**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of streptocyanine.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1B2(p,\*) | (2,2,2,1) | (1,0,1,0) | 7.815 | **6.757** | **7.171** | **7.338** | **7.128** | **7.214** | **7.283** |
| 3B2(p,\*) | (2,2,2,1) | (1,0,1,0) | 5.859 | **5.225** | **5.488** | **5.615** | **5.522** | **5.494** | **5.543** |

a Reference (8e,7o) active space including valence , two σCN and two σ\*CN orbitals.