Combined experimental and computational approach for the vibrational characteristics and theoretical evaluation of binding activities and ADME descriptors of 2,6-di-tert-butyl-p-cresol

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**Supplementary Material**

**Table S1.** Accumulation of natural charges and electron population of atoms in core, valence, Rydberg orbitals of 2,6-di-tert-butyl-p-cresol

|  |  |  |  |
| --- | --- | --- | --- |
| Atoms | Charge (e) | Natural Population (e) | Total (e) |
|  Core | Valence | Rydberg |
| $$C\_{1}$$ | 0.31896 | 1.99805 | 3.65999 | 0.02300 | 5.68104 |
| $$C\_{2}$$ | ‒0.08464 | 1.99895 | 4.06428 | 0.02141 | 6.08464 |
| $$ C\_{3}$$ | ‒0.19600 | 1.99865 | 4.18230 | 0.01505 | 6.19600 |
| $$C\_{4}$$ | ‒0.03641 | 1.99915 | 4.02019 | 0.01707 | 6.03641 |
| $$C\_{5}$$ | ‒0.19727 | 1.99865 | 4.18412 | 0.01450 | 6.19727 |
| $$C\_{6}$$ | ‒0.05417 | 1.99896 | 4.03434 | 0.02087 | 6.05417 |
| $$O\_{7}$$ | ‒0.73314 | 1.99975 | 6.71920 | 0.01419 | 8.73314 |
| $$H\_{8}$$ | 0.46677 | 0.0000 | 0.52628 | 0.00695 | 0.53323 |
| $$C\_{9}$$ | ‒0.07525 | 1.99917 | 4.05925 | 0.01683 | 6.07525 |
| $$C\_{10}$$ | ‒0.55896 | 1.99926 | 4.54831 | 0.01139 | 6.55896 |
| $$H\_{11}$$ | 0.19674 | 0.0000 | 0.80170 | 0.00156 | 0.80326 |
| $$H\_{12}$$ | 0.19682 | 0.0000 | 0.80163 | 0.00154 | 0.80318 |
| $$H\_{13}$$ | 0.20606 | 0.0000 | 0.79245 | 0.00149 | 0.79394 |
| $$C\_{14}$$ | ‒0.56413 | 1.99918 | 4.55059 | 0.01436 | 6.56413 |
| $$H\_{15}$$ | 0.17038 | 0.0000 | 0.82751 | 0.00211 | 0.82962 |
| $$H\_{16}$$ | 0.22615 | 0.0000 | 0.77217 | 0.00168 | 0.77385 |
| $$H\_{17}$$ | 0.21604 | 0.0000 | 0.78234 | 0.00162 | 0.78396 |
| $$C\_{18}$$ | ‒0.55788 | 1.99924 | 4.54752 | 0.01112 | 6.55788 |
| $$H\_{19}$$ | 0.19360 | 0.0000 | 0.80481 | 0.00159 | 0.80640 |
| $$H\_{20}$$ | 0.20313 | 0.0000 | 0.79538 | 0.00149 | 0.79687 |
| $$H\_{21}$$ | 0.19952 | 0.0000 | 0.79885 | 0.00163 | 0.80048 |
| $$H\_{22}$$ | 0.19883 | 0.0000 | 0.79901 | 0.00216 | 0.80117 |
| $$C\_{23}$$ | ‒0.57537 | 1.99927 | 4.56773 | 0.00837 | 6.57537 |
| $$H\_{24}$$ | 0.20279 | 0.0000 | 0.79547 | 0.00173 | 0.79721 |
