

Supporting Information

V=O···C Interactions in Crystal Structures of Oxovanadium-coordination Compounds

Vladimir Stilinović,^a Dejan-Krešimir Bučar,^{a,†} Ivan Halasz^a and Ernest Meštrović^{a,c}

Department of Chemistry, Faculty of Science, University of Zagreb, 102a Horvatovac, HR-10000, Zagreb, Croatia.

[‡] current address: Department of Chemistry, University of Iowa, 305 Chemistry Building, Iowa City, IA 52242, USA.

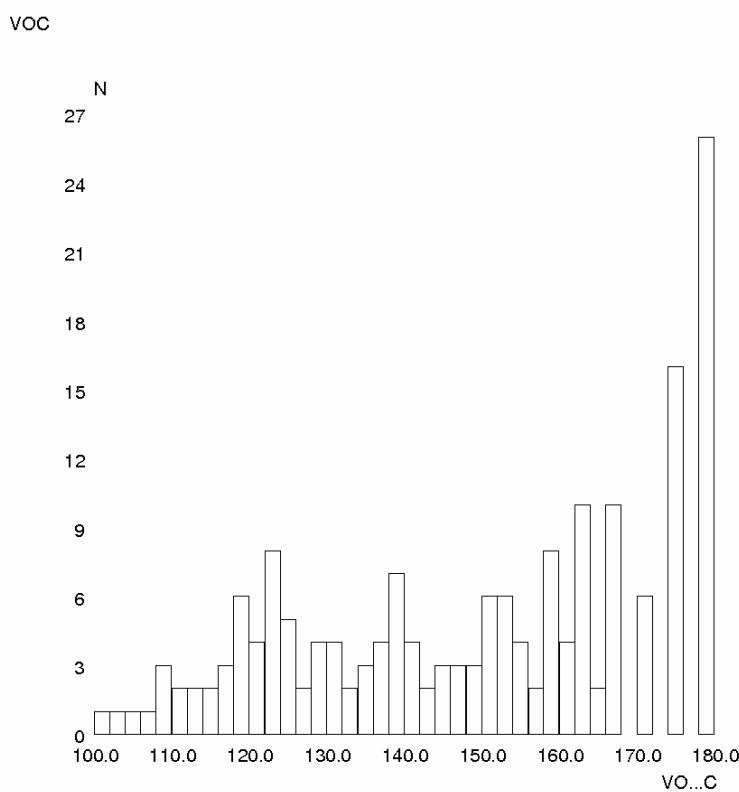


Figure S1. Histogram of VOC angles for dimers, oligomers and polymers with VOC ($d(\text{O}\cdots\text{C})$) is less than the sum of van der Waals radii).

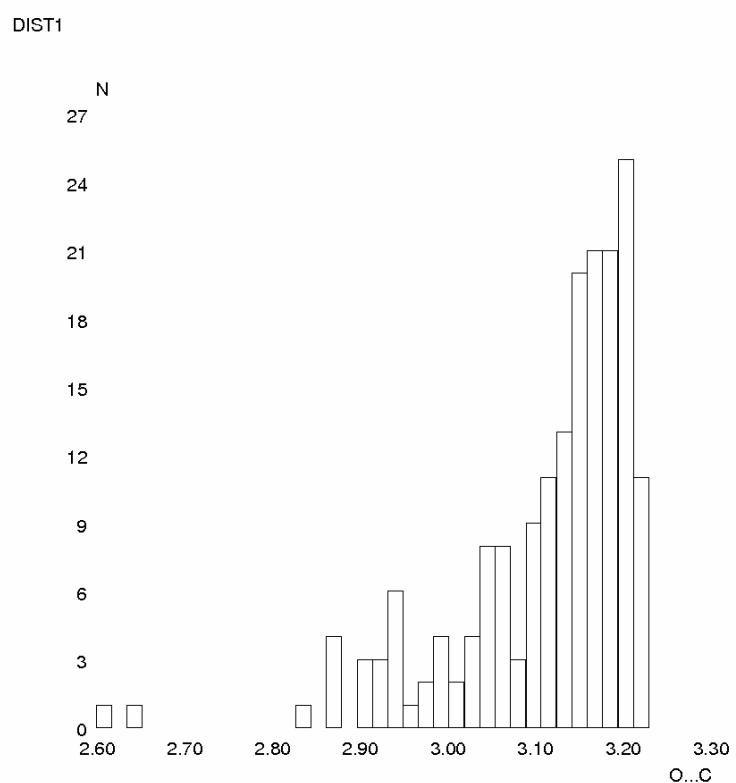


Figure S2. Histogram of OC distances for dimers, oligomers and polymers with VOC ($d(\text{O}\cdots\text{C})$ is less than the sum of van der Waals radii).

