Electronic Supplementary Information

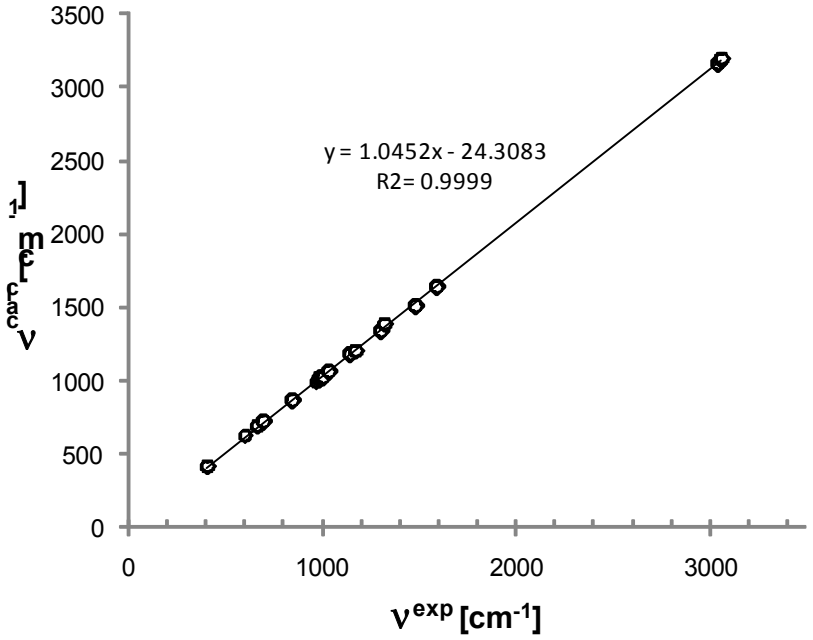

Fig.S1. The correlation between theoretical (B3LYP/6-311+G**) and experimental vibration frequencies [56]

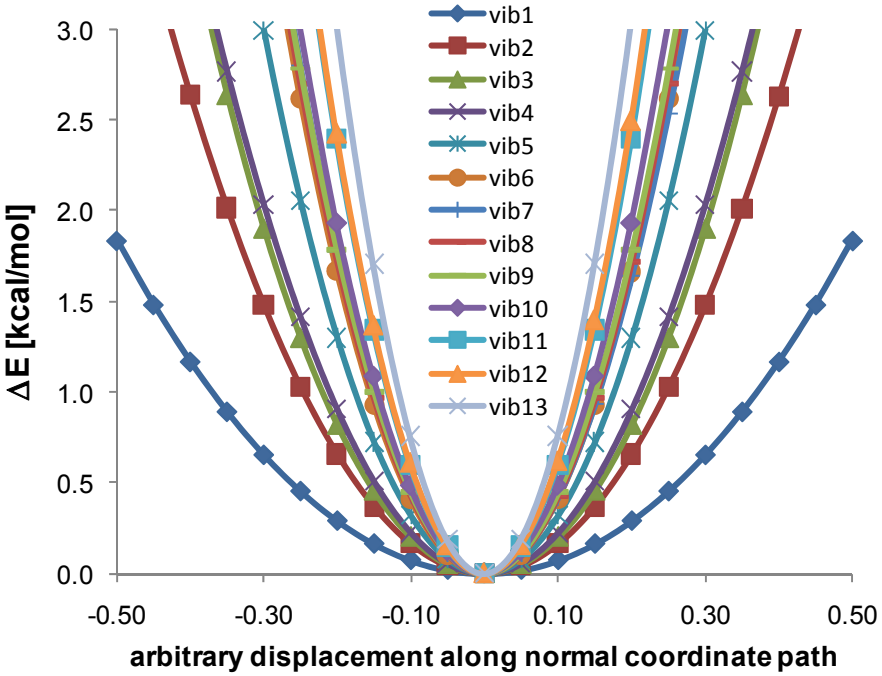

Fig.S2 Correlation between benzene molecule energy ($\Delta E_i(D_i) = \pi c h \Delta \nu_i$, with respect of the ground state ie. not-perturbed structure) and displacement along the normal coordinate paths for first 13 vibrations at room temperature. Presented points correspond to energy estimated at B3LYP/6-311++G** level of theory.

Table S1 Calculated and experimental frequencies, assignment and population of excited vibrational modes for normal vibrations of benzene contributing to thermal vibrations at normal temperature.

