**Экспериментальные и расчётные термодинамические параметры**

**предполагаемых реакций разложения диазониевых солей**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Реакция | Gaussian RB3LYP aug-cc-pVDZ | | | Эксперимент | | |
| DG298 | DH298 | DS\*298.15 | DH348 | DH353 | DH358 |
| 2-NO2-Ph-N2+ OTf- = 2-NO2-Ph-OTf + N2 | -268.6 | -230.1 | 38.5 | - | -330 | -416 |
| 3-NO2-Ph-N2+ OTf- = 3-NO2-Ph-OTf + N2 | -282.4 | -242.8 | 39.6 | -228 | -230 | -225 |
| 4-NO2-Ph-N2+ OTf- = 4-NO2-Ph-OTf + N2 | -287.6 | -248.0 | 39.6 | -200 | -235 | -250 |
| 4-NO2-Ph-N2+ OTs- = 4-NO2-Ph-OTs + N2 | -328.4 | -283.9 | 44.6 | -253 | -232 | -231 |
| 4-NO2-Ph-N2+ BF4- = 4-NO2-Ph-F + BF3 + N2 | -276.2 | -188.4 | 87.9 | -173 | -156 | -147 |
| 4-NO2-Ph-N2+ BF4- = 4-NO2-Ph-F\*BF3 + N2 | -250.3 | -191.7 | 58.7 | -173 | -156 | -147 |
| 4-CH3O-Ph-N2+ OTf- = 4-CH3O-Ph-OTf + N2 | -238.1 | -200.5 | 37.7 | -183 | -183 | - |