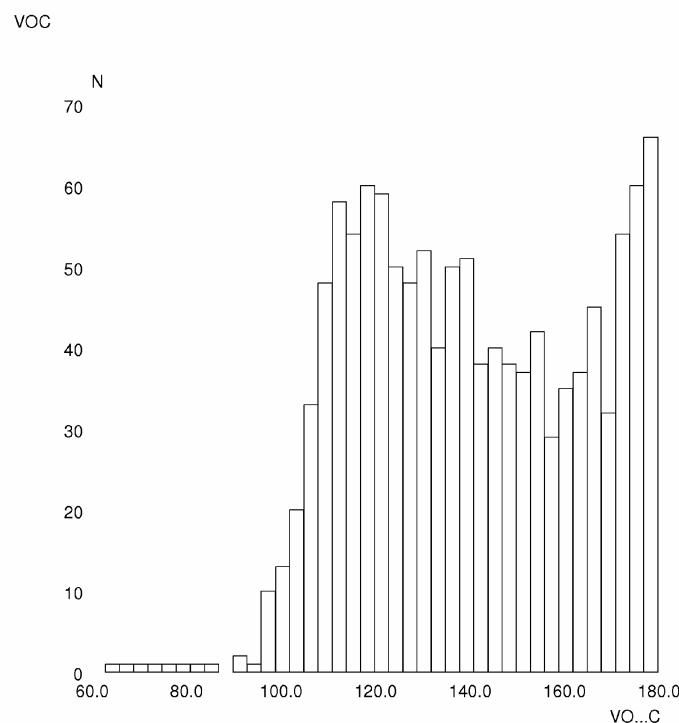


Figure S3. Histogram of VOC angle for all structures with VOC ($d(\text{O}\cdots\text{C})$ is less than the sum of van der Waals radii).

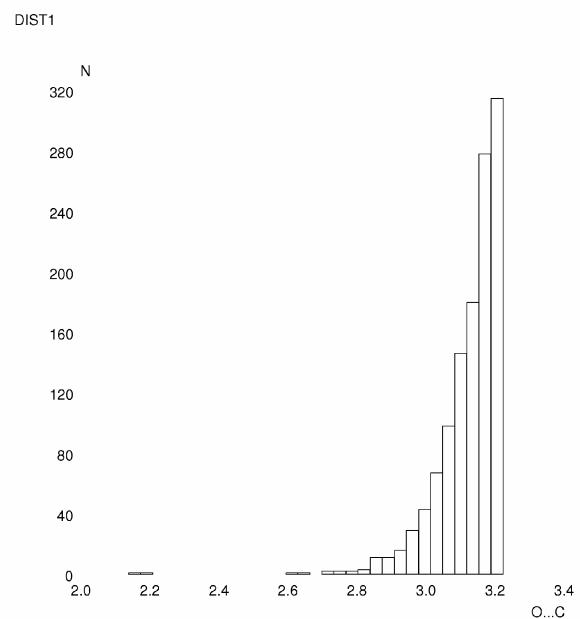


Figure S4. Histogram of OC distances for all structures with VOC ($d(O \cdots C)$ is less than the sum of van der Waals radii).

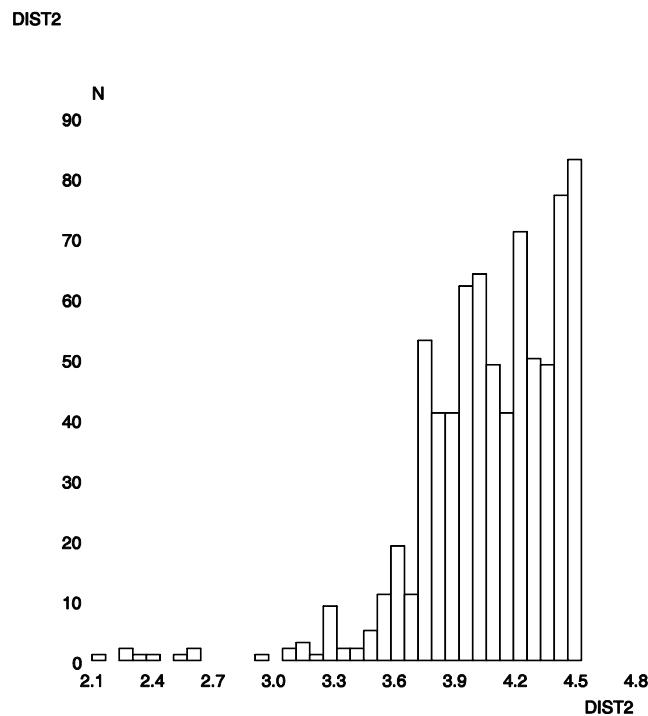


Figure S5. Histogram of V=O...V=O distances for all structures with VOC ($d(O \cdots V)$ is less than the sum of van der Waals radii + 1 Å).