| $$H\_{25}$$ | 0.20318 | 0.0000 | 0.79507 | 0.00174 | 0.79682 |
| $$H\_{26}$$ | 0.19894 | 0.0000 | 0.79941 | 0.00166 | 0.80106 |
| $$H\_{27}$$ | 0.20636 | 0.0000 | 0.79145 | 0.00219 | 0.79364 |
| $$C\_{28}$$ | ‒0.08121 | 1.99918 | 4.06527 | 0.01676 | 6.08121 |
| $$C\_{29}$$ | ‒0.55627 | 1.99924 | 4.54609 | 0.01094 | 6.55627 |
| $$H\_{30}$$ | 0.20738 | 0.0000 | 0.79111 | 0.00151 | 0.79262 |
| $$H\_{31}$$ | 0.18947 | 0.0000 | 0.80902 | 0.00150 | 0.81053 |
| $$H\_{32}$$ | 0.20035 | 0.0000 | 0.79828 | 0.00137 | 0.79965 |
| $$C\_{33}$$ | ‒0.56431 | 1.99927 | 4.55424 | 0.01081 | 6.56431 |
| $$H\_{34}$$ | 0.19633 | 0.0000 | 0.80198 | 0.00168 | 0.80367 |
| $$ H\_{35}$$ | 0.19602 | 0.0000 | 0.80233 | 0.00166 | 0.80398 |
| $$H\_{36}$$ | 0.19934 | 0.0000 | 0.79926 | 0.00140 | 0.80066 |
| $$H\_{37}$$ | ‒0.55730 | 1.99925 | 4.54718 | 0.01088 | 6.55730 |
| $$H\_{38}$$ | 0.21075 | 0.0000 | 0.78780 | 0.00145 | 0.78925 |
| $$H\_{39}$$ | 0.19952 | 0.0000 | 0.79911 | 0.00137 | 0.80048 |
| $$H\_{40}$$ | 0.18887 | 0.0000 | 0.80962 | 0.00150 | 0.81113 |

**Table S2.** Comparison of occupancies and energies of bonding and antibonding molecular orbitals between 2,6-di-tert-butyl-p-cresol and pure benzene.

|  |  |  |
| --- | --- | --- |
| Parameters | 2,6-di-tert-butyl-p-cresol | Benzene |
| Occupancies (e) | Energies (a.u.) | Occupancies (e) | Energies (a.u.) |
| BD ($C\_{1}‒C\_{2}$) | 1.96959 | ‒0.69515 | 1.9798 | ‒0.6989 |
| BD ($C\_{1}‒C\_{6}$) | 1.96740 | ‒0.69083 | 1.9799 | ‒0.6992 |
| BD ($C\_{1}‒O\_{7}$) | 1.99142 | ‒0.81883 |  |  |
| BD ($C\_{2}‒C\_{3}$) | 1.96434 | ‒0.68115 | 1.9799 | ‒0.6994 |
| BD ($C\_{2}‒C\_{9}$) | 1.96228 | ‒0.59657 |  |  |
| BD ($C\_{3}‒C\_{4}$) | 1.97194 | ‒0.67849 | 1.9798 | ‒0.6987 |
| BD ($C\_{3}‒H\_{22}$) | 1.97771 | ‒0.51449 |  |  |
| BD ($C\_{4}‒C\_{5}$) | 1.97203 | ‒0.67796 | 1.9799 | ‒0.6993 |
| BD ($C‒C\_{23}$) | 1.98240 | ‒0.58966 |  |  |
| BD ($C\_{5}‒C\_{6}$) | 1.96489 | ‒0.67699 | 1.9798 | ‒0.6990 |
| BD ($C\_{5}‒H\_{27}$) | 1.97674 | ‒0.51083 |  |  |
| BD ($C\_{6}‒C\_{28}$) | 1.96306 | ‒0.58053 |  |  |
| BD ($O\_{7}‒H\_{8}$) | 1.98583 | ‒0.78302 |  |  |
