**ELECTRONIC SUPPLEMENTARY INFORMATION**

**Table 1S:** Optimized geometrical parameters (bond lengths (Ǻ) and bond angles(°)) in various media at B3LYP/6-31+G(d,p) level.

**Table 2S**: Experimental and calculated vibrational frequencies (cm‐1) at the B3LYP/6-31+G(d,p) level.

**Table 3S:** B3LYP/6-31+G(d,p) total energies of radical (ET in a.u) and bond dissociation enthalpies (BDE in kJ/mol) in solution phase.

**Table 4S**: Bond dissociation free energy of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in in solution phase

**Table 5S**: Thermochemical parameters for interaction of investigated juglone derivatives with some of oxygen species obtained level (∆GR’ in kJ/mol) at B3LYP/6-31+G(d,p) level (∆GR’ in kJ/mol).

**Table 6S**: Thermodynamic energies of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in various media: ionization potentials (IP) and proton dissociation enthalpies (PDE).

**Table 7S**: Thermodynamic energies of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in various media: ionization potential free energies (IPFE) and proton dissociation free energies (PDFE).

**Table 8S**: Thermodynamic energies of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in various media: proton affinities (PA) and electron transfer enthalpies (ETE).

**Table 9S**: Thermodynamic energies of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in various media: proton affinity free energies (PAFE) and electron transfer free energy (ETFE).