No	$\tilde{\nu}_i^{calc}\ [cm^{-1}]$	$\tilde{\nu}_i^{exp}\ [cm^{-1}]$ [a]	symmetry	Assignment (% of PED[b])	% in the population
1	410.8	410	e2u	ring out-of-plane (degeneration=2) D1(8.9%), D5(8.9%), D13(8.9%), D17(8.9%), D2(6.8%), D6(6.8%), D15(6.8%), D18(6.8%), D3(4.7%), D7(4.7%), D14(4.7%), D19(4.7%), D4(2.6%), D8(2.6%), D16(2.6%), D20(2.6%)	29.1%
2	622.2	606	e2g	ring in-of-plane (degeneration=2) R2(9.4%), R6(9.4%), R5(7.9%), R11(7.9%), A9(5.1%), A17(5.1%), A5(4.6%), A14(4.6%), A8(4.1%), A18(4.1%), A2(3.5%), A12(3.5%), A4(3.2%), A13(3.2%), R1(3.1%), R8(3.1%), A1(2.3%), A10(2.3%), R7(2.1%), R12(2.1%)	15.3%
3	687.5	673	a2u	symmetric CH out-of-plane D2(8.3%), D3(8.3%), D6(8.3%), D7(8.3%), D10(8.3%), D11(8.3%), D14(8.3%), D15(8.3%), D18(8.3%), D19(8.3%), D22(8.3%), D23(8.3%)	6.6%
4	719.1	703	b2g	ring out-of-plane D1(8.2%), D5(8.2%), D9(8.2%), D13(8.2%), D17(8.2%), D21(8.2%), D2(4.2%), D3(4.2%), D6(4.2%), D7(4.2%), D10(4.2%), D11(4.2%), D14(4.2%), D15(4.2%), D18(4.2%), D19(4.2%), D22(4.2%), D23(4.2%)	6.1%
5	863.0	849	e1g	asymmetric CH out-of plane (degeneration=2) D3(8.3%), D7(8.3%), D12(8.3%), D14(8.3%), D19(8.3%), D24(8.3%), D2(6.7%), D8(6.7%), D11(6.7%), D16(6.7%), D18(6.7%), D23(6.7%)	8.6%
6	987.3	975	e2u	asymmetric CH out-of plane (degeneration=2) D12(11.3%), D24(11.3%), D4(6.3%), D20(6.3%), D2(5.8%), D18(5.8%), D6(5.5%), D15(5.5%), D8(5%), D16(5%), D11(4.7%), D23(4.7%), D10(4.1%), D22(4.1%), D9(2.5%), D21(2.5%)	6.4%
7	1010.6	992	a1g	Ring str R1(9.8%), R8(9.8%), R4(7.1%), R10(7.1%), A7(6.4%), A16(6.4%), A1(4.7%), A10(4.7%), A3(4%), A11(4%), A9(3.8%), A17(3.8%), A6(3.2%), A15(3.2%), R2(2.7%), R6(2.7%), A8(2.6%), A18(2.6%)	3.0%
8	1017.2	995	b2g	CH bend D4(8.3%), D8(8.3%), D12(8.3%), D16(8.3%), D20(8.3%), D24(8.3%), D2(3%), D3(3%), D6(3%), D7(3%), D10(3%), D11(3%), D14(3%), D15(3%), D18(3%), D19(3%), D22(3%), D23(3%), D1(2.3%), D5(2.3%), D9(2.3%), D13(2.3%), D17(2.3%), D21(2.3%)	3.0%
9	1022.4	1010	b1u	Ring out-of-plane R2(11.6%), R6(11.6%), R4(8.6%), R10(8.6%), A2(4.4%), A5(4.4%), A7(4.4%), A12(4.4%), A14(4.4%), A16(4.4%), A1(3.2%), A6(3.2%), A8(3.2%), A10(3.2%), A15(3.2%), A18(3.2%), R1(3.1%), R8(3.1%)	2.9%
10	1058.7	1038	e1u	CH bend (degeneration=2) R5(11%), R11(11%), A8(6.8%), A18(6.8%), A9(4.1%), A17(4.1%), R1(3.7%), R2(3.7%), R4(3.7%), R6(3.7%), R8(3.7%), R10(3.7%), R7(3.1%), R12(3.1%), A5(2.9%), A14(2.9%), A1(2.7%), A4(2.7%), A7(2.7%), A10(2.7%), A13(2.7%), A16(2.7%)	5.4%
11	1174.5	1150	b2u	CH bend R5(11.9%), R11(11.9%), R3(8.8%), R9(8.8%), A8(5.2%), A18(5.2%), A9(5%), A17(5%), A2(4%), A12(4%), A3(3.4%), A11(3.4%), R7(3.1%), R12(3.1%), R1(2.1%), R8(2.1%)	2.0%
12	1197.1	1178	e2g	CH bend (degeneration=2) R5(16.8%), R11(16.8%), A9(7.7%), A17(7.7%), A8(7.3%), A18(7.3%), R7(4.4%), R12(4.4%), A5(2.8%), A14(2.8%), R4(2.6%), R10(2.6%)	3.8%
13	1335.7	1310	b2u	Ring str R5(6.8%), R11(6.8%), R1(5.7%), R8(5.7%), A9(5.5%), A17(5.5%), R3(5%), R9(5%), A8(4.9%), A18(4.9%), A3(4.6%), A11(4.6%), R4(4.1%), R10(4.1%), A2(3%), A12(3%), A6(2.5%), A15(2.5%), A4(2.1%), A13(2.1%)	1.4%
14	1380.9	1326	a2g	CH bend (degeneration=2) R5(11.7%), R11(11.7%), R3(8.6%), R9(8.6%), A9(5.5%), A17(5.5%), A8(5.3%), A18(5.3%), A3(4.3%), A11(4.3%), A2(3.6%), A12(3.6%), R7(3.1%), R12(3.1%), A6(2%), A15(2%)	2.7%
15	1510.0	1486	e1u	Ring str + deform str (degeneration=2) R5(12.3%), R11(12.3%), A9(7.3%), A17(7.3%), A8(4.9%), A18(4.9%), R1(3.2%), R2(3.2%), R4(3.2%), R6(3.2%), R8(3.2%), R10(3.2%), R7(3%), R12(3%), A6(2.7%), A15(2.7%), A1(2.4%), A4(2.4%), A7(2.4%), A10(2.4%), A13(2.4%), A16(2.4%)	1.8%

