A New Benchmark Set for Excitation Energy of Charge Transfer States: Systematic Investigation of Coupled-Cluster Type Methods

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| Ammonia-fluor |          |          |          |
|--------------|----------|----------|----------|
| H            | 2.490675 | 0.939499 | -0.000156 |
| N            | 2.085280 | 0.000000 | 0.000003  |
| H            | 2.490739 | -0.469633| 0.813668  |
| H            | 2.490627 | -0.469860| -0.813586 |
| F            | -0.222963| 0.000000 | 0.000001  |
| F            | -1.710402| 0.000000 | 0.000000  |

| Aceton-fluor |          |          |          |
|--------------|----------|----------|----------|
| H            | -2.543489| 0.848415 | -1.328942|
| C            | -1.483454| 0.540423 | -1.289081|
| H            | -0.874751| 1.463810 | -1.326362|
| H            | -1.243732| -0.093252| -2.152254|
| C            | -1.199386| -0.211141| 0.000000 |
| O            | -0.766094| -1.362999| 0.000000 |
| C            | -1.483454| 0.544023 | 1.289082 |
| H            | -1.243732| -0.093253| 2.152254 |
| H            | -0.874757| 1.463813 | 1.326367 |
| H            | -2.543491| 0.848408 | 1.328938 |
| F            | 1.631766 | 0.853847 | 0.000000 |
| F            | 2.139396 | -0.495631| 0.000000 |

| Pyrazine-fluor |          |          |          |
|---------------|----------|----------|----------|
| N             | 0.995753 | 1.433963 | 0.000000 |
| C             | 0.995753 | 0.702894 | 1.137230 |
| C             | 0.995753 | -0.702894| 1.137230 |
| N             | 0.995753 | -1.433963| 0.000000 |
| C             | 0.995753 | -0.702894| -1.137230|
| C             | 0.995753 | 0.702894 | -1.137230|
| H             | 0.995753 | 1.261352 | 2.081529 |
| H             | 0.995753 | -1.261351| 2.081529 |
| H             | 0.995753 | -1.261352| -2.081529|
| H             | 0.995753 | 1.261351 | -2.081529|
| F             | -2.097479| 0.721626 | 0.000000 |
| F             | -2.097479| -0.721626| 0.000000 |
**Table 2: coordinates in Angstrom (cont. 2)**

### Acetone-nitromethane

|   | x     | y     | z     |
|---|-------|-------|-------|
| H | 1.811829 | 0.246785 | 1.837687 |
| C | 2.341053 | 0.546375 | 0.917315 |
| H | 3.348706 | 0.098100 | 0.941832 |
| H | 2.413351 | 1.642596 | 0.878699 |
| C | 1.569262 | 0.038569 | -0.286392 |
| O | 1.118023 | 0.805512 | -1.143722 |
| C | 1.383099 | -1.464592 | -0.377435 |
| H | 0.813573 | -1.715706 | -1.283526 |
| H | 2.363599 | -1.969922 | -0.397032 |
| H | 0.830656 | -1.814945 | 0.510807 |
| C | -1.970874 | 1.149505 | -0.504785 |
| H | -1.152760 | 1.388024 | -1.196400 |
| H | -2.893231 | 0.879281 | -1.034661 |
| H | -2.130317 | 1.966927 | 0.210009 |
| N | -1.514242 | -0.049172 | 0.261983 |
| O | -0.842687 | 0.159540 | 1.295692 |
| O | -1.782949 | -1.169899 | -0.22646 |

### Ammonia-oxigen-difluorid

|   | x     | y     | z     |
|---|-------|-------|-------|
| N | -2.420290 | -0.000734 | -0.132257 |
| H | -1.815288 | -0.803134 | 0.063560 |
| H | -1.818726 | 0.804803 | 0.061262 |
| H | -3.083243 | 0.003070 | 0.647931 |
| O | 0.983746 | 0.000141 | -0.561705 |
| F | 0.656308 | -1.133526 | 0.264727 |
| F | 0.655717 | 1.133681 | 0.264666 |