**Figure 1S**: Dependence of Experimental and calculated gas phase FT-IR frequencies (cm‐1) at B3LYP/6-31+G(d,p) level.

**Table 1S:** Optimized geometrical parameters (bond lengths (Ǻ) and bond angles (°)) in various media at B3LYP/6-31+G(d,p) level.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Gas** | | | **Benzene** | | | **Toluene** | | |
|  | Bond  lengths | | Bond angles | Bond  lengths | | Bond angles | Bond  lengths | | Bond angles |
|  | O1-H1…O2 | C1-O1 | O1-H1…O2 | O1-H1…O2 | C1-O1 | O1-H1…O2 | O1-H1…O2 | C1-O1 | O1-H1…O2 |
| J1 | 1.709 | 1.340 | 146.6 | 1.706 | 1.342 | 146.9 | 1.705 | 1.342 | 146.9 |
| J2 | 1.625 | 1.341 | 149.8 | 1.623 | 1.341 | 150.0 | 1.624 | 1.341 | 150.0 |
| J3 | 1.666 | 1.346 | 147.5 | 1.664 | 1.347 | 147.7 | 1.664 | 1.347 | 147.6 |
| J4 | 1.677 | 1.347 | 147.2 | 1.674 | 1.347 | 147.4 | 1.674 | 1.347 | 147.4 |
| J5 | 1.700  2.153\* | 1.349 | 145.9  112.8a | 1.700  2.162 a | 1.348 | 146.0  112.4 a | 1.700  2.162 a | 1.348 | 146.0  112.4 a |
| J6 | 1.688 | 1.336 | 147.4 | 1.683 | 1.338 | 147.7 | 1.683 | 1.338 | 147.7 |
| J7 | 1.639 | 1.342 | 149.8 | 1.637 | 1.343 | 149.9 | 1.637 | 1.343 | 149.9 |
| J8 | 1.683 | 1.343 | 147.8 | 1.681 | 1.344 | 148.0 | 1.680 | 1.344 | 148.0 |
| J9 | 1.707 | 1.335 | 146.4 | 1.705 | 1.337 | 146.6 | 1.705 | 1.337 | 146.6 |
| J10 | 1.685 | 1.333 | 147.4 | 1.682 | 1.335 | 147.5 | 1.682 | 1.335 | 147.5 |
| J11 | 1.686 | 1.334 | 147.3 | 1.683 | 1.335 | 147.5 | 1.683 | 1.335 | 147.5 |
| J12 | 1.658 | 1.339 | 148.8 | 1.658 | 1.341 | 148.9 | 1.658 | 1.341 | 148.9 |
| J13 | 1.671 | 1.340 | 148.2 | 1.668 | 1.342 | 148.4 | 1.668 | 1.342 | 148.4 |
| J14 | 1.679 | 1.337 | 147.6 | 1.676 | 1.338 | 147.8 | 1.675 | 1.338 | 147.8 |
| J15 | 1.621 | 1.348 | 148.6 | 1.619 | 1.347 | 148.6 | 1.619 | 1.347 | 148.6 |
| J16 | 1.693 | 1.331 | 146.7 | 1.691 | 1.335 | 146.8 | 1.691 | 1.332 | 146.8 |
| J17 | 1.670 | 1.327 | 147.9 | 1.662 | 1.328 | 148.3 | 1.662 | 1.328 | 148.3 |
|  | 1.664 |  | 145.9 |  |  |  |  |  |  |
| J18 | 1.685 | 1.333 | 147.2 | 1.682 | 1.335 | 147.3 | 1.680 | 1.334 | 147.5 |
|  | **Methanol** | | | **Acetonitrile** | | | **Water** | | |
|  | Bond  lengths | | Bond angles | Bond  lengths | | Bond angles | Bond  lengths | | Bond angles |
|  | O1-H1…O2 | C1-O1 | O1-H1…O2 | O1-H1…O2 | C1-O1 | O1-H1…O2 | O1-H1…O2 | C1-O1 | O1-H1…O2 |
| J1 | 1.700 | 1.344 | 147.2 | 1.700 | 1.344 | 147.3 | 1.699 | 1.345 | 147.2 |
| J2 | 1.620 | 1.342 | 150.2 | 1.619 | 1.342 | 150.2 | 1.619 | 1.342 | 150.2 |
| J3 | 1.660 | 1.346 | 147.9 | 1.656 | 1.346 | 147.9 | 1.658 | 1.346 | 147.9 |
| J4 | 1.670 | 1.347 | 147.7 | 1.670 | 1.347 | 147.7 | 1.670 | 1.347 | 147.7 |
| J5 | 1.700  2.170 a | 1.348 | 146.1  112.0 a | 1.699  2.171 a | 1.348 | 146.1  112.0 a | 1.700  2.171 a | 1.347 | 146.1  112.0 a |
| J6 | 1.673 | 1.340 | 148.1 | 1.673 | 1.341 | 148.0 | 1.673 | 1.341 | 148.1 |
| J7 | 1.634 | 1.344 | 150.2 | 1.634 | 1.344 | 150.2 | 1.633 | 1.344 | 150.0 |
| J8 | 1.675 | 1.345 | 148.3 | 1.675 | 1.345 | 148.3 | 1.675 | 1.345 | 148.4 |
| J9 | 1.697 | 1.339 | 147.0 | 1.697 | 1.340 | 146.9 | 1.699 | 1.340 | 147.0 |
| J10 | 1.672 | 1.337 | 148.0 | 1.672 | 1.337 | 148.0 | 1.672 | 1.337 | 148.0 |
| J11 | 1.673 | 1.337 | 148.0 | 1.673 | 1.337 | 148.0 | 1.672 | 1.337 | 148.0 |
| J12 | 1.655 | 1.342 | 149.2 | 1.655 | 1.342 | 149.2 | 1.655 | 1.343 | 149.2 |
| J13 | 1.661 | 1.343 | 148.7 | 1.661 | 1.343 | 148.7 | 1.661 | 1.343 | 148.7 |
| J14 | 1.671 | 1.338 | 148.1 | 1.670 | 1.338 | 148.0 | 1.670 | 1.338 | 148.0 |
| J15 | 1.619 | 1.346 | 148.4 | 1.619 | 1.346 | 148.4 | 1.619 | 1.346 | 148.4 |
| J16 | 1.681 | 1.334 | 147.3 | 1.680 | 1.334 | 147.3 | 1.680 | 1.335 | 147.3 |
| J17 | 1.642 | 1.329 | 149.2 | 1.642 | 1.329 | 149.2 | 1.642 | 1.329 | 149.3 |
| J18 | 1.671 | 1.337 | 147.9 | 1.671 | 1.337 | 147.9 | 1.668 | 1.337 | 148.0 |

**Table 2S**: Experimental and calculated FT-IR frequencies (cm‐1) at B3LYP/6-31+G(d,p) level.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | O-H | C=O  (H-bonded) | C=O | C-O | C-H |
| Experimental | 3465 [30] (a) | 1635[30] (a) | 1650[30] (a) | 1225[30] (b) | - |
| Theoretical | 3329 | 1653 | 1732 | 1346 | 3196-3226 |

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**Table 3S:** B3LYP/6-31+G(d,p) total energies of radical (ET in a.u) and bond dissociation energies (BDE in kJ/mol) in various media

