FOX7 and Trans-FOX7

(Last updated 16 January 2025)



Figure . The molecular diagram of (left) 1,1-diamino-2,2-dinitroethene and (right) (Z)-1,2-diamino-1,2-dinitroethene.

There are phase transitions at 389 and 446 K.

# CSP studies

|  |  |
| --- | --- |
| REFCODE | SEDTUQ |
| Formula | C2 H4 N4 O4 |
| Common Name | FOX-7 |
| IUPAC Systematic Name | 1,1-diamino-2,2-dinitroethene |
| CSD Refcodes | SEDTUQ30, SEDTUQ26, SEDTUQ25, SEDTUQ33 |
| Scientist | Sally Price |
| Date | 2008 |
| Publication | No publication planned. |
|  |  |
| Search Identifier | A |
| Energy Model | 1 |
| Study\_ID | 0 |
| Programs | MOLPAK, DMAREL (4.1.1) |
| Location on S Drive | \CHEMISTRY\_CPOSS\FOX7\ConOpt |
| Potential Description | GDMA2(MP2 6-31G(d,p)) + FIT |
| Search Identifier | B |
| Energy Model | 1 |
| Study\_ID | 1 |
| Programs | MOLPAK, DMACRYS (2.0.1) |
| Location on S Drive | \CHEMISTRY\_CPOSS\FOX7\Opt |
| Potential Description | GDMA2(MP2 6-31G(d,p)) + FIT |
|  |  |
| REFCODE | TRFOXS |
| Formula | C2 H4 N4 O4 |
| Common Name | TransFOX-7 |
| IUPAC Systematic Name | (Z)-1,2-diamino-1,2-dinitroethene |
| CSD Refcodes | N/A |
| Scientist | Sally Price |
| Date | 2008 |
| Publication | No publication planned. |
|  |  |
| Search Identifier | A |
| Energy Model | 1 |
| Study\_ID | 0 |
| Programs | MOLPAK, DMACRYS (2.0.1) |
| Location on S Drive | \CHEMISTRY\_CPOSS\FOX7\TransSearch |
| Potential Description | GDMA2(MP2 6-31G(d,p)) + FIT |

A screen shot of a graph

Description automatically generatedA chart with many small colored squares

Description automatically generated with medium confidenceA screen shot of a computer screen

Description automatically generated

Figure . Crystal energy landscape of FOX7 with the unconstrained optimized conformation, Trans-FOX7 with the unconstrained optimized conformation and FOX7 with the conformation constrained to have planar NH2 groups.

