
FOUNDATIONS
ADVANCES

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**Supporting information for article:**

# A universal algorithm for finding the shortest distance between systems of points

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**Table S1** The deviations ($E$, Å$^2$) of 2,5-dihydroxyterephthalate $C_8H_2O_6^{4-}$, terephthalate $C_8H_4O_4^{2-}$ and hexahydroterephthalate $C_8H_{10}O_4^{2-}$ ligands in coordination compounds. The reference ligand is italicized.

| Reference Code/N* | $E$, Å$^2$ | Reference Code/N* | $E$, Å$^2$ | $E$, Å$^2$ |
|---|---|---|---|---|
| $C_8H_2O_6^{4-}$ | *COKNIB01* | $C_8H_{10}O_4^{2-}$ | *Trans-isomer R1 (EDUVEF/3)* | *Cis-isomer R2 (KATVIL)* |
| COKNIB | 0.002 | BEKLUB | 0.063 | 0.762 |
| COKNIB01 | 0.000 | BEKMAI | 0.008 | 0.609 |
| COKNOH | 0.046 | ECEZES | 0.004 | 0.615 |
| COKNUN | 0.044 | EDUVEF/1 | 0.051 | 0.674 |
| COKNUN01 | 0.042 | EDUVEF/2 | 0.111 | 0.606 |
| LECQEQ | 0.045 | EDUVEF/3 | 0.000 | 0.636 |
| OLEYAH | 0.012 | EDUVEF/4 | 0.018 | 0.695 |
| OZUKOL | 0.051 | EMECOO | 0.001 | 0.639 |
| OZUKUR | 0.048 | FAGSUC | 0.082 | 0.601 |
| OZULUS | 0.010 | FORWUF/1 | 0.016 | 0.602 |
| OZUMAZ | 0.007 | FORWUF/2 | 0.002 | 0.630 |
| SATNOR | 0.046 | FORWUF/3 | 0.026 | 0.600 |
| VAMPOR | 0.046 | JECDUR | 0.209 | 0.726 |
| WOBHIF | 0.032 | JEYZUJ/1 | 0.003 | 0.648 |
| WOQTUT | 0.046 | JEYZUJ/2 | 0.003 | 0.642 |
| $C_8H_4O_4^{2-}$ | *HAZGOF10/1* | KATVIL | 0.636 | 0.000 |
| AVOFUM | 0.034 | KCYHXC10 | 0.035 | 0.621 |
| BADHUM/1 | 0.001 | KELKUK | 0.562 | 0.197 |
| BADHUM/2 | 0.031 | KICROG | 0.315 | 0.146 |
| EHAZES | 0.046 | LIBJAJ/1 | 0.020 | 0.610 |
| HAZGOF10/1 | 0.000 | LIBJAJ/2 | 0.013 | 0.695 |
| HAZGOF10/2 | 0.034 | RIHJIC/1 | 0.113 | 0.602 |
| MAQDUD | 0.003 | RIHJIC/2 | 0.012 | 0.682 |

| | | | | |
|---|---|---|---|---|
| NEZSOD | 0.004 | RIHJIC/3 | 0.052 | 0.671 |
| POXLEV/1 | 0.075 | RIHJIC/4 | 0.052 | 0.671 |
| POXLEV/2 | 0.004 | RIHJIC/5 | 0.000 | 0.643 |
| PTRPHT02 | 0.002 | SIWGUB/1 | 0.027 | 0.698 |
| QQQDHD01 | 0.039 | SIWGUB/2 | 0.014 | 0.627 |
| QQQDHD02 | 0.010 | SIWHAI | 0.615 | 0.004 |
| RUBZIY | 0.038 | SUNDIP | 0.539 | 0.063 |
| SAXZIA | 0.045 | | | |
| SEVROC | 0.070 | | | |
| TAJTAC/1 | 0.001 | | | |
| TAJTAC/2 | 0.039 | | | |
| TAJTIK/1 | 0.003 | | | |
| TAJTIK/2 | 0.034 | | | |
| YOQYIO | 0.005 | | | |
| ZUBKEO/1 | 0.070 | | | |
| ZUBKEO/2 | 0.014 | | | |

* N is the number of a symmetrically inequivalent ligand in the structure with a given reference code.

**Table S2** The deviations ($E$) of coordination networks with the diamond underlying topology. All unit cells were reduced to the volume of the diamond unit cell (45.385 Å$^3$).

| Composition | Reference Code | $E$, Å$^2$ | Composition | Reference Code | $E$, Å$^2$ |
|---|---|---|---|---|---|
| $C_{10}H_{20}CaO_{15}V$ | FUTQAO | 1.649 | $C_{12}H_{30}O_{26}Tb_2$ | WEMFEB | 0.990 |
| $C_{12}H_{30}Dy_2O_{26}$ | WEMFIF | 0.990 | $C_{12}H_{30}O_{26}Yb_2$ | WEMCAU | 0.963 |
| $C_{12}H_{30}Er_2O_{26}$ | WEMBUN | 0.976 | $C_{20}H_{28}InO_8$ | ISOJOQ | 1.163 |
| $C_{12}H_{30}Eu_2O_{26}$ | WEMDUP | 1.002 | $C_{30}H_{26}CdO_6$ | VOTZEL | 1.315 |
| $C_{12}H_{30}Gd_2O_{26}$ | WEMFAX | 1.002 | $C_{30}H_{26}MnO_6$ | QOZYUA | 1.217 |
| $C_{12}H_{30}Ho_2O_{26}$ | WEMFOL | 0.978 | | QOZYUA01 | 1.232 |
| $C_{12}H_{30}Nd_2O_{26}$ | WEMDID | 1.032 | | QOZYUA02 | 1.239 |
| $C_{12}H_{30}O_{26}Sm_2$ | WEMDOJ | 1.015 | | QOZYUA03 | 1.217 |