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Radical | ET | BDE (kJ/mol) | | | |
| **gas** | **Benzene** | **Toluene** | **methanol** | **Acetonitrile** |
| J1radO1 | -609.713789 | 410 | 410 | 401 | 401 |
| J2 radO1 | -743.709533 | 359 | 359 | 345 | 345 |
| J3radO1 | -704.403282 | 356 | 356 | 344 | 344 |
| J3radN | -704.406538 | 379 | 379 | 377 | 377 |
| J4radO1 | -665.100663 | 361 | 363 | 351 | 351 |
| J4radN | -665.099789 | 374 | 374 | 377 | 377 |
| J5radO1 | -684.958850 | 375 | 375 | 368 | 368 |
| J5radO | -684.966485 | 355 | 355 | 348 | 348 |
| J6 radO1 | -724.248178 | 391 | 391 | 386 | 386 |
| J7 radO1 | -766.984233 | 403 | 403 | 395 | 395 |
| J8 radO1 | -688.356060 | 404 | 404 | 394 | 394 |
| J9 radO1 | -708.950745 | 403 | 403 | 394 | 394 |
| J10 radO1 | -1069.305661 | 405 | 405 | 396 | 396 |
| J11 radO1 | -3180.839552 | 406 | 406 | 397 | 397 |
| J12 radO1 | -840.786874 | 399 | 399 | 390 | 390 |
| J13 radO1 | -687.124896 | 392 | 396 | 386 | 386 |
| J14 radO1 | -723.038254 | 417 | 415 | 407 | 407 |
| J15 radO1 | -798.296631 | 405 | 404 | 398 | 398 |
| J15radO | -798.272218 | 462 | 461 | 477 | 477 |
| J16 radO1 | -701.951118 | 416 | 415 | 407 | 406 |
| J17 radO1 | -814.203712 | 427 | 427 | 409 | 409 |
| J18 radO1 | -946.763265 | 413 | 417 | 408 | 408 |

Relative to N-H BDE values. bO-H BDE values

**Table 4S**: Bond dissociation free energy of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in in solution phase

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Molecules | BDFE (kJ/mol) | | | | | |
| **Gas** | **Benzene** | **Toluene** | **Methanol** | **Acetonitrile** | **Water** |
| J1 | 377 | 371 | 370 | 360 | 360 | 360 |
| J2 | 329 | 319 | 318 | 305 | 305 | 305 |
| J3 | 350  346 a | 313  345 a | 315  345 a | 304  342 a | 304  342 a | 303  342 a |
| J4 | 333  338a | 328  340 a | 323  340 a | 338  343 a | 311  343 a | 311  343 a |
| J5 | 341  323b | 336  320 b | 336  319 b | 329  313 b | 329  313 b | 328  313 b |
| J6 | 355 | 349 | 349 | 346 | 346 | 346 |
| J7 | 369 | 363 | 363 | 353 | 353 | 353 |
| J8 | 369 | 363 | 363 | 350 | 350 | 350 |
| J9 | 367 | 364 | 364 | 352 | 352 | 351 |
| J10 | 370 | 363 | 363 | 355 | 355 | 354 |
| J11 | 372 | 366 | 366 | 357 | 357 | 356 |
| J12 | 366 | 361 | 360 | 351 | 351 | 351 |
| J13 | 369 | 358 | 357 | 346 | 345 | 345 |
| J14 | 380 | 375 | 375 | 367 | 367 | 367 |
| J15 | 373 | 360 | 360 | 357 | 357 | 357 |
| J16 | 381 | 375 | 374 | 366 | 365 | 365 |
| J18 | 383 | 378 | 377 | 367 | 367 | 364 |

Relative to N-H BDFE values. bO-H BDFE values

**Table 5S**: Thermochemical parameters for interaction of investigated juglone derivatives with some of oxygen species at B3LYP/6-31+G(d,p) level (∆GR’ in kJ/mol).

