602	598	673	55.77	670	51.38	660	50.62	665	60.85	$\gamma_{NH}, \delta_{C-C-C}$
547	544	641	23.07	640	23.72	635	18.64	636	19.81	$\delta_{C-N-C}, \delta_{C-C-C}$
503	496	610	25.15	610	26.1	593	14.48	595	16.04	γ_C
470	468	543	3.09	543	2.85	534	2.22	535	1.9	δ_{C-C-C}
449	445	492	7.29	491	7.94	492	5.93	492	5.78	τ_{C-N}, γ_C
434	435	471	11.49	468	13.63	461	6.52	459	9.59	δ_{C-N-C}, γ_C
-	369	434	5.27	433	5.39	430	3.65	429	3.98	δ_{C-N-C}
-	365	424	8.08	423	7.66	418	6.01	417	6.09	$\gamma_C, \tau_{C-N}, \gamma_N$
-	325	380	2.57	381	1.63	376	2.02	377	1.49	$\delta_{C-C-Cl}, \delta_{C-N-C}$
-	281	367	1.68	365	1.55	365	3.2	363	2.6	γ_C, δ_{C-N-C}
-	257	344	3.24	345	3.56	337	1.44	338	1.77	$\delta_{C-C-O}, \delta_{N-C-O}$
-	227	299	6.6	296	4.63	295	6.87	290	4.46	$\delta_{N-C-N}, \delta_{N-C-S}$
-	202	280	5.4	280	5.43	267	3.21	270	3.52	γ_N, τ_{C-N}
-	180	233	5.71	232	5.41	227	4.73	226	4.56	γ_N, τ_{C-N}
-	166	218	0.47	216	0.47	211	3.45	210	3.13	$\delta_{N-C-S}, \delta_{N-C-O}$
-	139	209	4.13	206	4.31	201	0.36	206	1.12	$\delta_{C-C-C}, \tau_{C-N}$
-	122	167	0.42	166	0.52	167	0.75	165	0.8	$\delta_{C-C-C}, \delta_{N-C-C}, \tau_{C-C}$
-	110	141	1.65	143	0.88	137	0.84	136	0.72	τ_{C-C}
-	86	133	0.67	138	1.16	126	0.82	131	0.6	γ_N, τ_{C-N}
-	61	109	0.8	110	0.94	103	0.64	107	1.14	$\delta_{C-C-N}, \delta_{C-N-C}, \delta_{C-C-C}$
-	53	97	4.27	95	4.38	99	3.1	98	2.92	τ_{C-C}, τ_{C-N}
-	42	69	2.1	68	2.16	67	2.09	67	2.14	τ_{C-N}, τ_{C-C}
-	27	38	2.63	38	2.71	37	2.17	37	2.3	τ_{C-N}, τ_{C-C}
-	10	26	1.06	25	1.07	28	1.05	28	1.02	τ_{C-C}, τ_{C-N}

^aTaken from Ref [14]. ^b NCA; The calculated vibrational frequencies which have been carried out on the basis of normal coordinate analysis using simple general valence force field in Wilson's GF matrix method with the SPSIM computer program [14], ^c v, stretching; δ , in-plane bending; γ , out-of-plane bending; τ , torsion; sym, symmetric; asym, asymmetric; ar, aromatic group.