### Ammonia-pyrazin

|   | x     | y     | z     |
|---|-------|-------|-------|
| N | 0.551070 | 1.435370 | 0.000026 |
| C | 0.551176 | 0.702702 | 1.134927 |
| C | 0.551384 | -0.702642 | 1.134899 |
| N | 0.551493 | -1.435265 | -0.00032 |
| C | 0.551386 | -0.702589 | -1.134927 |
| C | 0.551179 | 0.702756 | -1.134889 |
| H | 0.551093 | 1.259441 | 2.080741 |
| H | 0.551464 | -1.259418 | 2.080691 |
| H | 0.551470 | -1.259320 | -2.080746 |
| H | 0.551098 | 1.259531 | -2.080682 |
| N | -2.516082 | -0.000399 | 0.000002 |
| H | -2.940485 | 0.466335 | -0.807243 |
| H | -2.940280 | -0.932952 | 0.000820 |
| H | -2.940487 | 0.467759 | 0.806414 |
Table 3: coordinates in Angstrom (cont. 3)

Pyrrole-pyrazine (H-bond)

| Atom | X (Å)     | Y (Å)     | Z (Å)      |
|------|-----------|-----------|------------|
| N    | -1.116277 | -0.000150 | 0.019717   |
| C    | -1.840966 | 1.141214  | 0.010095   |
| C    | -3.246427 | 1.141801  | -0.008562  |
| N    | -3.972069 | 0.001043  | -0.018193  |
| C    | -3.248391 | -1.140963 | -0.008585  |
| C    | -1.842932 | -1.142795 | 0.010072   |
| H    | -1.279558 | 2.083082  | 0.017546   |
| H    | -3.807049 | 2.084137  | -0.016006  |
| H    | -3.810634 | -2.082333 | -0.016048  |
| H    | -1.282199 | -2.085066 | 0.017517   |
| N    | 1.906183  | -0.000072 | 0.015242   |
| C    | 2.699989  | 1.126323  | 0.003913   |
| C    | 2.700047  | -1.126427 | 0.003917   |
| C    | 4.034805  | 0.715035  | -0.015132  |
| C    | 4.034842  | -0.715070 | -0.015130  |
| H    | 0.879481  | -0.000601 | 0.029892   |
| H    | 2.260267  | 2.123953  | 0.010185   |
| H    | 2.260376  | -2.124079 | 0.010193   |
| H    | 4.904166  | 1.372849  | -0.027538  |
| H    | 4.904236  | -1.372840 | -0.027534  |

Pyrrole-pyrazine (stacked)

| Atom | X (Å)     | Y (Å)     | Z (Å)     |
|------|-----------|-----------|-----------|
| H    | 2.068365  | -1.554770 | -1.258236 |
| H    | -2.068564 | -1.553940 | -1.258236 |
| H    | 2.068365  | -1.554770 | 1.258236  |
| H    | -2.068564 | -1.553940 | 1.258236  |
| C    | 1.135821  | -1.554583 | -0.697884 |
| C    | -1.136020 | -1.554127 | -0.697884 |
| C    | 1.135821  | -1.554583 | 0.697884  |
| C    | -1.136020 | -1.554127 | 0.697884  |
| N    | -0.000100 | -1.554355 | -1.417402 |
| N    | -0.000100 | -1.554355 | 1.417402  |
| H    | -0.770304 | 1.855801  | -2.114612 |
| H    | -0.770304 | 1.855801  | 2.114612  |
| H    | 1.850809  | 1.855275  | -1.358585 |
| H    | 1.850809  | 1.855275  | 1.358585  |
| H    | 2.130086  | 1.856074  | 0.000000  |
| C    | -0.333285 | 1.855713  | -1.125828 |
| C    | -0.333285 | 1.855713  | 1.125828  |
| C    | 0.985374  | 1.855448  | -0.709235 |
| C    | 0.985374  | 1.855448  | 0.709235  |
| N    | -1.119278 | 1.855871  | 0.000000  |
Table 4: coordinates in Angstrom (cont. 4)

Tetrafluor-ethylene-ethylene (3.5 Å)

|   |   |   |
|---|---|---|
| F | -1.394866 | -1.110938 | -0.741831 |
| F | -1.394866 | 1.110938  | -0.741831 |
| F |  1.394866 | -1.110938 | -0.741831 |
| F |  1.394866 | 1.110938  | -0.741831 |
| C | -0.667784 | 0.000000  | -0.759941 |
| C |  0.667784 | 0.000000  | -0.759941 |
| H | -1.244242 | 0.935429  |  2.658551 |
| H | -1.244242 | -0.935429 |  2.658551 |
| H |  1.244242 | 0.935429  |  2.658551 |
| H |  1.244242 | -0.935429 |  2.658551 |
| C | -0.674558 | 0.000000  |  2.662317 |
| C |  0.674558 | 0.000000  |  2.662317 |

