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|---------------------------|--------------|---------------|
| Nandini Bajaj - 18CY20020 | | |
| H2 | Basis | Energy |
| | 631G | -1.175482 |
| | 6311G | -1.176632 |
| | 6311G, d, p | -1.179571 |
| | | |
| CH3Cl | Basis | Energy |
| | 6311G, d, p | -500.150712 |
| | | |
| CH3Br | Basis | Energy |
| | 6311G, d, p | -2614.073536 |
| | | |
| BrCH3Cl (TS) | Basis | Energy |
| | 6311G, d, p | -3074.386961 |
| | | |
| BrCH3Cl (TS-IRC) | Basis | Energy |
| | 6311G, d, p | -3074.37855 |