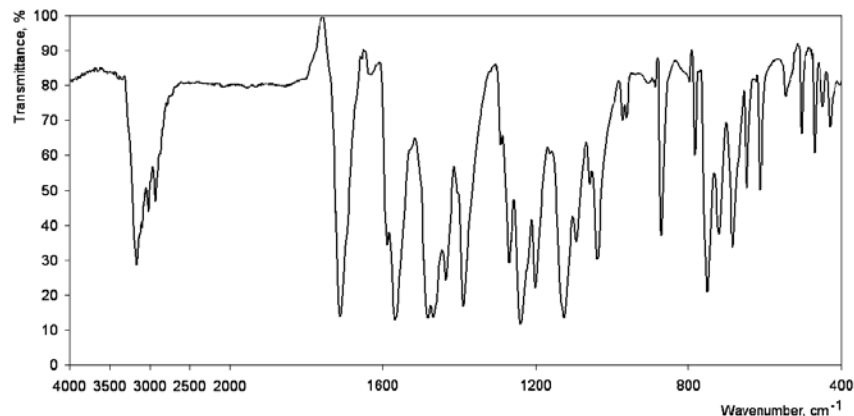


Fig. 2. Infrared spectrum of DMBT

TABLE-3
COEFFICIENT CORRELATION DATA BETWEEN EXPERIMENTAL
AND CALCULATED VIBRATIONAL FREQUENCIES

	Exp.	NCA	HF		B3LYP	
			6-31G(d)	6-311G(d)	6-31G(d)	6-311G(d)
Exp.	1.0000					
NCA	0.9999	1.0000				
HF	6-31G(d)	0.9975	0.9983	1.0000		
	6-311G(d)	0.9972	0.9981	1.0000	1.0000	
B3LYP	6-31G(d)	0.9978	0.9985	0.9998	0.9997	1.0000
	6-311G(d)	0.9974	0.9983	0.9998	0.9998	1.0000

The vibration mode calculated at 3444 cm^{-1} (DFT-B3LYP/6-31G(d)) is assigned to (N–H) stretching mode of vibrations. This band is calculated at 3166 cm^{-1} by Arslan *et al.*¹⁴ for DMBT with normal coordinate analysis. The difference between experimental (3166 cm^{-1}) and calculated $\nu(\text{N–H})$ is *ca.* 278 cm^{-1} (DFT-B3LYP/6-31G(d)). This striking discrepancy is due to the formation of intermolecular hydrogen bonding with N–H (intermolecular hydrogen-bonding D–H...A parameters is: N1–H1...S1 (-x, 1-y, -z) with H...A = 2.54 \AA and a D–H...A angle of 159° (CCDC-273278) (values normalized for N–H = 1.03 \AA). It is also noted that the experimental results belong to solid phase and theoretical calculations belong to gaseous phase.

The strong $\nu(\text{C=O})$ stretching band in the FT-IR spectrum of DMBT appears at about 1710 cm^{-1} . This band calculated at 1705 , 1730 and 1805 cm^{-1} with NCA, B3LYP/6-31G(d) and HF/6-31G(d) methods, respectively. As can be seen from Table-3, the best results calculated with NCA and DFT-B3LYP/6-31G(d) methods.

The C–H stretching vibrations of substituted phenyl ring are assigned to one band observed at 3091 cm⁻¹ in the FT-IR spectrum of DMBT. The B3LYP/6-31G(d)-calculated wavenumbers of this band well reproduce the experimental and NCA ones (Table-2). The methyl group asymmetric and symmetric $\nu(\text{C-H})$ stretching vibrations are established at 3019 and 2924 cm⁻¹, respectively. These assignments were also supported by the literature^{14,19}.

Conclusion

In this work, we have calculated the geometric parameters and vibrational frequencies of the *N,N*-dimethyl-*N'*(2-chloro-benzoyl)thiourea by using B3LYP and HF method with the standard 6-31G(d) and 6-311G(d) basis sets. We have used the scaling factor values of 0.8929 and 0.9613 for HF and B3LYP methods, respectively, to fit the theoretical results with experimental ones. Scaling factors results gained seemed to be in a good agreement with experimental ones. In particular, the results of DFT-B3LYP/6-31G(d) method have shown better fit to experimental ones than *ab initio* HF/6-31G(d), HF/6-311G(d) and DFT-B3LYP/6-311G(d) in evaluating vibrational frequencies.

The good correlation ($r = 0.9985$) between DFT-B3LYP/6-31G(d) method and normal coordinate analysis using simple general valence force field in Wilson's GF matrix method is also found.

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250 First Avenue, Suite 300, Needham, MA 02494
Tel.: 781-972-5400; Fax: 781-972-5425
Toll-free in the U.S.: 888-999-6288