| BD ($C\_{9}‒C\_{10}$) | 1.97452 | ‒0.59506 |  |  |
| BD ($C\_{9}‒C\_{14}$) | 1.97636 | ‒0.60644 |  |  |
| BD ($C\_{9}‒C\_{18}$) | 1.97011 | ‒0.59387 |  |  |
| BD ($C\_{10}‒H\_{11}$) | 1.98752 | ‒0.51271 |  |  |
| BD ($C\_{10}‒H\_{12}$) | 1.98858 | ‒0.51176 |  |  |
| BD ($C\_{10}‒H\_{13}$) | 1.98845 | ‒0.50883 |  |  |
| BD ($C\_{14}‒H\_{15}$) | 1.94058 | ‒0.53581 |  |  |
| BD ($C\_{14}‒H\_{16}$) | 1.98549 | ‒0.52500 |  |  |
| BD ($C\_{14}‒H\_{17}$) | 1.98498 | ‒0.52443 |  |  |
| BD ($C\_{18}‒C\_{19}$) | 1.98740 | ‒0.51061 |  |  |
| BD ($C\_{18}‒H\_{20}$) | 1.98812 | ‒0.50898 |  |  |
| BD ($C\_{18}‒H\_{21}$) | 1.98796 | ‒0.51046 |  |  |
| BD ($C\_{23}‒H\_{24}$) | 1.98328 | ‒0.50386 |  |  |
| BD ($C\_{23}‒H\_{25}$) | 1.98254 | ‒0.50369 |  |  |
| BD ($C\_{23}‒H\_{26}$) | 1.99051 | ‒0.50507 |  |  |
| BD ($C\_{28}‒C\_{29}$) | 1.97094 | ‒0.57045 |  |  |
| BD ($C\_{28}‒C\_{33}$) | 1.97846 | ‒0.57641 |  |  |
| BD ($C\_{28}‒C\_{37}$) | 1.97103 | ‒0.56994 |  |  |
| BD ($C\_{29}‒H\_{30}$) | 1.98917 | ‒0.48456 |  |  |
| BD ($C\_{29}‒H\_{31}$) | 1.98873 | ‒0.48829 |  |  |
| BD ($C\_{29}‒H\_{32}$) | 1.98883 | ‒0.48654 |  |  |
| BD ($C\_{33}‒H\_{34}$) | 1.98799 | ‒0.49722 |  |  |
| BD ($C\_{33}‒H\_{35}$) | 1.98796 | ‒0.49739 |  |  |
| BD ($C\_{33}‒H\_{36}$) | 1.98855 | ‒0.49726 |  |  |
| BD ($C\_{37}‒H\_{38}$) | 1.98886 | ‒0.48335 |  |  |
| BD ($C\_{37}‒H\_{39}$) | 1.98891 | ‒0.48548 |  |  |
| BD ($C\_{37}‒H\_{40}$) | 1.98850 | ‒0.48750 |  |  |
| BD\* ($C\_{1}‒C\_{6}$) | 0.02992 | 0.56967 | 0.0164 | 0.5792 |
| BD\* ($C\_{1}‒O\_{7}$) | 0.02758 | 0.28802 |  |  |
| BD\* ($C\_{2}‒C\_{3}$) | 0.02349 | 0.56820 | 0.0163 | 0.5793 |
| BD\* ($C\_{2}‒C\_{9}$) | 0.03764 | 0.40402 |  |  |
| BD\* ($C\_{3}‒C\_{4}$) | 0.02428 | 0.57891 | 0.0164 | 0.5783 |
| BD\* ($C\_{3}‒H\_{22}$) | 0.01611 | 0.46696 |  |  |
| BD\* ($C\_{4}‒C\_{5}$) | 0.02378 | 0.58419 | 0.0163 | 0.5792 |
| BD\* ($C\_{4}‒C\_{23}$) | 0.01696 | 0.39919 |  |  |
| BD\* ($C\_{5}‒C\_{6}$) | 0.35619 | 0.05249 | 0.0164 | 0.5788 |
| BD\* ($C\_{5}‒H\_{27}$) | 0.01607 | 0.47377 |  |  |
| BD\* ($C\_{6}‒C\_{28}$) | 0.03685 | 0.41859 |  |  |