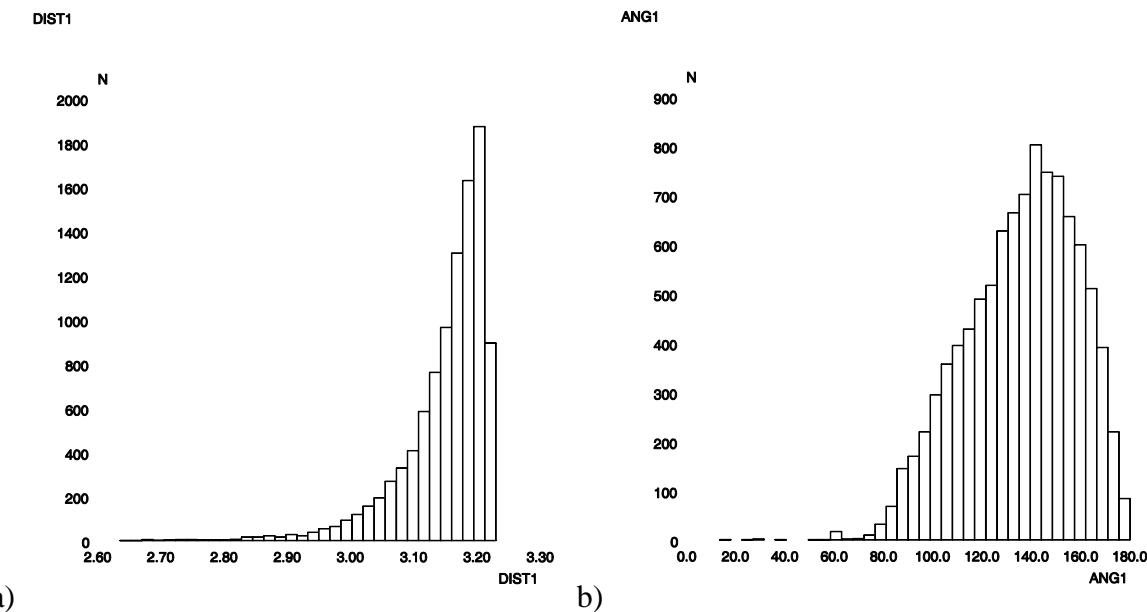


Figure S6. Geometry of C=O…C contacts. a) C=O…C distances for all structures with C=O…C contacts ($d(\text{O} \cdots \text{C})$ is less than the sum of van der Waals radii), b) C=O…C angles for all structures with C=O…C contacts.

The V=O…C interaction is probably quite similar to the well known C=O…C interaction. However, there are noticeable differences in the geometries of the two. Firstly, the distribution of O…C distances is quite wider in the first case than in the former (see Figures S4 and S6a). Secondly the V=O…C angle shows an apparent bimodal distribution, with the likeliest angles around 115° and 180° (Figure S3), whereas in the case of C=O…C interactions the C=O…C angle distribution has only a single maximum at ca. 140°.

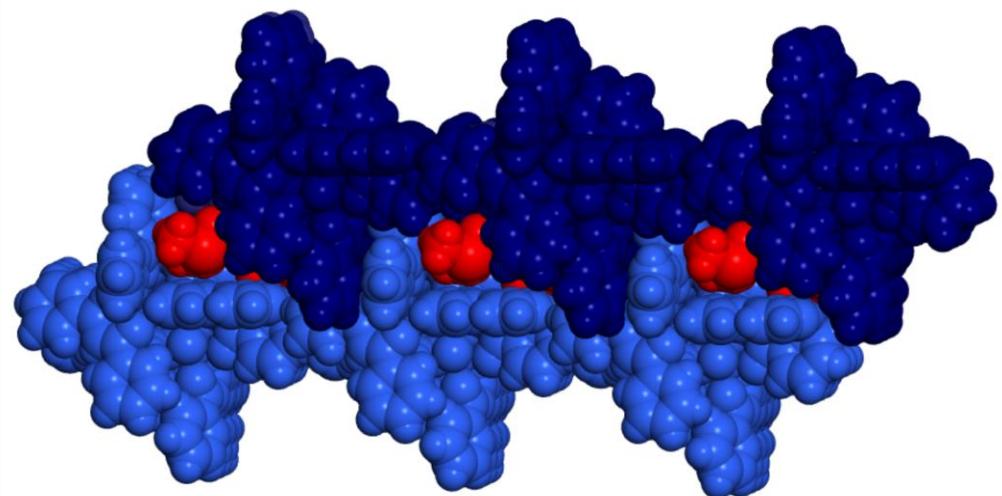


Figure S7. Perspective view of two dimer layers (blue shades) of **2**. The pores in-between the layers are filled with **dmso** (red) molecules.