# CSD structures (CSD version 5.43 with Mar, Jun, Sep and Nov 2022 updates)

Table . Crystallographic information for CSD entries for XXX. Different polymorphs are coloured differently.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| REFCODE | space group | Z’ | a / Å | b / Å | c / Å | α / ° | β / ° | γ / ° | density / g cm-3 | Form |
| SEDTUQ | P21/n | 1 | 6.941 | 6.569 | 11.315 | 90 | 90.55 | 90 | 1.907 | alpha |
| SEDTUQ01 | P21/n | 1 | 6.9396 | 6.6374 | 11.3406 | 90 | 90.611 | 90 | 1.883 | alpha |
| SEDTUQ02 | P21/n | 1 | 6.9209 | 6.5515 | 11.2741 | 90 | 90.06 | 90 | 1.924 | alpha |
| SEDTUQ03 | P21/n | 1 | 6.934 | 6.6228 | 11.3119 | 90 | 90.065 | 90 | 1.893 | alpha |
| SEDTUQ04 | P21/n | 1 | 6.9414 | 6.6534 | 11.3316 | 90 | 90.082 | 90 | 1.879 | alpha |
| SEDTUQ05 | P21/n | 1 | 6.9467 | 6.6887 | 11.35 | 90 | 90.143 | 90 | 1.865 | alpha |
| SEDTUQ06 | P212121 | 1 | 6.9738 | 6.635 | 11.6475 | 90 | 90 | 90 | 1.825 | beta |
| SEDTUQ07 | P212121 | 1 | 6.972 | 6.663 | 11.666 | 90 | 90 | 90 | 1.815 | beta |
| SEDTUQ08 | P212121 | 1 | 6.974 | 6.675 | 11.673 | 90 | 90 | 90 | 1.81 | beta |
| SEDTUQ09 | P21/n | 1 | 6.922 | 6.501 | 11.262 | 90 | 90.485 | 90 | 1.941 | alpha |
| SEDTUQ10 | P212121 | 1 | 6.66 | 6.985 | 11.672 | 90 | 90 | 90 | 1.811 | beta |
| SEDTUQ11 | P21/n | 1 | 6.922 | 6.501 | 11.262 | 90 | 90.485 | 90 | 1.941 | alpha |
| SEDTUQ12 | P21/n | 1 | 6.9295 | 6.5301 | 11.275 | 90 | 90.53 | 90 | 1.928 | alpha |
| SEDTUQ13 | P21/n | 1 | 6.7118 | 6.0361 | 10.9581 | 90 | 90.077 | 90 | 2.215 | a' |
| SEDTUQ15 | P21/n | 1 | 6.9129 | 6.4872 | 11.2465 | 90 | 90.4816 | 90 | 1.95 | alpha |
| SEDTUQ16 | P21/n | 1 | 6.9146 | 6.4963 | 11.252 | 90 | 90.49 | 90 | 1.946 | alpha |
| SEDTUQ17 | P21/n | 1 | 6.9165 | 6.5072 | 11.2575 | 90 | 90.4987 | 90 | 1.941 | alpha |
| SEDTUQ18 | P21/n | 1 | 6.9184 | 6.5187 | 11.2646 | 90 | 90.5108 | 90 | 1.936 | alpha |
| SEDTUQ19 | P21/n | 1 | 6.9209 | 6.5336 | 11.2726 | 90 | 90.5215 | 90 | 1.93 | alpha |
| SEDTUQ20 | P21/n | 1 | 6.9254 | 6.5582 | 11.2866 | 90 | 90.5441 | 90 | 1.919 | alpha |
| SEDTUQ21 | P21/n | 1 | 6.9303 | 6.5873 | 11.3017 | 90 | 90.5672 | 90 | 1.906 | alpha |
| SEDTUQ22 | P21/n | 1 | 6.935 | 6.619 | 11.3172 | 90 | 90.5886 | 90 | 1.893 | alpha |
| SEDTUQ23 | P21/n | 1 | 6.9413 | 6.6532 | 11.3353 | 90 | 90.608 | 90 | 1.879 | alpha |
| SEDTUQ24 | P21/n | 1 | 6.9484 | 6.6942 | 11.3547 | 90 | 90.618 | 90 | 1.862 | alpha |
| SEDTUQ25 | P21/n | 2 | 13.354 | 6.895 | 12.05 | 90 | 111.102 | 90 | 1.9 | gamma |
| SEDTUQ26 | P212121 | 1 | 6.986 | 6.686 | 11.687 | 90 | 90 | 90 | 1.802 | beta |
| SEDTUQ27 | P21/n | 1 | 6.922 | 6.501 | 11.262 | 90 | 90.485 | 90 | 1.941 | alpha |
| SEDTUQ28 | P21/n | 1 | 6.922 | 6.501 | 11.262 | 90 | 90.485 | 90 | 1.941 | alpha |
| SEDTUQ29 | P21/n | 1 | 6.922 | 6.501 | 11.262 | 90 | 90.485 | 90 | 1.941 | alpha |
| SEDTUQ30 | P21/n | 1 | 6.922 | 6.501 | 11.262 | 90 | 90.485 | 90 | 1.941 | alpha |
| SEDTUQ31 | P212121 | 1 | 6.986 | 6.671 | 11.681 | 90 | 90 | 90 | 1.807 | gamma |
| SEDTUQ32 | P212121 | 1 | 6.986 | 6.66 | 11.674 | 90 | 90 | 90 | 1.811 | beta |
| SEDTUQ33 | P1 | 2 | 6.0745 | 6.6924 | 6.6972 | 119.505 | 93.913 | 110.042 | 2.308 | polymorph |
| SEDTUQ34 | P1 | 2 | 6.0745 | 6.6924 | 6.6972 | 119.505 | 93.913 | 110.042 | 2.308 | polymorph |
| SEDTUQ35 | P21/n | 1 | 6.948 | 6.6364 | 11.3413 | 90 | 90.569 | 90 | 1.881 |  |
| SEDTUQ36 | P21/n | 1 | 6.8931 | 6.5058 | 11.2567 | 90 | 90.48 | 90 | 1.948 |  |
| SEDTUQ37 | P21/n | 1 | 6.8358 | 6.3591 | 11.163 | 90 | 90.314 | 90 | 2.027 |  |
| SEDTUQ38 | P21/n | 1 | 6.822 | 6.3249 | 11.1378 | 90 | 90.263 | 90 | 2.047 |  |
| SEDTUQ39 | P21/n | 1 | 6.8011 | 6.2779 | 11.1042 | 90 | 90.249 | 90 | 2.075 |  |
| SEDTUQ40 | P21/n | 1 | 6.7982 | 6.2473 | 11.1067 | 90 | 90.215 | 90 | 2.085 |  |
| SEDTUQ41 | P21/n | 1 | 6.7789 | 6.7789 | 11.0632 | 90 | 90.2 | 90 | 1.935 |  |
| SEDTUQ42 | P21/n | 1 | 6.7562 | 6.1435 | 11.0371 | 90 | 90.166 | 90 | 2.147 |  |
| SEDTUQ43 | P21/n | 1 | 6.7472 | 6.1083 | 11.0236 | 90 | 90.141 | 90 | 2.165 |  |
| SEDTUQ44 | P21/n | 1 | 6.7111 | 6.0339 | 10.9621 | 90 | 90.086 | 90 | 2.216 |  |
| SEDTUQ45 | P1 | 2 | 5.9859 | 6.6716 | 6.6854 | 119.463 | 94.11 | 110.145 | 2.358 |  |
| SEDTUQ46 | P1 | 2 | 5.8965 | 6.6394 | 6.6545 | 119.395 | 94.308 | 110.262 | 2.421 |  |
| SEDTUQ47 | P1 | 2 | 5.8695 | 6.6197 | 6.6343 | 119.409 | 94.338 | 110.317 | 2.449 |  |
| SEDTUQ48 | P1 | 2 | 5.7268 | 6.603 | 6.6195 | 119.381 | 94.429 | 110.739 | 2.534 |  |
| SEDTUQ49 | P1 | 2 | 5.6947 | 6.5793 | 6.5961 | 119.356 | 94.461 | 110.881 | 2.57 |  |

