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N,*N*′-二-[3-羟基-4-(2-苯并噻唑)苯基]脲的光谱实验与密度泛函理论研究

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Experimental and Density Functional Theoretical Studies on the Spectra of *N*,*N*′-di[3-hydroxy-4-(2-benzothiazole)phenyl]urea

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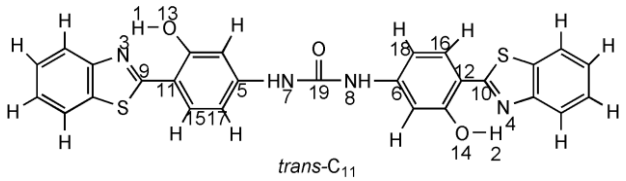
表 S1　*trans*-C_{11} 几何结构参数

Table S1　The geometrical structure parameters of *trans*-C_{11}



trans-C_{11}

Structures	B3LYP/6-31+g(*d*)	B3LYP/6-311+g(*d*,*p*)	BPV86/6-31+g(*d*)	BPV86/6-311++g(*d*,*p*)	PBEPBE/6-31+g(*d*)	PBEPBE/6-311+g(*d*,*p*)	MPW1PW91/6-31+g(*d*)	MPW1PW91/6-311+g(*d*,*p*)
H_1-N_3[a]	0.177	0.175	0.171	0.169	0.171	0.168	0.174	0.172
H_2-N_4	0.177	0.175	0.171	0.168	0.171	0.169	0.174	0.172
C_5-N_7	0.141	0.141	0.141	0.141	0.141	0.141	0.140	0.140
C_6-N_8	0.141	0.141	0.141	0.141	0.141	0.141	0.140	0.140
C_9-C_{11}	0.145	0.145	0.145	0.145	0.145	0.145	0.145	0.145
C_{10}-C_{12}	0.145	0.145	0.145	0.145	0.145	0.145	0.145	0.145
O_{13}-H_1-N_3[b]	145.996	146.726	148.071	149.030	148.102	149.126	146.667	147.716
O_{14}-H_2-N_4	145.990	146.699	148.073	149.049	148.125	149.122	146.691	147.668
N_3-C_9-C_{11}	123.502	123.486	123.098	123.071	123.101	123.023	123.244	123.202
N_4-C_{10}-C_{12}	123.368	123.366	122.996	122.985	123.016	123.126	123.134	123.101
C_5-N_7-C_{19}	128.380	128.357	128.271	128.294	128.317	128.435	128.202	128.215
C_6-N_8-C_{19}	128.399	128.388	128.344	128.374	128.392	128.411	128.230	128.253
N_7-C_{19}-N_8	112.088	111.834	111.824	111.584	111.800	111.525	112.018	111.755
N_3-C_9-C_{11}-C_{15}	180.000	180.000	180.000	180.000	180.000	180.000	180.000	180.000
N_4-C_{10}-C_{12}-C_{16}	180.000	180.000	180.000	180.000	180.000	180.000	180.000	180.000
C_{17}-C_5-N_7-C_{19}	180.000	180.000	180.000	180.000	180.000	180.000	180.000	180.000
C_{18}-C_6-N_8-C_{19}	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

[a] bond lengths in nm; [b] angles in degree

表 S2　*trans*-C_{11} 理论计算和实验红外光谱及其归属

Table S2　Calculated and Observed IR Wavenumbers of *trans*-C_{11} with Band Assignments

No.	Calc./cm^{-1} B3LYP/6-31+g(*d*)	B3LYP/6-311+g(*d*,*p*)	BPV86/6-31+g(*d*)	BPV86/6-311++g(*d*,*p*)	PBEPBE/6-31+g(*d*)	PBEPBE/6-311+g(*d*,*p*)	MPW1PW91/6-31+g(*d*)	MPW1PW91/6-311+g(*d*,*p*)	Calc. assignment	Obs./cm^{-1}	Obs. assignment
1	3607.16	3623.49	3498.64	3518.76	3508.84	3528.03	3655.67	3668.65	ν(N—H)	-	-
	3592.40	3609.12	3485.13	3505.75	3494.93	3514.33	3642.44	3655.67			
2	3290.02	3298.31	2973.88	2964.65	2984.07	2974.00	3297.68	3285.76	ν(O—H in hydrogen bond)	3275.65	ν(O—H in hydrogen bond)
	3270.76	3281.37	2950.77	2941.46	2961.20	2947.81	3277.42	3267.08			
3	3282.33	3258.68	3195.38	3177.99	3199.76	3183.34	3304.48	3280.84	ν(C—H in aromatic ring)	3060.44	ν(C—H in aromatic ring)
	3278.33	3254.10	3192.30	3173.83	3196.05	3176.08	3302.04	3277.32			
	3216.96	3198.35	3140.55	3128.20	3148.09	3134.89	3248.91	3228.45			
	3216.61	3198.14	3140.20	3128.09	3147.84	3134.70	3248.60	3228.32			
	3210.38	3192.16	3134.16	3122.16	3141.88	3128.74	3242.47	3222.61			
	3210.11	3191.80	3134.01	3122.01	3141.43	3128.60	3242.31	3222.19			
	3200.41	3182.15	3124.20	3112.36	3132.12	3119.14	3232.44	3212.22			
	3200.37	3182.08	3124.11	3112.30	3131.98	3119.13	3232.38	3212.09			
	3196.95	3179.61	3114.24	3103.69	3121.24	3110.53	3223.30	3205.37			
	3191.35	3172.57	3113.19	3101.58	3121.18	3108.62	3221.63	3201.00			
	3189.80	3171.55	3113.10	3101.32	3120.85	3108.30	3221.46	3200.59			
	3189.59	3171.10	3110.15	3099.37	3115.85	3102.78	3217.65	3200.13			
	3187.66	3170.71	3106.84	3094.24	3113.57	3099.72	3215.51	3195.60			
	3174.25	3159.53	3095.26	3086.36	3102.13	3093.87	3204.13	3187.53			