Tetrafluor-ethylene-ethylene (5 Å)

|   |   |   |
|---|---|---|
| F | -1.394866 | -1.110938 | -1.070259 |
| F | -1.394866 | 1.110938  | -1.070259 |
| F |  1.394866 | -1.110938 | -1.070259 |
| F |  1.394866 | 1.110938  | -1.070259 |
| C | -0.667784 | 0.000000  | -1.088369 |
| C |  0.667784 | 0.000000  | -1.088369 |
| H | -1.244242 | 0.935429  |  3.830123 |
| H | -1.244242 | -0.935429 |  3.830123 |
| H |  1.244242 | 0.935429  |  3.830123 |
| H |  1.244242 | -0.935429 |  3.830123 |
| C | -0.674558 | 0.000000  |  3.833889 |
| C |  0.674558 | 0.000000  |  3.833889 |
| system            | Assignment of the excitation | Excitation energy / eV | TheoDORE characters |
|-------------------|-------------------------------|-----------------------|---------------------|
| ammonia-fluorine  | 1 A' → 1 → 2 (1)             | 4.28                  | 1.26                |
|                   |                               | 4.08                  | 1.34                |
|                   |                               | 4.06                  | 1.50                |
|                   |                               | 4.00                  | 1.55                |
|                   |                               | 3.99                  | 1.71                |
|                   |                               | 4.00                  | 1.97                |
|                   |                               | 3.97                  | 4.07                |
|                   |                               | 4.07                  | 4.27                |
|                   |                               | 4.13                  | 1.26                |
|                   |                               | 4.15                  | 1.01                |
| acetone-fluorine  | 2 A' → 2                    | 4.43                  | 1.26                |
|                   |                               | 4.27                  | 1.34                |
|                   |                               | 4.23                  | 1.50                |
|                   |                               | 4.20                  | 1.55                |
|                   |                               | 4.19                  | 1.71                |
|                   |                               | 4.20                  | 1.97                |
|                   |                               | 4.20                  | 1.97                |
|                   |                               | 4.20                  | 4.07                |
|                   |                               | 4.20                  | 4.27                |
|                   |                               | 4.15                  | 1.26                |
| pyrazine-fluorine | 2 A' → 2                    | 5.18                  | 1.26                |
|                   |                               | 6.28                  | 1.34                |
|                   |                               | 6.10                  | 1.50                |
|                   |                               | 5.83                  | 1.55                |
|                   |                               | 5.90                  | 1.71                |
|                   |                               | 5.85                  | 1.97                |
|                   |                               | 5.85                  | 4.07                |
|                   |                               | 5.85                  | 4.27                |
|                   |                               | 5.13                  | 1.26                |
| ammonia-difluoride| 2 A' → 2                    | 4.44                  | 1.26                |
|                   |                               | 4.22                  | 1.34                |
|                   |                               | 4.18                  | 1.50                |
|                   |                               | 4.18                  | 1.55                |
|                   |                               | 4.17                  | 1.71                |
|                   |                               | 4.17                  | 1.71                |
|                   |                               | 4.17                  | 1.97                |
|                   |                               | 4.17                  | 1.97                |
|                   |                               | 4.17                  | 4.07                |
|                   |                               | 4.17                  | 4.27                |
|                   |                               | 4.15                  | 1.26                |
| acetone-          | 1 A → 1 → 2 (1)             | 3.80                  | 1.26                |
| nitromethane      |                               | 4.44                  | 1.34                |
|                   |                               | 4.42                  | 1.50                |
|                   |                               | 4.41                  | 1.55                |
|                   |                               | 4.40                  | 1.71                |
|                   |                               | 4.40                  | 1.71                |
|                   |                               | 4.40                  | 1.97                |
|                   |                               | 4.40                  | 1.97                |
|                   |                               | 4.40                  | 4.07                |
|                   |                               | 4.40                  | 4.27                |
| ammonia-pyrazine  | 1 A → 1 → 2 (1)             | 4.98                  | 1.26                |
|                   |                               | 5.05                  | 1.34                |
|                   |                               | 5.05                  | 1.50                |
|                   |                               | 4.97                  | 1.55                |
|                   |                               | 4.95                  | 1.71                |
|                   |                               | 4.93                  | 1.71                |
|                   |                               | 4.93                  | 1.97                |
|                   |                               | 4.93                  | 1.97                |
|                   |                               | 4.93                  | 4.07                |
|                   |                               | 4.93                  | 4.27                |
| pyrrole-pyrazine  (H3 bond) | 1 A → 1 → 2 (1) | 7.23                  | 1.26                |