Table . Experimental information for CSD entries for XXX.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| REFCODE | space group | R factor | T / K | Year | Comments |
| SEDTUQ | P21/n | 3.12 | 173 | 1998 | Crystallized from cold N,N-dimethylformamide1 |
| SEDTUQ01 | P21/n | 3.02 | 295 | 1999 | Private communication |
| SEDTUQ02 | P21/n | 3.61 | 200 | 2006 | Slow cooling from DMF or DMSO; Oxford Cryosystems temperature controller on diffractometer2 |
| SEDTUQ03 | P21/n | 4.02 | 298 | 2006 | Slow cooling from DMF or DMSO; Oxford Cryosystems temperature controller on diffractometer2 |
| SEDTUQ04 | P21/n | 4.1 | 333 | 2006 | Slow cooling from DMF or DMSO; Oxford Cryosystems temperature controller on diffractometer2 |
| SEDTUQ05 | P21/n | 5.42 | 373 | 2006 | Slow cooling from DMF or DMSO; Oxford Cryosystems temperature controller on diffractometer2 |
| SEDTUQ06 | P212121 | 3.59 | 393 | 2006 | Slow cooling from DMF or DMSO; Oxford Cryosystems temperature controller on diffractometer2 |
| SEDTUQ07 | P212121 | 12.3 | 403 | 2006 | Powder data; finely ground2 |
| SEDTUQ08 | P212121 | 12.4 | 423 | 2006 | Powder data; finely ground2 |
| SEDTUQ09 | P21/n | 2.1 | 100 | 2008 | Synchrotron radiation; recrystallized from 2-propanol3 |
| SEDTUQ10 | P212121 | 4.08 | 400 | 2012 | Private communication |
| SEDTUQ11 | P21/n | 2.14 | 100 | 2016 | Re-refinement of data collected in SEDTUQ094 |
| SEDTUQ12 | P21/n | 3.92 | 153 | 2018 | Crystallized concomitantly with phenanthroline cocrystal5 |
| SEDTUQ13 | P21/n | 11.04 | 293 | 2016 | Synchrotron; Grown from DMSO solution6 |
| SEDTUQ15 | P21/n | 2.67 | 80 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ16 | P21/n | 2.61 | 100 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ17 | P21/n | 2.79 | 120 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ18 | P21/n | 2.99 | 140 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ19 | P21/n | 3.09 | 164 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ20 | P21/n | 3.34 | 200 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ21 | P21/n | 3.87 | 240 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ22 | P21/n | 5.74 | 280 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ23 | P21/n | 7.74 | 320 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ24 | P21/n | 9.49 | 360 | 2022 | Synchrotron; Slow evaporation from DMSO7 |
| SEDTUQ25 | P21/n | 6.02 | 200 | 2007 | Slow heating on diffractometer of crystal prepared for SEDTUQ268 (does not revert to other phases on cooling carefully) |
| SEDTUQ26 | P212121 | 2.82 | 423 | 2007 | Slow cooling of DMF or DMSO solutions8 |
| SEDTUQ27 | P21/n | 2.49 | 100 | 2020 | Re-refinement of data collected in SEDTUQ099 |
| SEDTUQ28 | P21/n | 2.64 | 100 | 2020 | Re-refinement of data collected in SEDTUQ099 |
| SEDTUQ29 | P21/n | 1.95 | 100 | 2020 | Re-refinement of data collected in SEDTUQ099 |
| SEDTUQ30 | P21/n | 1.38 | 100 | 2020 | Re-refinement of data collected in SEDTUQ099 |
| SEDTUQ31 | P212121 | 2.96 | 413 | 2007 | Intermediate data collections between SEDTUQ26 and SEDTUQ258 |
| SEDTUQ32 | P212121 | 2.89 | 403 | 2007 | Intermediate data collections between SEDTUQ26 and SEDTUQ258 |
| SEDTUQ33 | P1 | 14.9 | 293 | 2016 | Synchrotron data, 5.9 GPa6 According to a different reference, this is called epsilon |
| SEDTUQ34 | P1 | 14.9 | 293 | 2016 | Synchrotron data, 5.9 GPa6 |
| SEDTUQ35 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ36 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ37 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ38 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ39 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ40 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ41 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ42 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ43 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ44 | P21/n | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ45 | P1 | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ46 | P1 | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ47 | P1 | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ48 | P1 | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |
| SEDTUQ49 | P1 | 0 | 298 | 2016 | Synchrotron data, I don’t understand the publication reference6 |

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