1. The structure of R*i*MR*i*3+ is optimized in the gas phase at the PBE0/6-311G\*-RECP level.
2. The constrained minima of the MR*i*3+ complexes (*i* = 1~8) with the M-N-C angle constrained to approximate the M3+ location observed in the complex M(PhR*i*)3+ calculated by using the PBE0/ZORA/DKH/6-311G\*-RECP methods and the CPCM solvation model in aqueous phase
3. The structure of MR*l*Ph 3+ is optimized in the gas phase at the PBE0/6-311G\*-RECP level.
4. The structure of MR*l*Ph(NO3)3 is optimized in the gas phase at the PBE0/6-311G\*-RECP level.
5. The structure of MR*l*PhR*r*3+is optimized in the gas phase at the PBE0/6-311G\*-RECP level.
6. The structure of MR*l*PhR*r* (NO3)3 is optimized in the gas phase at the PBE0/6-311G\*-RECP level.