Table S1. Broad list of refcodes of compound containing the V=O···C contact forming dimers, oligomers or polymers in the solid state.

Dimers

ABUZAY, ADIDAS, ASAVAR, BAPDOM, BEQVOJ, BILREU, CEFROU, DANROA, DAQSIX, EBUZIK, EDELUU, EFITOC, EVAKER, FAHXUI, FOCTIB, FUWYAX, GECFEZ, GECFIB, GOGCOU, HAMNOZ, HAXPEB, HEXTOT, HEXTUZ, HIZKAC, HOHZAF, HUILON, IWOKEK, IXIFUQ, JAHVUK, JETWUB, JOGDEO, KACROV, KEGYIE, KOHQON, KOQFOL, KOQFUR, KUZZXOS, LEPJEV, LOXVAV, MUXVEG, NABKOR, NECCON, NIQCAR, OBOYOU, OGERAT, PACDIH, PACDON, PAGXOK, PAVHEA, PERHAW, PORZOL, PORZUR, POWFOW, PUSSIF, QABZAU, QAKSEB, QALWOQ, QATXOY, QEYXUN, QIHWOT01, QOJNAE, QUDGIF, QUFLMIN, QUKDAB, QUKJAH, SEDNEV, SEDTOK, SEDVAY, SEHLOH, SUGXIW, SUVRUW, TABMIT, TIZPIB, TOZQUU, TUNXIJ, UCUHUW, UHOGIH, VEKBIX, VEKBOD, VEMQUA, WABQAR, WAMPEG, WEKDAR, WIHQIN, WOBCAR, WOTTII, WUTVUC, WUVNIK, WUVNOQ, XACPLV01, XAPCAT, XOVBOZ, XUTMAA, YAZGOV, YECDEQ, YUGRAT, ZOJJEN, ZUFJUF.

Oligomers

AROJOG, PECJIQ

Polymers

ACILIH, ALADEW, AOXOVA, AQHPRV, AVIDUE, AVIFAM, BAFNEB, BAFQAA, BAPDUS, BICKUU, BICLEF, BIGFAY, BOBDUR, CEBPIJ, CENJEK, CESQOH, CINKUF, DESFEM, EBUZAC, EWOSAK, FOKHEJ, FIGMAK, FISVEJ, GUTPEQ, HAKROA, HARHOX, HENHIS, HENHOY, HENHUE, HENJAM, HEPXOQ, HETYEK, HETYIO, HIQFAO, IFUSOR, IKUWAM, ILOYEN, ILOYOX, IMAROD, IQEPOJ, IZITUG, JAMCOP10, JEBJOP, JOXMUE, KABZAP,

KEBWIY, KEJTUP, KEPQIG, KIVYIX, KOHQED, KOHQIH, KUPDII, LAHWIB, LAKFAE,
LAPWAA, LATRIH, LUWXUW, MANPAT, MEMFOZ, MEZCUP, MIVZAS, MUHPUA, MUHSEM,
MUHSEN03, MUJSEP, MUJSIT, NAPJEU, NAQKUL, NAQLAS, NAVLEB, NIJDUF, NOKNAC,
OBOXUZ, OBOYAG, OBOJEK, OBOJIO, OCADOM, OCAGOO, ODUBOE, OEDTAV, OFABON,
OFUSEN, OJEDIQ, OLUBEC, PAQVIM, PAQVUZ, PATCET, PATCIX, PATCUJ, PATDAQ,
PATDEU, PATDOE, PATDUK, PAVHUQ, PAWYES, PAXLAB, PUGWOD, QAKSEB, QEPBUI,
QEPCET, QOLWOD, RAGDEI, REFCAG, REILUO, RELLOJ, REYRIW, RIPFAX, RIRMOU,
ROCKAV, SEGDOY, SETXAR, SILBEU, TECFAJ, TEGROM, TEMHOJ, TIMJUU01, TOZREF,
UCUJAE, UCUJEI, UDOQAF, ULUWON, VAQMUW, VEBNEW, VIZFEP, VONACN10,
WAWKOV, WEFGAP, WENVUG, WIHQEJ, WIRGAF, WOTTEE, XAHKOG, XAKXOX, XAPJUU,
XEBXIL, XEMXAO, XENCUO, XETFEH, XEZYUW, XEZZEH, XODROX, XOTPOL, XUDLUD,
XUVYIW01, YACDUB, YAMQIN, YARTOA, YATTET, YEDBUE, YEDCAL, YEHWEM,
YEMSUG01, YENTOB, YETFEI, YETFIM, YOWGEW, YUVFEA, ZOJVID, ZUWNIO.