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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A1"(n,\*) | (2,4,1,2) | (1,2,0,2) | 5.881a | **3.899** | **4.624** | **4.707** | **4.608** | **4.987** | **5.000** |
| 1A2"(n,\*) | (2,4,1,2) | (1,1,0,0) | 5.142a | **4.386** | **4.767** | **4.942** | **4.895** | **4.874** | **4.895** |
| 1E''(n,\*) | (2,4,1,2) | (1,2,0,2) | 5.514a | **4.142** | **4.762** | **4.944** | **4.881** | **4.980** | **5.006** |
| 1A2'(,\*) | (0,6,0,3) | (1,0,1,0) | 5.550b | **5.325** | **5.758** | **5.978** | **5.950** | **5.719** | **5.755** |
| 1A1'(,\*) | (0,6,0,3) | (2,0,0,0) | 8.204b | **6.892** | **7.429** | **7.421** | **7.300** | **7.409** | **7.499** |
| 1E'(n,3s) | (3,4,1,2) | (2,0,2,0) | 7.400c | **7.154** | **7.484** | **7.507** | **7.448** | **7.494** | **7.526** |
| 1E''(n,\*) | (2,4,1,2) | (1,1,0,1) | 8.265a | **7.038** | **7.748** | **8.069** | **7.983** | **7.896** | **7.924** |
| 1E'(,\*) | (0,6,0,3) | (4,0,3,0) | 10.029b | **7.700** | **8.651** | **8.594** | **8.340** | **8.719** | **8.831** |
| 3A2"(n,\*) | (2,4,1,2) | (1,1,0,0) | 4.737a | **3.989** | **4.371** | **4.551** | **4.515** | **4.493** | **4.513** |
| 3E''(n,\*) | (2,4,1,2) | (1,2,0,2) | 5.143a | **3.878** | **4.474** | **4.657** | **4.606** | **4.679** | **4.706** |
| 3A1"(n,\*) | (2,4,1,2) | (1,2,0,2) | 5.882a | **3.943** | **4.697** | **4.807** | **4.711** | **5.040** | **5.059** |
| 3A1'(,\*) | (0,6,0,3) | (2,0,0,0) | 4.464b | **4.545** | **4.878** | **5.058** | **5.046** | **4.751** | **4.805** |
| 3E'(,\*) | (0,6,0,3) | (3,0,1,0) | 5.570b | **5.201** | **5.617** | **5.765** | **5.729** | **5.574** | **5.624** |
| 3A2'(,\*) | (0,6,0,3) | (1,0,1,0) | 7.696b | **6.117** | **6.621** | **6.472** | **6.360** | **6.681** | **6.756** |

a Using reference (12e,9o) active space including valence  and nN orbitals. b Using reference (6e,9o) active space including valence  and three 3px orbitals. c Using reference (12e,10o) active space including valence , nN and 3s orbitals.