Figure S1: B3LYP/6-311G(d,p) geometries along the reaction path in the reaction of H-C≡C-OH + CO.
Figure S2: B3LYP/6-311G(d,p) geometries along the reaction path in the reaction of H-C≡O-H + CS.
Figure S3: B3LYP/6-311G(d,p) geometries along the reaction path in the reaction of H₂C≡N+NH₂+CO.
**Figure S4**: Geometries along the reaction path in the reaction of H-C≡C-NH₂ + CS. Optimized values obtained at B3LYP/6-311G(d,p) except Shaz1, Shatr1 taken from HF/6-31G(d).
Figure S5: Geometries along the reaction path in the reaction of H-C≡C-C₆H₅ + CO. Optimized values obtained at B3LYP/6-311G(d,p).
Figure S6: Geometries along the reaction path in the reaction of H-C≡C-C₆H₅ + CS. Optimized values obtained at B3LYP/6-311G(d,p).
Figure S7: Geometries along the reaction path in the reaction of OH-C≡C-CH₃ + CO. Optimized values obtained at B3LYP/6-311G(d,p).
Figure S8: Geometries along the reaction path in the reaction of OH\(\cdot\)C\(\equiv\)C\(\cdot\)CH\(_3\) + CS. Optimized values obtained at B3LYP/6-31G(d,p) except Smoz2.

Smotr2 taken from HF/6-31G(d).
Figure S9: B3LYP/6-311G(d,p) geometries along the reaction path in the reaction of OH+C-C3H8+CO.
**Figure S10**: Geometries along the reaction path in the reaction of OH-C≡C₆H₅ + CS. Optimized values obtained at B3LYP/6-311G(d,p) except Spoz2, Spotr2 taken from HF/6-31G(d).