**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of AlCH2.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 | MS-PT2  IPEA | XMS-PT2  IPEA |
| 12A1(s,p) | (5,3,2,0) | (1,0,1,0) | 1.052a | **0.897** | **0.914** | **0.962** | **0.964** | **0.944** | **0.948** | **–** | **–** |
| 12A2(s,s)b | (5,3,2,0) | (0,0,1,1) | 1.990a | **2.184** | **2.251** | **2.206** | **2.212** | **2.255** | **2.280** | **–** | **–** |
| 22A1(s,p\*)b | (5,3,2,0) | (2,0,1,0) | 3.893a | **3.270** | **3.558** | **3.592** | **3.490** | **3.471** | **3.563** | **–** | **–** |
| 22A2(s,px(Al)) | (5,3,2,0) | (0,0,1,2) | 3.630a | **3.315** | **3.606** | **3.599** | **3.532** | **3.498** | **3.605** | **–** | **–** |
| 12B1(s2,ppx(Al))c | (5,3,2,0) | (0,2,1,0) | 3.884a | **3.776** | **3.996** | **4.020** | **4.000** | **3.985** | **4.036** | **3.996** | **3.995** |
| 22B1(p,px(Al))d | (5,3,2,0) | (0,2,1,0) | 4.512a | **4.383** | **4.644** | **4.645** | **4.583** | **4.546** | **4.634** | **4.633** | **4.639** |
| 32A1(s,p\*) | (5,3,2,0) | (0,0,1,3) | 5.466a | **4.475** | **4.846** | **4.823** | **4.652** | **4.681** | **4.817** | **4.847** | **4.851** |
| 22B2(p,p\*)b,e | (6,3,3,0) | (0,0,5,0) | 5.035f | **4.769** | **5.051** | **5.049** | **4.978** | **4.972** | **5.060** | **5.008** | **4.993** |
| 32B2(s2,pp\*)e | (6,3,3,0) | (0,0,5,0) | 4.910f | **5.052** | **5.185** | **5.165** | **5.147** | **5.186** | **5.227** | **5.198** | **5.195** |
| 42B2(s,3s)b | (6,3,3,0) | (0,0,5,0) | 5.340f | **5.290** | **5.472** | **5.460** | **5.422** | **5.458** | **5.509** | **5.500** | **5.505** |
| 52B2(p,p\*) | (6,3,3,0) | (0,0,5,0) | 5.734f | **5.332** | **5.659** | **5.655** | **5.544** | **5.508** | **5.625** | **5.679** | **5.692** |
| 14A2(s,px(Al)) | (5,3,2,0) | (0,0,1,1) | 1.691a | **1.926** | **1.984** | **1.937** | **1.947** | **1.984** | **2.010** | **–** | **–** |
| 14A1(s,p\*) | (5,3,2,0) | (1,0,1,0) | 2.480a | **2.499** | **2.555** | **2.555** | **2.566** | **2.539** | **2.563** | **–** | **–** |
| 14B2(s,3s) | (6,3,3,0) | (0,0,2,0) | 4.441f | **4.549** | **4.638** | **4.621** | **4.607** | **4.639** | **4.669** | **–** | **–** |

a Using reference (9e,10o) full valence active space. b Involving partial double character. c Involving partial double character at SA3 level, but strong double character at SA2 level. The first two B1 states are mixed at SA3 level. d Involving partial double character. The first two B1 states are mixed. e Gaining partial Rydberg character upon including 3s Rydberg orbital. f Using reference (9e,12o) full valence active space plus one 3s and one 3py orbitals.