
FOUNDATIONS
ADVANCES

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**Supporting information for article:**

# Fast analytical evaluation of intermolecular electrostatic interaction energies using the pseudoatom representation of the electron density. III. Application to crystal structures via the Ewald and direct summation methods

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# Supporting information

**Table S1** Crystallographic data for the benchmark systems.

| | **ACG**[1] | **BENZ**[2] | **LAC**[3] | **LDOPA**[4] | **PARA**[5] |
|---|---|---|---|---|---|
| CSD code | ACYGLY11 | BENZEN | YILLAG | LDOPAS03 | HXACAN13 |
| Formula | $C_4H_7NO_3$ | $C_6H_6$ | $C_3H_6O_3$ | $C_9H_{11}NO_4$ | $C_8H_9NO_2$ |
| Space group | $P2_1/c$ | Pbca | $P2_12_12_1$ | $P2_1$ | $P2_1/a$ |
| *a* | 4.859 | 7.440 | 5.490 | 13.619 | 12.667 |
| *b* (Å) | 11.546 | 9.550 | 8.422 | 5.232 | 9.166 |
| *c* | 9.811 | 6.920 | 9.345 | 6.062 | 7.073 |
| α | 90 | 90 | 90 | 90 | 90 |
| β (°) | 97.060 | 90 | 90 | 97.56 | 115.51 |
| γ | 90 | 90 | 90 | 90 | 90 |
| *V* (Å$^3$) | 546.2 | 491.7 | 432.1 | 428.2 | 741.2 |
| *Z* | 4 | 4 | 4 | 2 | 4 |

| | **ABA**[6] | **ALA**[7] | **GLY**[8] | **SER**[9] | **VAL**[10] |
|---|---|---|---|---|---|
| CSD code | GAMBUT02 | LALNIN03 | GLYCIN85 | LSERIN01 | VALIDL02 |
| Formula | $C_4H_9NO_2$ | $C_3H_7NO_2$ | $C_2H_5NO_2$ | $C_3H_7NO_3$ | $C_2H_{11}NO_2$ |
| Space group | $P2_1/a$ | $P2_12_12_1$ | $P2_1/n$ | $P2_12_12_1$ | $P\bar{1}$ |
| *a* | 8.214 | 5.928 | 5.087 | 8.599 | 5.222 |
| *b* (Å) | 10.000 | 12.260 | 11.773 | 9.348 | 5.406 |
| *c* | 7.208 | 5.794 | 5.460 | 5.618 | 10.838 |
| α | 90 | 90 | 90 | 90 | 90.89 |
| β (°) | 110.59 | 90 | 111.99 | 90 | 92.34 |
| γ | 90 | 90 | 90 | 90 | 110.02 |
| *V* (Å$^3$) | 554.2 | 421.1 | 303.2 | 451.6 | 287.1 |
| *Z* | 4 | 4 | 4 | 4 | 2 |

[1] Mackay, 1975; standard crystallographic settings, originally reported unit cell is 4.859 Å, 11.546 Å, 14.633 Å, 90°, 138.29°, 90°.

[2] Bacon, Curry & Wilson, 1964

[3] Schouten, Kanters & Krieken, 1994

[4] Howard *et al.*, 1995

[5] Wilson, 2000

[6] Weber, Craven & McMullan, 1983

[7] Destro, Marsh & Bianchi, 1988

[8] Destro *et al.*, 2000

[9] Kistenmacher, Rand & Marsh, 1974

[10] Dalhus & Görbitz, 1996

**Table S2** Electrostatic interaction energies (kJ/mol) for the individual multipolar terms from the DS/aMM (first row; $R_{\text{DS cutoff}}$ = 300 Å) and ES/aMM (second row) calculations for all the small-molecule benchmark systems.

