**Supplementary Section**



**M06-2X**

**Fig. 1S**. Calculated IR spectra for **5**.

****

**Fig. 2S.** Relationship between the experimental and computed frequencies of **5**.



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**Fig. 3S.** Calculated 1H NMR spectra of **5**.



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**Fig. 4S**. Calculated 13C NMR spectra of **5**.

**Table. 1S**. Theoretically computed total energies (kcal.mol−1), zero-point vibrational energies (kcal.mol−1), rotational constants (GHz), entropies (cal.mol−1.K−1), enthalpies (kcal. mol−1), Gibbs-free energies (kcal. mol−1), dipole moment (Debye) and some physico-chemical properties at M06-2X/6-311++G(2d,p) level.

|  |  |  |
| --- | --- | --- |
| Parameters | M06-2X/6-311++G(2d,p) |  |
| Total energy | -615494.160 |  |
| Zero-point energy | -615203.373 |  |
| Rotational constants | 0.4720513 |  |
|  | 0.1377180 |  |
|  | 0.1148729 |  |
| Entropy |  |  |
| Total | 152.187 |  |
| Translational | 43.140 |  |
| Rotational | 34.992 |  |
| Vibrational | 74.055 |  |
| Enthalpy | -615189.141 |  |
| Gibbs-free energy | -615234.515 |  |
| Dipole moment (D) |  |  |
| X | -1.8788 |  |
| Y | -0.6383  |  |
| Z | 1.9260 |  |
| Total | 2.7653 |  |
| Properties | Values |  |
| Molar Refractivitya (cm3) | 93.92 ± 0.4 |
| Molar Volumea (cm3) | 286.2 ± 5.0 |
| Parachora (cm3) | 744.2 ± 6.0 |
| Index of refractiona | 1.570 ± 0.03 |
| Surface tensiona (dyne/cm) | 45.7 ± 5.0 |
| Densitya (g/cm3) | 1.10 ± 0.1 |
| Polarizabilitya (cm3) | 37.23 ± 0.5 ×10-24 |
| Log *P* | 2.37b |

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**Table. 2S.** Second order perturbation theory analysis of Fock Matrix in NBO basis for **5** at the M06/2X method with 6-311++G(2d,p) basis set.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Donor NBO(I) | Acceptor NBO(j) | E2(kcal/mole) M06-2x | Ej-Ei(a.u) M06-2x | F(i,j)(a.u) M06-2x |
|  |  |
| π(C1-C2) | π\*(C9-C8) |  | 31.68 |  | 0.32 |  | 0.091 |
| π(C1-C2) | π\*(C10-C11) |  | 28.38 |  | 0.35 |  | 0.090 |
| π(C8-C9) | π\*(C1-C2) |  | 25.34 |  | 0.21 |  | 0.068 |
| π(C8-C9) | π\*(C10-C11) |  | 27.22 |  | 0.35 |  | 0.089 |
| π(C10-C11) | π\*(C1-C2) |  | 30.90 |  | 0.26 |  | 0.083 |
| π(C10-C11) | π\*(C8-C9) |  | 28.10 |  | 0.32 |  | 0.087 |
| Lp(1)N3 | π\*(C1-C2) |  | 74.67 |  | 0.36 |  | 0.157 |
| Lp(1)N3 | σ\*(C4-C24) |  | 7.79 |  | 0.82 |  | 0.074 |
| Lp(1)N7 | σ\*(C4-C26) |  | 16.05 |  | 2.60 |  | 0.189 |
| Lp(1)N15 | π\*(C14-O16) |  | 71.25 |  | 0.40 |  | 0.150 |
| Lp(1)N15 | σ\*(C18-C23) |  | 7.63 |  | 0.77 |  | 0.073 |
| Lp(2)O16 | σ\*(C14-N15) |  | 31.02 |  | 0.86 |  | 0.147 |
| Lp(2)O16 | σ\*(C6-C14) |  | 23.40 |  | 0.76 |  | 0.121 |