4	1783.77	1775.16	1729.26	1720.93	1735.60	1727.86	1822.75	1814.84	ν(C=O)	1597.50	ν(C=O)
5	1679.31 1677.72 1376.59 1364.80 1350.33 1306.22	1668.93 1667.01 1364.70 1350.78 1338.19 1294.93	1633.42 1630.73 1406.04 1318.28 1279.38	1624.32 1621.35 1396.81 1307.21 1265.40	1638.09 1635.57 1412.06 1373.97 1323.67 1297.90	1630.86 1626.15 1404.33 1364.81 1311.48 1269.22	1708.37 1706.47 1467.60 1425.94 1401.15 1393.51 1374.22 1326.83	1699.33 1697.04 1460.19 1418.21 1391.44 1382.18 1363.02 1315.83	ν(C = C in phenol)	1545.06	ν(C=C)
6	1643.33 1630.91	1629.57 1620.011	1594.43 1583.77	1582.94 1574.89	1596.95 1586.98	1585.96 1578.19	1666.28 1656.09	1654.73 1646.44	ν(Ph—N—CO—N—Ph)		The stretching vibration of molecular relevant to conjugate system
7	1609.41 1609.29	1598.50 1598.23	1561.94 1591.67	1551.66 1551.47	1566.14 1565.89	1556.88 1556.38	1636.67 1636.41	1627.05 1626.73	ν(C = C in benzene ring of benzothiazole)	1474.22 1436.92 1397.03 1217.56	
8	1575.75 1566.80	1564.99 1556.33	1518.06	1506.65	1519.17 1510.93	1506.95 1459.95	-	-	ν(C = N—Ph)		
9	1561.49 1555.24 1524.66 1519.22	1549.32 1543.11 1512.42 1507.04	1529.81 1522.53 1507.11	1520.38 1513.13 1506.65	1534.05 1527.33	1525.51 1519.18	1585.13 1575.15 1579.06 1541.03	1572.43 1562.88 1537.07 1528.69	ν(C = N—Ph—N—CO—N—Ph—N=C)		
10	1500.86 1499.57 1491.57 1490.06 1327.92 1327.46	1490.00 1488.99 1481.40 1479.80 1318.08 1317.57	1465.38 1458.90 1358.93 1357.70 1298.61 1297.81	1346.96 1343.60 1341.62 1288.92 1288.14 1340.80	1470.20 1464.22 1365.62 1364.83 1359.95 1359.33	1464.02 1454.33 1354.04 1352.14 1348.95 1349.63	1523.47 1519.14 1508.87 1507.74 1349.25 1348.67	1513.63 1508.29 1497.98 1496.89 1339.38 1338.78	The stretching vibration between benzothiazole and phenol		
11	1642.14 1641.60 1479.61 1478.78 1362.42 1362.25	1631.35 1630.50 1467.19 1466.38 1346.62 1346.41	1592.91 1592.09 1449.66 1449.23 1435.67 1434.60	1582.16 1581.26 1447.97 1439.08 1422.80 1421.89	1598.12 1597.30 1451.64 1451.48 1437.83 1437.00 1303.59 1301.97	1588.30 1587.56 1441.54 1441.50 1425.02 1424.66 1294.31 1292.08	1671.57 1670.96 1496.32 1495.94 1391.73 1391.20	1661.43 1660.69 1483.49 1483.12 1378.18 1377.39	The stretching vibration of benzothiazole		
12	1435.76 1403.92	1564.99 1556.33	1477.86 1471.48 1370.64 1354.27 1352.92	1494.22 1465.70 1458.26 1456.35 1361.51	1481.66 1474.74	1498.75 1470.18	1604.01 1593.91	1594.02 1584.52	*ν*(C = N—Ph—N)		