|                   |                               | 7.13                  | 1.34                |
|                   |                               | 7.14                  | 1.50                |
|                   |                               | 7.03                  | 1.55                |
|                   |                               | 7.04                  | 1.71                |
|                   |                               | 7.04                  | 1.71                |
|                   |                               | 7.04                  | 1.97                |
|                   |                               | 7.04                  | 1.97                |
|                   |                               | 7.04                  | 4.07                |
|                   |                               | 7.04                  | 4.27                |
| pyrrole-pyrazine  (stacked) | 1 A → 1 → 2 (1) | 4.34                  | 1.26                |
|                   |                               | 4.49                  | 1.34                |
|                   |                               | 4.48                  | 1.50                |
|                   |                               | 4.48                  | 1.55                |
|                   |                               | 4.48                  | 1.71                |
|                   |                               | 4.48                  | 1.71                |
|                   |                               | 4.48                  | 1.97                |
|                   |                               | 4.48                  | 1.97                |
|                   |                               | 4.48                  | 4.07                |
|                   |                               | 4.48                  | 4.27                |
| tetrafluoro-      | 1 A → 1 → 2 (1)             | 5.07                  | 1.26                |
| ethylene-         |                               | 5.60                  | 1.34                |
| ethylene-         |                               | 5.80                  | 1.50                |
| ethylene          |                               | 5.25                  | 1.55                |
|                 |                               | 5.27                  | 1.71                |
|                 |                               | 5.27                  | 1.71                |
|                 |                               | 5.27                  | 1.97                |
|                 |                               | 5.27                  | 1.97                |
|                 |                               | 5.27                  | 4.07                |
|                 |                               | 5.27                  | 4.27                |
| ethylene-         | 1 A → 1 → 2 (1)             | 5.93                  | 1.26                |
| ethylene-         |                               | 6.47                  | 1.34                |
| ethylene          |                               | 6.55                  | 1.50                |
|                 |                               | 6.14                  | 1.55                |
|                 |                               | 6.17                  | 1.71                |
|                 |                               | 6.17                  | 1.71                |
|                 |                               | 6.17                  | 1.97                |
|                 |                               | 6.17                  | 1.97                |
|                 |                               | 6.17                  | 4.07                |
|                 |                               | 6.17                  | 4.27                |
| tetrafluoro-      | 1 A → 1 → 2 (1)             | 4.18                  | 1.26                |
| ethylene-         |                               | 4.44                  | 1.34                |
| ethylene-         |                               | 4.44                  | 1.50                |
| ethylene          |                               | 4.44                  | 1.55                |
|                 |                               | 4.44                  | 1.71                |
|                 |                               | 4.44                  | 1.71                |
|                 |                               | 4.44                  | 1.97                |
|                 |                               | 4.44                  | 1.97                |
|                 |                               | 4.44                  | 4.07                |
|                 |                               | 4.44                  | 4.27                |
| tetrafluoro-      | 1 A → 1 → 2 (1)             | 5.05                  | 1.26                |
| ethylene-         |                               | 5.08                  | 1.34                |
| ethylene-         |                               | 5.33                  | 1.50                |
| ethylene          |                               | 5.33                  | 1.55                |
|                 |                               | 5.33                  | 1.71                |
|                 |                               | 5.33                  | 1.71                |
|                 |                               | 5.33                  | 1.97                |
|                 |                               | 5.33                  | 1.97                |
|                 |                               | 5.33                  | 4.07                |
|                 |                               | 5.33                  | 4.27                |
| tetrafluoro-      | 1 A → 1 → 2 (1)             | 5.93                  | 1.26                |
| ethylene-         |                               | 6.47                  | 1.34                |
| ethylene-         |                               | 6.55                  | 1.50                |
| ethylene          |                               | 6.14                  | 1.55                |
|                 |                               | 6.17                  | 1.71                |
|                 |                               | 6.17                  | 1.71                |
|                 |                               | 6.17                  | 1.97                |
|                 |                               | 6.17                  | 1.97                |
|                 |                               | 6.17                  | 4.07                |
|                 |                               | 6.17                  | 4.27                |