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Supporting information for article:

HBr or not HBr? That is the question: crystal structure of 6-hydroxy-1,4-diazepane-1,4-diium dibromide redetermined

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Full list of refcodes for CSD search

By studying some related literature, we became aware that the report of Liu *et al*. (1996) might not be the only example, where the nature of `Hbr' in a crystal structure should be questioned. A search in the latest version (2018, Version 5.20) of the Cambridge Structural Database (CSD; Groom *et al*., 2016), looking for molecular H---Br (*i.e.* for an H atom directly connected to a Br atom by a single bond) revealed a total of 69 entries:

ANOPEA, AWIVUY, BEPQIY, DAFFOH, EVAMIX, EWAZEJ, GICSOC, GIGYED, HACBOE, HEQGOZ, IVAWUY, JADVAM, KEGXUP, KEKQAS, KONVEO, KUFZOB, KUYQUS, MDOIMP, MIYZOK, MOKTAJ, MOMVIV, MOMVIV01, MPPYRL, MUFKON, MUSTEB, NAVFOI01, NIJGOC, NMTHFA01, PAJDIN, PASOHB, PEXHAB, PIMMAZ, PUPKOC, QEVSUF, QEVSUF01, QICGUF, QQQAQP, QQQASS, QQQATJ, QQQAVY, QQQGQY, SIJYAN, SOCZUH, TAZQAM, TMEPYR, TOKTIW (Liu's paper), TPPOBR, UFOYIX, UHEPII, UMTHFA01, UNESAI, VISBOP, VOKCII, YALFAS, YEBZEN, YISZUV, YITTOL,YOTSIJ, ZZZDIO, ZZZDNY, ZZZGUI, ZZZNGC, ZZZPOK, ZZZPSW, ZZZPTA, ZZZQRK, ZZZSZW, ZZZVJP, ZZZVLE.