16	1633.1	1596	e2g	Ring str(degeneration=2) R1(7.1%), R8(7.1%), R3(7%), R9(7%), A3(5.9%), A11(5.9%), R5(5.4%), R11(5.4%), A9(4.6%), A17(4.6%), A7(4.1%), A16(4.1%), R4(3.2%), R10(3.2%), A2(3.2%), A12(3.2%), A1(2.7%), A10(2.7%), A6(2.2%), A15(2.2%)	1.3%
17	3155.5	3047	e2g	CH str (degeneration=3) R7(11.1%), R12(11.1%), R3(8.1%), R9(8.1%), A5(6%), A14(6%), A6(5.8%), A15(5.8%), A2(4.6%), A12(4.6%), A3(4.2%), A11(4.2%), R5(3%), R11(3%)	0.0%
18	3180.7	3062	a1g	CH str (degeneration=2) R3(12.2%), R9(12.2%), R7(9%), R12(9%), A2(6.4%), A12(6.4%), A3(5.7%), A11(5.7%), A6(4.2%), A15(4.2%), A5(3.5%), A14(3.5%), R5(2%), R11(2%)	0.0%
19	3190.9	3063	e1u	CH str R7(12%), R12(12%), R3(8.7%), R9(8.7%), A5(5.8%), A14(5.8%), A6(5.6%), A15(5.6%), A2(4.4%), A12(4.4%), A3(3.9%), A11(3.9%), R5(3.3%), R11(3.3%)	0.0%

[a] T. Shimanouchi, "Molecular Vibrational Frequencies" in NIST Chemistry WebBook, NIST Standard Reference Database Number 69, Eds. P.J. Linstrom and W.G. Mallard, National Institute of Standards and Technology, Gaithersburg MD, 20899, http://webbook.nist.gov, (retrieved December 11, 2010).
[b] only most significant contributions (2%) are listed here

Table S2 The values of parabola parameter approximating benzene energy as a function of displacement along normal coordinates ($E_n(d) = A \cdot d^2$). The scaling factors χ_i were obtained according to formula: $E_i = \chi_i \cdot E_i$. The last column comprises amplitudes of displacement along normal coordinate of first 13 modes at room temperature.

	A_i	χ_i	D_i
vib1	7.24	1.000	0.390
vib2	16.43	0.441	0.322
vib3	20.79	0.348	0.307
vib4	22.60	0.320	0.300
vib5	32.84	0.221	0.275
vib6	41.93	0.173	0.257
vib7	42.70	0.170	0.255
vib8	43.23	0.168	0.254
vib9	44.55	0.163	0.253
vib10	48.39	0.150	0.249
vib11	60.02	0.121	0.236
vib12	61.72	0.117	0.234
vib13	76.38	0.095	0.222