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | ∆GOR1 | ∆GOR2 | ∆GOR3 | ∆GOR4 | ∆GOO- | ∆GOOR1 | ∆GOOR2 | ∆GOOR3 | ∆GOOR4 |
| J1 | -75 | -5 | -18 | -3 | 158 | 64 | 71 | 43 | 72 |
| J2 | -123 | -53 | -66 | -51 | 110 | 16 | 23 | -5 | 24 |
| J3 | -102 | -32 | -45 | -30 | 131 | 37 | 44 | 16 | 45 |
|  | -106a | -36 a | -49 a | -34 a | 127 a | 33 a | 40 a | 12 a | 41 a |
| J4 | -119 | -49 | -62 | -47 | 114 | 20 | 27 | -1 | 28 |
|  | -114 a | -44 a | -57 a | -42 a | 119 a | 25 a | 32 a | 4 a | 33 a |
| J5 | -111 | -41 | -54 | -39 | 122 | 28 | 35 | 7 | 36 |
|  | -129b | -59 b | -72 b | -57 b | 104 b | 10 b | 17 b | -11 b | 18 b |
| J6 | -97 | -27 | -40 | -25 | 136 | 42 | 49 | 21 | 50 |
| J7 | -83 | -13 | -26 | -11 | 150 | 56 | 63 | 35 | 64 |
| J8 | -83 | -13 | -26 | -11 | 150 | 56 | 63 | 35 | 64 |
| J9 | -85 | -15 | -28 | -13 | 148 | 54 | 61 | 33 | 62 |
| J10 | -82 | -12 | -25 | -10 | 151 | 57 | 64 | 36 | 65 |
| J11 | -80 | -10 | -23 | -8 | 153 | 59 | 66 | 38 | 67 |
| J12 | -86 | -16 | -29 | -14 | 147 | 53 | 60 | 32 | 61 |
| J13 | -83 | -13 | -26 | -11 | 150 | 56 | 63 | 35 | 64 |
| J14 | -72 | -2 | -15 | 0 | 161 | 67 | 74 | 46 | 75 |
| J15 | -79 | -9 | -22 | -7 | 154 | 60 | 67 | 39 | 68 |
|  | -19 b | 51 b | 38 b | 53 b | 214 b | 120 b | 127 b | 99 b | 128 b |
| J16 | -71 | -1 | -14 | 1 | 162 | 68 | 75 | 47 | 76 |
| J18 | -69 | 1 | -12 | 3 | 164 | 70 | 77 | 49 | 78 |

aRelative to N-H thermochemical parameter values. bO-H thermochemical parameter values .

**Table 6S**: Thermodynamic energies of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in various media: ionization potentials (IP) and proton dissociation (PDE).

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Molecules | IP (kJ/mol) | | | | PDE (kJ/mol) | | | |
| **Benzene** | **Toluene** | **methanol** | **Acetonitrile** | **Benzene** | **Toluene** | **methanol** | **Acetonitrile** |
| J1 | 713 | 709 | 557 | 550 | **-5** | 70 | 19 | 31 |
| J2 | 589 | 585 | 441 | 434 | 68 | 143 | 79 | 91 |
| J3 | 607 | 604 | 458 | 451 | 45  69 a | 121  144 a | 61  94 a | 62  106 a |
| J4 | 624 | 633 | 471 | 464 | 34  47 a | 112  123 a | 55  80 a | 67  93 a |
| J5 | 684 | 680 | 529 | 452 | -12  -32 b | 64  43 b | 14  -5 b | 26  7 b |
| J6 | 661 | 655 | 514 | 507 | 27 | 105 | 49 | 61 |
| J7 | 687 | 683 | 538 | 531 | 14 | 89 | 31 | 44 |
| J8 | 692 | 688 | 541 | 534 | 10 | 85 | 29 | 41 |
| J9 | 723 | 719 | 566 | 560 | -23 | 53 | 2 | 15 |
| J10 | 715 | 711 | 562 | 554 | -12 | 63 | 10 | 22 |
| J11 | 710 | 706 | 558 | 551 | -6 | 69 | 14 | 26 |
| J12 | 660 | 655 | 518 | 511 | 35 | 112 | 47 | 51 |
| J13 | 669 | 665 | 520 | 513 | 20 | 100 | 34 | 54 |
| J14 | 748 | 744 | 585 | 578 | -36 | 40 | -2 | 10 |
| J15 | 757 | 753 | 595 | 588 | -56 | 20 | -21 | -8 |
| J16 | 751 | 752 | 591 | 584 | -39 | 32 | -9 | 3 |
| J17 | 761 | 757 | 601 | 594 | -37 | 39 | -15 | -4 |
| J18 | 757 | 743 | 587 | 580 | -32 | 43 | -3 | 8 |

aRelative to N-H thermodynamic parameter values . bO-H thermodynamic parameter values .