| BD\* ($O\_{7}‒H\_{8}$) | 0.06001 | 0.48883 |  |  |
| BD\* ($C\_{9}‒C\_{10}$) | 0.02077 | 0.37612 |  |  |
| BD\* ($C\_{9}‒C\_{14}$) | 0.02342 | 0.36463 |  |  |
| BD\* ($C\_{9}‒C\_{18}$) | 0.02569 | 0.37501 |  |  |
| BD\* ($C\_{10}‒H\_{11}$) | 0.00648 | 0.43706 |  |  |
| BD\* ($C\_{10}‒H\_{12}$) | 0.00677 | 0.43968 |  |  |
| BD\* ($C\_{10}‒H\_{13}$) | 0.00588 | 0.44109 |  |  |
| BD\* ($C\_{14}‒H\_{15}$) | 0.00870 | 0.40547 |  |  |
| BD\* ($C\_{14}‒H\_{16}$) | 0.00789 | 0.42540 |  |  |
| BD\* ($C\_{14}‒H\_{17}$) | 0.01459 | 0.44503 |  |  |
| BD\* ($C\_{18}‒H\_{19}$) | 0.00739 | 0.43636 |  |  |
| BD\* ($C\_{18}‒H\_{20}$) | 0.00626 | 0.44088 |  |  |
| BD\* ($C\_{18}‒H\_{21}$) | 0.00613 | 0.44077 |  |  |
| BD\* ($C\_{23}‒H\_{24}$) | 0.00746 | 0.43827 |  |  |
| BD\* ($C\_{23}‒H\_{25}$) | 0.00791 | 0.43837 |  |  |
| BD\* ($C\_{23}‒H\_{26}$) | 0.00343 | 0.43894 |  |  |
| BD\* ($C\_{28}‒C\_{29}$) | 0.02268 | 0.39918 |  |  |
| BD\* ($C\_{28}‒C\_{33}$) | 0.01902 | 0.39709 |  |  |
| BD\* ($C\_{28}‒C\_{37}$) | 0.02243 | 0.39967 |  |  |
| BD\* ($C\_{29}‒H\_{30}$) | 0.00583 | 0.46640 |  |  |
| BD\* ($C\_{29}‒H\_{31}$) | 0.00749 | 0.45850 |  |  |
| BD\* ($C\_{29}‒H\_{32}$) | 0.00481 | 0.46087 |  |  |
| BD\* ($C\_{33}‒H\_{34}$) | 0.00731 | 0.45153 |  |  |
| BD\* ($C\_{33}‒H\_{35}$) | 0.00717 | 0.45126 |  |  |
| BD\* ($C\_{33}‒H\_{36}$) | 0.00693 | 0.45880 |  |  |
| BD\* ($C\_{37}‒H\_{38}$) | 0.00608 | 0.46941 |  |  |
| BD\* ($C\_{37}‒H\_{39}$) | 0.00518 | 0.46195 |  |
| BD\* ($C\_{37}‒H\_{40}$) | 0.00771 | 0.45901 |  |

**Table S3.** Observed and calculated vibrational wavenumbers ($cm^{-1}$) and vibrational assignments of 2,6 di-tert-butyl-p-cresol.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Unscaled wavenumber | Scaled wavenumber | IR | Raman | aAssignments with Major contribution of PED |
| Wavenumber | Transmittance | Wavenumber | Raman Activity |
| 3883 | 3671 | 3650 | 64 | 3629 | 13 | 𝜈(O-H)(100) |
| 3203 | 3064 | 3067 | 30 | − | − | 𝜈(C-H)Ring(96) |
| 3137 | 3004 | − | − | 3003 | 28 | 𝜈(C-H)Ring(94) |
| 3103 | 2973 | − | − | 2971 | 87 | 𝜈(C-H)Ring(94) |
