The shortest Th–Th distance from a new type of quadruple bond

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Supporting Information

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I. Additional computational details

For calculations in the ADF 2014.01 program, the criteria of the grid size, SCF and geometry convergence are 6.0 (Accint), 1e-6 (SCFconv) and 1e-4 (TolE and TolG) and the others (TolR & TolA) were set as defaults. As Cy$_3$PThThPCy$_3$ and Ph$_3$PThThPPh$_3$ are rather large systems, Slater type orbital basis sets of double-zeta plus one polarization function (DZP) were used for the atoms of these two molecules except Th, for which TZP was used.

For calculations in the Molpro 2015.1 program, the global threshold for the smallest allowed eigenvalue of the overlap matrix (THROVL) was set as 1.d-9, all other parameters were employed at their default value. D$_{3d}$ symmetry was used for all \textit{ab initio} studies on H$_3$PThThPH$_3$, including CASPT2, CCSD(T) and SOC calculations. Although the D$_{3d}$ structure is not quite the most stable at the PBE level (0.54 kJ/mol less stable than the C$_1$ structure, with a small imaginary frequency of 21.2$^i$ cm$^{-1}$), high symmetry is so helpful for state specification in \textit{ab initio} calculations that we felt the constraint to D$_{3d}$ symmetry appropriate. The \textit{xyz} coordinates of both of the D$_{3d}$ and C$_1$ structures are given in Section III. Note that the Th–Th bond lengths are very similar between these two structures, 2.604 Å (D$_{3d}$) vs 2.607 Å (C$_1$).
II. Table

Table S1. An–An bond distances reported in the literature. See main text for the source reference numbers.

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Table S2. The $\angle_{L\text{-Th-Th}}$ angles (°) and total bonding energies $E$ (kJ/mol) of the optimised LThThL molecules. Also provided are the $\angle_{L\text{-Th-Th}}$ angles and energies for modified geometries, derived from the optimised geometries as follows. Starred structures are optimised with symmetry constraints that enforce linearity (e.g. $D_{3d}$ for $H_3AsThThAsH_3$). For other compounds this approach did not lead to either SCF or geometry convergence, and hence the other angle data in the same column indicate structures based on the optimised geometries but fixing $\angle_{L\text{-Th-Th}}$ to be either linear (180°) or trans-bent (170°), depending on the angle in the fully optimised structure. The energy difference $\Delta E$ between the two forms is also given.

| Compounds       | Optimised Geometry | | | | | |
|------------------|--------------------|-----------------|-----------------|-----------------|-----------------|
|                  | $\angle_{L\text{-Th-Th}}$ | $E$             | $\angle_{L\text{-Th-Th}}$ | $E$             | $\Delta E$      |
| $H_3AsThThAsH_3$ | 169.2              | -3387.49        | 180.0*           | -3387.70        | 0.21            |
| $H_3PThThPH_3$   | 175.4              | -3626.69        | 180.0*           | -3626.15        | -0.54           |
| $Me_3PThThPMe_3$ | 179.5              | -13339.22       | 170.0            | -13336.1        | -3.12           |
| Cy3PThThPCy3     | 176.2              | -56433.08       | 180.0            | -56432.40       | -0.68           |
| Ph3PThThPPh3     | 173.8              | -43077.79       | 180.0            | -43074.78       | -3.01           |
| $H_3NThThNH_3$   | 180.0              | -4451.27        | 170.0            | -4446.04        | -5.23           |
| NHCThThNHC       | 177.9              | -11722.65       | 180.0*           | -11722.56       | -0.09           |
| $H_2FPThThPFH_2$ | 169.4              | -3904.76        | 180.0            | -3901.16        | -3.60           |
| HF2PThThPF2H     | 168.2              | -4194.84        | 180.0            | -4184.96        | -9.88           |
| OCThThCO         | 180.0              | -3665.02        | 170.0            | -3663.43        | -1.59           |
| ONThThNO         | 180.0              | -3487.95        | 170.0            | -3482.85        | -5.10           |
III. xyz coordinates (Å) and total SCF energies from DFT (PBE) optimisations of the studied compounds.

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**Notes:**
- $\text{E}$ represents the total SCF energy.
- The xyz coordinates are given in ångströms (Å).
- The compounds are named according to their structure.
- The energies are given in Hartree (Hart).
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