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Molecules | IPFE (kJ/mol) | | | | | | PDFE (kJ/mol) | | | | | |
| **Gas** | **Benzene** | **Toluene** | **methanol** | **Acetonitrile** | **Water** | **Gas** | **Benzene** | **Toluene** | **methanol** | **Acetonitrile** | **Water** |
| J1 | 824 | 653 | 701 | 502 | 509 | 482 | 865 | -86 | 105 | -60 | 79 | -42 |
| J2 | 689 | 529 | 580 | 386 | 393 | 367 | 951 | -15 | 176 | 1 | 140 | 18 |
| J3 | 712 | 549 | 598 | 402 | 409 | 384 | 950 | -41 | 152 | -16 | 123 | 0 |
| 946a | -9 a | 182 a | 22 a | 161 a | 40 a |
| J4 | 734 | 565 | 631 | 418 | 425 | 399 | 910 | -41 | 145 | -26 | 114 | -7 |
| 916 a | -29 a | 162 a | 6 a | 145 a | 25 a |
| J5 | 795 | 624 | 672 | 474 | 481 | 454 | 858 | -92 | 99 | -64 | 75 | -46 |
| 840b | -109 b | 83 b | -80 b | 59 b | -61 b |
| J6 | 763 | 592 | 650 | 458 | 465 | 439 | 903 | -47 | 135 | -30 | 109 | -12 |
| J7 | 787 | 625 | 673 | 483 | 489 | 463 | 894 | -66 | 125 | -48 | 91 | -30 |
| J8 | 795 | 631 | 679 | 484 | 491 | 465 | 886 | -71 | 119 | -53 | 87 | -34 |
| J9 | 835 | 663 | 711 | 512 | 519 | 492 | 843 | -103 | 88 | -79 | 60 | -61 |
| J10 | 823 | 655 | 703 | 507 | 513 | 487 | 859 | -97 | 94 | -70 | 69 | -52 |
| J11 | 817 | 650 | 698 | 503 | 510 | 484 | 866 | -88 | 103 | -65 | 74 | -47 |
| J12 | 754 | 600 | 649 | 464 | 471 | 445 | 924 | -43 | 147 | -31 | 108 | -14 |
| J13 | 776 | 611 | 659 | 466 | 473 | 447 | 904 | -57 | 133 | -38 | 100 | -22 |
| J14 | 851 | 685 | 733 | 529 | 536 | 510 | 840 | -114 | 77 | -80 | 59 | -62 |
| J15 | 870 | 696 | 743 | 537 | 543 | 516 | 815 | -141 | 52 | -98 | 41 | -79 |
| J16 | 863 | 691 | 743 | 536 | 543 | 516 | 829 | -120 | 66 | -89 | 51 | -70 |
| J17 | 872 | 700 | 749 | 546 | 553 | 526 | 833 | -112 | 79 | -95 | 41 | -77 |
| J18 | 859 | 687 | 735 | 532 | 538 | 512 | 836 | -113 | 78 | -83 | 56 | -67 |

**Table 7S**: Thermodynamic energies of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in various media: ionization potential free energies (IPFE) and proton dissociation free energies (PDFE).

aRelative aRelative to N-H PDFE values. b O-H PDFE values

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Molecules | PA (kJ/mol) | | | | ETE (kJ/mol) | | | |
| Benzene | Toluene | methanol | Acetonitrile | Benzene | Toluene | methanol | Acetonitrile |
| J1 | 312 | 380 | 380 | 178 | 396 | 399 | 398 | 392 |
| J2 | 313 | 381 | 381 | 179 | 343 | 346 | 341 | 335 |
| J3 | 340  332 a | 408  401 a | 408  401 a | 205  214 a | 313  344 a | 317  346 a | 314  338 a | 308  332 a |
| J4 | 304  319 a | 372  388 a | 372  388 a | 170  206 a | 355  352 a | 360  355 a | 356  346 a | 350  340 a |
| J5 | 273  253 b | 342  328 b | 342  328 b | 148  136 b | 399  393 b | 402  395 b | 394  387 b | 388  381 b |
| J6 | 312 | 380 | 380 | 174 | 376 | 380 | 389 | 383 |
| J7 | 315 | 383 | 383 | 185 | 386 | 388 | 384 | 379 |
| J8 | 316 | 384 | 384 | 182 | 385 | 388 | 387 | 381 |
| J9 | 290 | 358 | 358 | 159 | 411 | 413 | 409 | 403 |
| J10 | 289 | 358 | 358 | 160 | 413 | 413 | 411 | 405 |
| J11 | 290 | 358 | 358 | 161 | 414 | 413 | 411 | 405 |
| J12 | 307 | 376 | 376 | 177 | 389 | 392 | 388 | 392 |
| J13 | 304 | 372 | 372 | 174 | 385 | 392 | 387 | 381 |
| J14 | 298 | 366 | 366 | 165 | 414 | 417 | 417 | 411 |
| J15 | 228  222c | 296  297c | 296  117c | 112  123c | 473 | 477 | 461 | 455 |
| J16 | 268 | 336 | 336 | 146 | 470 | 447 | 436 | 430 |
| J17 | 260 | 329 | 329 | 140 | 464 | 467 | 445 | 438 |
| J18 | 281 | 353 | 353 | 156 | 434 | 432 | 427 | 421 |