| | | ACG | BENZ | LAC | LDOPA | PARA | ABA | ALA | GLY | SER | VAL |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Interactions involving monopoles (M) and dipoles (D) only** | **M-M** | -8.91863262 | -3.81766106 | -12.86873414 | -112.04801966 | -9.20914481 | -159.49707908 | -118.09477935 | -118.60964175 | -129.03444119 | -111.59391134 |
| | | -8.91868741 | -3.81766101 | -12.86829403 | -112.04619992 | -9.20922800 | -159.46944974 | -118.11080761 | -118.63684329 | -129.02068032 | -111.59848296 |
| | **M-D** | -29.47829738 | 28.04224602 | -35.39004786 | -61.65454380 | -38.60937838 | -75.85196984 | -78.08443165 | -65.89087531 | -89.70921258 | -69.70288856 |
| | | -29.47836276 | 28.04224565 | -35.38917660 | -61.65449859 | -38.60879125 | -75.84577522 | -78.09041189 | -65.90083245 | -89.70112853 | -69.70475744 |
| | **D-D** | -18.50599044 | -49.92567967 | -29.66074415 | -52.78145748 | -28.31073533 | -12.40889387 | -7.18905041 | -10.28614827 | -23.88005426 | -11.32864910 |
| | | -18.50599523 | -49.92567897 | -29.66042482 | -52.78149793 | -28.30994842 | -12.40843168 | -7.18967505 | -10.28721427 | -23.87879914 | -11.32883318 |
| **Interactions involving quadrupoles (Q)** | **M-Q** | 2.70443415 | -9.93826163 | 3.91524886 | 6.16924399 | 8.89508324 | 14.81740676 | 15.72851855 | 5.62649572 | 7.27480351 | 8.29448228 |
| | | 2.70443540 | -9.93826149 | 3.91524839 | 6.16925284 | 8.89508993 | 14.81742029 | 15.72852161 | 5.62649668 | 7.27481234 | 8.29448282 |
| | **D-Q** | -2.85742377 | 33.54210484 | 4.51417570 | 23.85716028 | 2.33879915 | 0.74346747 | -7.32077948 | -6.02041705 | 5.48353381 | -1.44124730 |
| | | -2.85742361 | 33.54210433 | 4.51417384 | 23.85716300 | 2.33880432 | 0.74346701 | -7.32078003 | -6.02041643 | 5.48353789 | -1.44124701 |
| | **Q-Q** | 4.75308242 | -5.14285317 | 1.40145229 | -3.43194696 | 3.78813382 | 4.96849535 | 5.59355727 | 6.28523639 | 0.08933372 | 4.20947853 |
| | | 4.75308241 | -5.14285307 | 1.40145228 | -3.43194716 | 3.78813371 | 4.96849534 | 5.59355730 | 6.28523640 | 0.08933372 | 4.20947855 |
| **Interactions involving octupoles (O)** | **M-O** | -1.29999385 | 0.36698428 | 0.21857847 | -1.02624656 | -1.25591781 | 8.93937123 | 5.16001519 | 4.09499270 | 6.75139304 | 3.09428792 |
| | | -1.29999385 | 0.36698428 | 0.21857844 | -1.02624649 | -1.25591781 | 8.93937131 | 5.16001520 | 4.09499257 | 6.75139307 | 3.09428777 |
| | **D-O** | -2.45472299 | -1.79579262 | -0.40066845 | -1.49222518 | -3.14257605 | 1.41332529 | -2.32032034 | -2.37003496 | 5.94765628 | -3.09703020 |
| | | -2.45472299 | -1.79579262 | -0.40066847 | -1.49222518 | -3.14257605 | 1.41332530 | -2.32032035 | -2.37003500 | 5.94765628 | -3.09703024 |
| | **Q-O** | 2.82282859 | 0.89673479 | -0.06654613 | 1.95216898 | 1.48322268 | 2.11390430 | 4.37859497 | 4.54205095 | -2.92122727 | 4.69186298 |
| | | 2.82282859 | 0.89673479 | -0.06654613 | 1.95216898 | 1.48322268 | 2.11390430 | 4.37859497 | 4.54205095 | -2.92122727 | 4.69186298 |
| | **O-O** | -1.12648590 | 0.04134159 | 0.38200178 | -0.00343326 | -0.33864445 | -0.29269105 | 0.35633325 | 0.11912223 | -1.26649039 | 0.57568481 |
| | | -1.12648590 | 0.04134159 | 0.38200178 | -0.00343326 | -0.33864445 | -0.29269105 | 0.35633325 | 0.11912223 | -1.26649039 | 0.57568481 |
| **Interactions involving hexadecapoles (H)** | **M-H** | 0.06653978 | -0.23481120 | -0.31908021 | 1.65722468 | 0.00757743 | 0.80363037 | 1.37228373 | 1.88292424 | 0.57349207 | 2.60080489 |
| | | 0.06653978 | -0.23481120 | -0.31908021 | 1.65722468 | 0.00757743 | 0.80363037 | 1.37228373 | 1.88292424 | 0.57349207 | 2.60080489 |
| | **D-H** | -0.50234452 | 1.12219117 | 0.02367041 | 0.37408444 | 1.16194865 | -0.07393367 | 0.13744369 | 0.10519078 | -0.50254554 | 0.28407468 |
| | | -0.50234452 | 1.12219117 | 0.02367041 | 0.37408444 | 1.16194865 | -0.07393367 | 0.13744369 | 0.10519078 | -0.50254554 | 0.28407468 |
| | **Q-H** | 0.50876642 | -0.56147032 | -0.15805768 | 0.31079765 | -0.86056414 | 0.87427729 | 0.26256168 | 0.26010576 | 0.31410704 | -0.33797081 |
| | | 0.50876642 | -0.56147032 | -0.15805768 | 0.31079765 | -0.86056414 | 0.87427729 | 0.26256168 | 0.26010576 | 0.31410704 | -0.33797081 |
| | **O-H** | 0.06414855 | -0.12631477 | -0.03543382 | -0.27046928 | -0.14292541 | 0.06013713 | -0.00059629 | 0.27491959 | 0.01334528 | 0.46840227 |
| | | 0.06414855 | -0.12631477 | -0.03543382 | -0.27046928 | -0.14292541 | 0.06013713 | -0.00059629 | 0.27491959 | 0.01334528 | 0.46840227 |
| | **H-H** | -0.04014342 | -0.01426239 | -0.03507946 | 0.02593193 | -0.00357719 | 0.04771998 | 0.05193381 | 0.24209525 | 0.03694305 | 0.20140992 |
| | | -0.04014342 | -0.01426239 | -0.03507946 | 0.02593193 | -0.00357719 | 0.04771998 | 0.05193381 | 0.24209525 | 0.03694305 | 0.20140992 |

## S1. References


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