Electronic Supplementary Material (ESI) for New Journal of Chemistry.


**Table S4 –** Calculated (mPW1PW/6-31G*) structural parameters for the most stable conformers of 1,3-dap in the different chemical environments considered.

| | *Isolated molecule* | | *Condensed phase* | | *Aqueous Solution* | | *$CCl_4$ solution* | |
|---|---|---|---|---|---|---|---|---|
| Parameter[a] | GGG'G | TG'GG' | TTTG | TGTT | TTTG | TGTT | TTTG | TG'GG' |
| *Bond length (pm)* | | | | | | | | |
| $C^4C^7$ | 152.6 | 153.5 | 152.3 | 153.2 | 152.3 | 153.2 | 152.3 | 153.3 |
| $C^4H^5$ | 110.4 | 109.6 | 110.4 | 109.8 | 110.4 | 109.8 | 110.5 | 109.7 |
| $C^4H^6$ | 109.7 | 109.8 | 109.7 | 109.7 | 109.7 | 109.7 | 109.7 | 109.9 |
| $C^7C^{10}$ | 152.6 | 152.6 | 152.9 | 152.9 | 152.9 | 152.9 | 152.9 | 152.7 |
| $C^7H^8$ | 109.8 | 110.0 | 109.8 | 109.9 | 109.8 | 109.9 | 109.7 | 109.9 |
| $C^7H^9$ | 109.7 | 109.8 | 110.0 | 110.0 | 110.0 | 110.0 | 110.0 | 109.8 |
| $C^{10}H^{11}$ | 110.7 | 109.7 | 109.7 | 109.8 | 109.8 | 109.8 | 109.7 | 109.7 |
| $C^{10}H^{12}$ | 109.7 | 110.3 | 109.7 | 109.7 | 109.8 | 109.7 | 109.7 | 110.3 |
| $N^1C^4$ | 146.3 | 145.6 | 146.2 | 146.1 | 146.3 | 146.2 | 146.0 | 146.3 |
| $N^1H^2$ | 101.6 | 101.7 | 102.0 | 101.9 | 102.1 | 101.9 | 101.8 | 102.1 |
| $N^1H^3$ | 101.7 | 101.9 | 102.1 | 102.0 | 102.1 | 102.1 | 101.8 | 102.1 |
| $N^{13}C^{10}$ | 145.7 | 146.4 | 146.1 | 146.1 | 146.2 | 146.2 | 145.9 | 146.6 |
| $N^{13}H^{14}$ | 101.6 | 101.7 | 102.1 | 102.1 | 102.1 | 102.1 | 101.8 | 102.1 |
| $N^{13}H^{15}$ | 101.8 | 101.6 | 102.1 | 102.1 | 102.1 | 102.1 | 101.8 | 102.0 |
| *Bond angle(º)* | | | | | | | | |
| $C^4C^7C^{10}$ | 114.8 | 114.6 | 113.2 | 114.3 | 113.2 | 114.3 | 113.3 | 114.5 |
| $C^4C^7H^8$ | 109.9 | 109.4 | 108.9 | 108.9 | 108.9 | 108.9 | 108.6 | 109.3 |
| $C^4$ $C^7H^9$ | 107.6 | 109.2 | 109.3 | 109.2 | 109.3 | 109.1 | 109.3 | 109.1 |
| $C^7C^{10}H^{11}$ | 108.3 | 108.7 | 109.3 | 109.2 | 109.3 | 109.2 | 109.4 | 108.7 |
| $C^7C^{10}H^{12}$ | 108.5 | 109.1 | 109.5 | 109.8 | 109.5 | 109.8 | 109.6 | 108.9 |
| $C^7C^{10}N^{13}$ | 111.1 | 112.0 | 115.8 | 115.8 | 115.7 | 115.7 | 116.0 | 112.2 |