**Table 8S**: Thermodynamic energies of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in various media: proton affinities (PA) and electron transfer enthalpies (ETE).

aRelative to N-H thermochemical parameter values. bO-H thermochemical parameter values

cRelated to H-OOC thermochemical parameter values

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Molecules | PAFE (kJ/mol) | | | | | | ETFE (kJ/mol) | | | | | |
| **Gas** | **Benzene** | **Toluene** | **Methanol** | **Acetonitrile** | **Water** | **Gas** | **Benzene** | **Toluene** | **Methanol** | **Acetonitrile** | **Water** |
| J1 | 1386 | 230 | 414 | 98 | 236 | 109 | 302 | 336 | 391 | 343 | 350 | 330 |
| J2 | 1386 | 233 | 417 | 101 | 239 | 112 | 254 | 282 | 336 | 285 | 293 | 272 |
| J3 | 1414  1412a | 258  258 a | 442  442 a | 126  141 a | 263  279 a | 137  153 a | 247 | 250 | 307 | 259 | 267 | 246 |
| 277 a | 283 a | 337 a | 282 a | 290 a | 270 a |
| J4 | 1379  1385 a | 223  244 a | 407  428 a | 91  132 a | 229  270 a | 102  144 a | 266 | 301 | 351 | 301 | 309 | 289 |
| 265 a | 292 a | 347 a | 292 a | 299 a | 279 a |
| J5 | 1366  1352b | 195  182 b | 379  366 | 71  61 b | 208  199 b | 82  73 b | 309 | 337 | 391 | 339 | 346 | 326 |
| 305 b | 333 b | 388 b | 333 b | 340 b | 320 b |
| J6 | 1410 | 232 | 416 | 95 | 232 | 106 | 278 | 313 | 368 | 333 | 341 | 321 |
| J7 | 1404 | 233 | 417 | 106 | 244 | 117 | 299 | 326 | 381 | 328 | 336 | 315 |
| J8 | 1409 | 237 | 421 | 102 | 239 | 113 | 293 | 321 | 376 | 330 | 337 | 317 |
| J9 | 1385 | 209 | 393 | 78 | 216 | 92 | 316 | 351 | 406 | 355 | 362 | 340 |
| J10 | 1381 | 208 | 392 | 82 | 219 | 93 | 323 | 351 | 406 | 354 | 362 | 341 |
| J11 | 1381 | 208 | 392 | 82 | 220 | 94 | 324 | 354 | 409 | 356 | 363 | 343 |
| J12 | 1395 | 227 | 411 | 99 | 237 | 110 | 305 | 329 | 384 | 333 | 341 | 320 |
| J13 | 1397 | 223 | 408 | 96 | 233 | 107 | 306 | 330 | 384 | 331 | 338 | 318 |
| J14 | 1388 | 216 | 400 | 86 | 224 | 97 | 325 | 355 | 409 | 362 | 370 | 350 |
| J15 | 1311 | 148 | 331 | 35 | 173 | 47 | 396 | 408 | 463 | 403 | 411 | 389 |
| J16 | 1353 | 185 | 369 | 66 | 204 | 78 | 361 | 386 | 440 | 381 | 388 | 367 |
| J17 | 1345 | 180 | 364 | 61 | 199 | 73 | 382 | 408 | 463 | 389 | 393 | 375 |
| J18 | 1345 | 199 | 387 | 77 | 215 | 89 | 349 | 375 | 425 | 371 | 378 | 355 |

**Table 9S**: Thermodynamic energies of Jn (in kJ/mol) at B3LYP/6-31+G(d,p) level in various media: proton affinity free energies (PAFE) and electron transfer free energy (ETFE).

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aRelative to N-H thermodynamic parameter values (PAFE and ETFE). bO-H thermodynamic parameter values (PAFE and ETFE).



**Figure 1S**: Dependence of Experimental and calculated gas phase FT-IR frequencies (cm‐1) at B3LYP/6-31+G(d,p) level.