|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Conformations** | **φ****C2-N3-C4-C5** | **ψ****N3-C4-C5-N6** | **χ1****N3-C4-C12-C14** | **χ2****C4-C12-C14-C15** | **ΔHf** **)Kcalmol-1(** | **Δ )ΔHf(****)Kcalmol-1(** |
| **αD)g+ g+(** | 23.2 | 57.0 | 41.2 | 82.3 | -53.777370 | 7.01 |
| **αD)a g+(** | 76.8 | 29.1 | -129.2 | 95.6 | -53.149132 | 7.64 |
| **αD)g- g-(** | 10.8 | 65.5 | -58.2 | -82.2 | -55.699348 | 5.09 |
|  |  |  |  |  |  |  |
| **βL)g+g+(**  | -150.0 | 167.2 | 64.8 | 5.3 | -55,881470 | 4.91 |
| **βL)g+ a(**  | -125.2 | 170.7 | 74.8 | 171.4 | -55.683189 | 5.10 |
| **βL)a g+ (** | -146.8 | 170.8 | -144.6 | 65.4 | -58.818661 | 1.97 |
| **βL)a g- (** | -146.2 | 170.4 | -144.8 | -116.0 | -58.818691 | 1.97 |
| **βL)g- g-(** | -119.2 | 132.1 | -57.6 | -31.2 | -58.322929 | 2.46 |
|  |  |  |  |  |  |  |
| **γL)g+ g+ (** | -82.7 | 60.6 | 39.3 | 78.3 | -60.282001 | 0.51 |
| **γL)g+ g-)** | -84.1 | 58.1 | 39.3 | -94.9 | -60.373520 | 0.41 |
| **γL)a g+(** | -81.0 | 74.9 | -156.2 | 89.3 | -59.510700 | 1.28 |
| **γL)a g-(** | -82,4 | 70.6 | -155.5 | -95.2 | -59.291512 | 1.50 |
|  **γL)g- g+(** | -80.3 | 66.0 | -19.2 | 101.2 | -60.792629 | 0.00 |
| **γL)g- g-(** | -84.1 | 66.8 | -10.3 | -82.3 | -60.778450 | 0.01 |
|  |  |  |  |  |  |  |
| **γD)g+ g+)**  | 44.7 | -80.4 | 42.2 | 101.6 | -53,932598 | 6.86 |
| **γD)a g+(**  | 75.4 | -65.6 | -167.6 | 68.4 | -58,116692 | 2.67 |
| **γD)a a (**  | 77.5 | -55.1 | -130.4 | 131.7 | -58.390171 | 2.40 |
| **γD)a g-(**  | 77.2 | -55.0 | -130.0 | -49.7 | -58.387901 | 2.40 |
| **γD)g- g+)**  | 75.6 | -62.0 | -68.8 | 109.8 | -60.154072 | 0.63 |
| **γD)g- a)**  | 74.2 | -66.4 | -83.0 | -162.7 | -58.079609 | 1.71 |
| **γD)g- g-)**  | 75.5 | -62.4 | -69.2 | -70.0 | -60.154499 | 0.63 |
|  |  |  |  |  |  |  |
| **δD)g+ g+ (** | -115.2 | -53.4 | 49,3 | 99.4 | -57.406090 | 3.38 |
| **δD)g+ g-(** | -113.9 | -52.0 | 49.4 | -82.9 | -57.542358 | 3.25 |
| **δD)a g+(**  | -129.1 | -69 .5 | -178.5 | 64.0 | -55.683590 | 5.10 |
| **δD)a g-)** | -129.3 | -69.6 | -178.6 | -117 .5 | -55.687199 | 5.10 |
|  |  |  |  |  |  |  |
| **εD )a g+(** | 91,9 | -158,2 | -151.9 | 56.9 | -55,966282 | 4.82 |
| **εD )a a(** | 94.7 | -150.4 | -154.8 | -127.3 | -55.948681 | 4.84 |
| **εD )g- g+(** | 79.2 | 169.4 | -63.4 | 105.1 | -54.185909 | 6.60 |

 a torsion angles in degrees

**Table S2 : Torsion angles(a), heats of formation ΔHf and relative heats of formation**

**Δ(ΔHf) of 28 structures of HCO-L-Phe-NH2 located at MNC/AM1**