| $C^{10}N^{13}H^{14}$ | 109.7 | 109.4 | 108.7 | 108.7 | 108.6 | 108.6 | 109.1 | 108.9 |
| $C^{10}N^{13}H^{15}$ | 107.7 | 109.9 | 108.8 | 108.8 | 108.6 | 108.6 | 109.2 | 109.2 |
| $H^2N^1C^4$ | 110.0 | 109.0 | 109.0 | 109.9 | 108.9 | 109.8 | 109.5 | 108.1 |
| $H^2N^1H^3$ | 106.5 | 105.8 | 105.2 | 105.6 | 105.0 | 105.5 | 105.6 | 104.9 |
| $H^3N^1C^4$ | 109.5 | 107.3 | 108.7 | 109.2 | 108.5 | 109.0 | 109.1 | 106.0 |
| $H^5C^4C^7$ | 108.7 | 109.0 | 108.9 | 109.4 | 108.9 | 109.4 | 109.0 | 109.2 |
| $H^5C^4H^6$ | 106.5 | 105.9 | 106.3 | 106.1 | 106.3 | 106.1 | 106.3 | 106.1 |
| $H^6C^4C^7$ | 108.9 | 108.5 | 109.1 | 108.8 | 109.1 | 108.8 | 109.0 | 108.5 |
| $H^8C^7C^{10}$ | 108.3 | 109.6 | 109.7 | 108.7 | 109.6 | 108.7 | 109.9 | 109.6 |
| $H^8C^7H^9$ | 106.8 | 106.0 | 106.6 | 106.4 | 106.6 | 106.4 | 106.5 | 106.2 |
| $H^9C^7C^{10}$ | 109.2 | 107.7 | 109.0 | 109.1 | 109.0 | 109.1 | 109.0 | 107.8 |
| $H^{11}C^{10}H^{12}$ | 106.3 | 106.4 | 106.1 | 106.2 | 106.1 | 106.2 | 106.0 | 106.4 |
| $H^{11}C^{10}N^{13}$ | 114.2 | 107.3 | 107.8 | 107.9 | 107.9 | 108.0 | 107.7 | 107.5 |
| $H^{12}C^{10}N^{13}$ | 108.0 | 113.2 | 107.8 | 107.6 | 107.9 | 107.6 | 107.7 | 112.9 |
| $H^{14}N^{13}H^{15}$ | 107.6 | 106.1 | 105.1 | 105.0 | 104.9 | 104.9 | 105.4 | 105.5 |
| $N^1C^4C^7$ | 111.9 | 117.0 | 110.9 | 116.8 | 111.0 | 116.7 | 110.8 | 116.3 |
| $N^1C^4H^5$ | 113.3 | 108.1 | 113.6 | 107.6 | 113.5 | 107.7 | 113.8 | 108.1 |
| $N^1C^4H^6$ | 107.3 | 107.8 | 107.8 | 107.6 | 107.9 | 107.7 | 107.7 | 108.0 |

| *Dihedral angle(º)* | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| $C^4C^7C^{10}H^{11}$ | -51.9 | -54.9 | 58.0 | 57.5 | 58.1 | 57.6 | 58.0 | -56.1 |
| $C^4C^7C^{10}H^{12}$ | -166.9 | -170.6 | -57.8 | -58.5 | -57.8 | -58.4 | -57.8 | -171.6 |
| $C^4C^7C^{10}N^{13}$ | 74.4 | 63.4 | -180.0 | 179.5 | -179.9 | 179.6 | 180.0 | 62.6 |
| $C^7C^{10}N^{13}H^{14}$ | -178.9 | 68.3 | -56.8 | -55.8 | -56.6 | -55.5 | -57.3 | 68.2 |
| $C^7C^{10}N^{13}H^{15}$ | -62.0 | -175.6 | 57.0 | 58.0 | 56.9 | 58.0 | 57.5 | -177.0 |
| $H^2N^1C^4C^7$ | 179.7 | -65.0 | 179.5 | -62.5 | 179.9 | -62.6 | 178.5 | -64.7 |
