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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,au,bu,bg) | State-average  (Ag,Au,Bu,Bg) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PV-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1Bu(,\*) | (0,4,0,4) | (1,0,2,0) | 6.647a | **6.523** | **6.762** | **6.723** | **6.683** | **6.653** | **6.720** |
| 1Bg(,3s) | (4,2,3,2) | (1,0,0,1) | 5.942b | **6.315** | **6.490** | **6.484** | **6.440** | **6.380** | **6.429** |
| 1Ag(,\*2) | (3,2,3,2) | (2,0,0,0) | 6.990c | **6.384**d | **6.736** | **6.780** | **6.700** | **6.627**d | **6.718** |
| 1Au(,3px) | (3,2,5,2) | (1,2,0,0) | 5.947e | **6.642** | **6.745** | **6.806** | **6.836** | **6.673** | **6.704** |
| 1Au(,3py) | (3,2,5,2) | (1,2,0,0) | 6.123e | **6.838** | **6.952** | **7.004** | **7.015** | **6.864** | **6.902** |
| 1Bu(,3pz) | (0,4,0,4) | (1,0,2,0) | 7.928a | **7.298** | **7.603** | **7.526** | **7.449** | **7.541** | **7.622** |
| 3Bu(,\*) | (3,2,3,2) | (1,0,1,0) | 3.553c | **3.190** | **3.404** | **3.431** | **3.397** | **3.348** | **3.398** |
| 3Ag(,\*) | (3,2,3,2) | (2,0,0,0) | 5.519c | **4.927** | **5.317** | **5.358** | **5.299** | **5.187** | **5.286** |
| 3Bg(,3s) | (4,2,3,2) | (1,0,0,1) | 5.892b | **6.266** | **6.439** | **6.431** | **6.385** | **6.326** | **6.376** |

a Using reference (4e,8o) active space including valence  and 4 3pz. b Using reference (10e,11o) active space including valence , σCC, σ\*CC and 3s orbitals. c Using reference (10e,10o) active space including valence , σCC and σ\*CC orbitals. d Level shift = 0.4 au. e Using reference (10e,12o) active space including valence , σCC, σ\*CC, 3px and 3py orbitals.