| 3092 | 2963 | − | − | 2963 | 84 | 𝜈as(C-H)methyl(96) |
| 3082 | 2954 | 2955 | 77 | − | − | 𝜈as(C-H)methyl(95) |
| 3065 | 2939 | 2939 | 4 | − | − | 𝜈s(C-H)methyl(93) |
| 3035 | 2911 | 2925 | 8 | 2916 | 96 | 𝜈as(C-H)methyl(94) |
| 3015 | 2893 | 2871 | 7 | − | − | 𝜈s(C-H)methyl(91) |
| 1641 | 1611 | − | − | 1607 | 34 | 𝜈(C-C)(63) |
| 1505 | 1481 | 1482 | 84 | − | − | 𝜈(C-C)(56) |
| 1496 | 1472 | − | − | 1472 | 31 | 𝜈(C-C)(58) |
| 1482 | 1459 | − | − | 1453 | 37 | β(C-H)(52) |
| 1480 | 1457 | 1450 | 62 | − | − | β(C-H)(69) |
| 1466 | 1443 | 1432 | 36 | − | − | β(C-H)(52) |
| 1414 | 1394 | 1397 | 21 | 1397 | 14 | β(CH3)(70) |
| 1405 | 1385 | − | − | 1380 | 36 | β(CH3)(67) |
| 1394 | 1374 | 1377 | 66 | − | − | β(CH3)(52) |
| 1393 | 1374 | 1362 | 64 | − | − | β(CH3)(51) |
| 1310 | 1294 | 1307 | 49 | − | − | β(C-H)(64) |
| 1295 | 1279 | 1266 | 70 | − | − | 𝜈(C-C)(48) |
| 1265 | 1250 | 1246 | 64 | 1233 | 14 | β(C-H)(69) |
| 1255 | 1240 | 1231 | 53 | − | − | 𝜈(C-C)sub(43) |
| 1237 | 1223 | 1214 | 38 | 1215 | 33 | 𝜈C−O(63) |
| 1215 | 1202 | 1200 | 44 | 1201 | 51 | β(C-H)(55) |
| 1174 | 1162 | 1152 | 58 | 1155 | 14 | 𝜈(C-C)(49) |
| 1140 | 1129 | 1121 | 32 | − | − | γ(CH3)(51) |
| 1045 | 1036 | − | − | 1035 | 13 | 𝜈(C-C)sub(45) |
| 1042 | 1033 | 1027 | 52 | − | − | 𝜈(C-C)sub(51) |
| 968 | 961 | − | − | − | − |  𝜈(C-C)(42) |
| 959 | 952 | − | − | 952 | 84 | 𝜈(C-C)sub(52) |
| 939 | 933 | 935 | 74 | 936 | 53 | 𝜌(CH3)(72) |
| 889 | 883 | 888 | 79 | − | − | 𝜌(CH3)(76) |
| 882 | 877 | 867 | 74 | − | − | β(C-C-C)(40) |
| 780 | 777 | 775 | 81 | 777 | 51 | β(C-C-C)(47) |
| 758 | 755 | 769 | 57 | 759 | 16 | βRing(51) |
| 634 | 633 | − | − | 633 | 23 | γRing(82) |
| 625 | 624 | 619 | 42 | − | − | β(C-C-C)(52) |
| 590 | 589 | 580 | 84 | − | − | γRing(79) |
| 561 | 561 | − | − | 558 | 95 | γ(O-H)(82)  |
| 458 | 458 | 464 | 72 | 472 | 70 | τCH3(90) |
| 388 | 389 | − | − | 391 | 19 | τCH3(83) |
| 325 | 327 | − | − | 325 | 36 | γ(C-C-C)(56) |
| 280 | 281 | − | − | 286 | 70 | γ(C-C-C)(57) |
| 225 | 226 | − | − | 226 | 43 | τCH3(100) |

a𝜈; stretching, β; in-plane bending, γ; out-of-plane bending, 𝜌; rocking, τ; torsion.