| $H^2N^1C^4H^5$ | -57.0 | 58.4 | -57.4 | 60.8 | -57.0 | 60.8 | -58.3 | 58.6 |
| $H^2N^1C^4H^6$ | 60.2 | 172.5 | 60.1 | 174.8 | 60.4 | 174.8 | 59.3 | 173.0 |
| $H^3N^1C^4C^7$ | -63.6 | 49.1 | -66.3 | 52.9 | -66.2 | 52.5 | -66.4 | 47.3 |
| $H^3N^1C^4H^5$ | 59.7 | 172.6 | 56.8 | 176.2 | 56.8 | 175.9 | 56.9 | 170.6 |
| $H^3N^1C^4H^6$ | 177.0 | -73.4 | 174.3 | -69.8 | 174.3 | -70.1 | 174.5 | -75.0 |
| $H^5C^4C^7C^{10}$ | 173.5 | 167.5 | 56.1 | -57.8 | 56.1 | -57.6 | 56.2 | 167.3 |
| $H^5C^4C^7H^8$ | -64.1 | -69.0 | 178.4 | 63.9 | 178.4 | 64.1 | 178.7 | -69.3 |
| $H^5C^4C^7H^9$ | 51.7 | 46.6 | -65.5 | 179.7 | -65.5 | 179.9 | -65.5 | 46.4 |
| $H^6C^4C^7C^{10}$ | 57.9 | 52.6 | -59.5 | -173.3 | -59.5 | -173.1 | -59.4 | 52.1 |
| $H^6C^4C^7H^8$ | -179.7 | 176.1 | 62.8 | -51.5 | 62.7 | -51.4 | 63.0 | 175.5 |
| $H^6C^4C^7H^9$ | -63.8 | -68.3 | 178.8 | 64.2 | 178.8 | 64.4 | 178.9 | -68.8 |
| $H^8C^7C^{10}H^{11}$ | -175.1 | -178.3 | -63.8 | -64.3 | -63.8 | -64.2 | -63.7 | -179.3 |
| $H^8C^7C^{10}H^{12}$ | 69.9 | 66.0 | -179.7 | 179.7 | -179.7 | 179.8 | -179.6 | 65.2 |
| $H^8C^7C^{10}N^{13}$ | -48.8 | -60.0 | 58.2 | 57.7 | 58.2 | 57.8 | 58.2 | -60.6 |
| $H^9C^7C^{10}H^{11}$ | 69.0 | 66.8 | 179.9 | -180.0 | 179.9 | -179.9 | 179.9 | 65.5 |
| $H^9C^7C^{10}H^{12}$ | -46.0 | -48.8 | 64.0 | 64.0 | 64.1 | 64.1 | 64.1 | -50.0 |
| $H^9C^7C^{10}N^{13}$ | -164.7 | -174.9 | -58.1 | -58.0 | -58.1 | -57.9 | -58.1 | -175.7 |
| $H^{11}C^{10}N^{13}H^{14}$ | -55.9 | -172.6 | 66.0 | 66.9 | 66.1 | 67.1 | 65.5 | -172.3 |
| $H^{11}C^{10}N^{13}H^{15}$ | 61.0 | -56.4 | 179.8 | -179.3 | 179.7 | -179.4 | -179.7 | -57.6 |
| $H^{12}C^{10}N^{13}H^{14}$ | 62.2 | -55.5 | -179.9 | -178.9 | -179.6 | -178.6 | 179.5 | -55.3 |
| $H^{12}C^{10}N^{13}H^{15}$ | 179.0 | 60.7 | -66.0 | -65.1 | -66.0 | -65.1 | -65.7 | 59.5 |
| $N^1C^4C^7H^8$ | 61.7 | 54.0 | -55.8 | -173.6 | -56.0 | -173.4 | -55.3 | 53.5 |
| $N^1C^4C^7H^9$ | 177.6 | 169.6 | 60.2 | -57.8 | 60.1 | -57.6 | 60.5 | 169.2 |
| $N^1C^4C^7C^{10}$ | -60.6 | -69.5 | -178.2 | 64.7 | -178.3 | 64.9 | -177.83 | -69.9 |

[a] *See Figure 1 for atom numbering*