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The crystal structure of 3-oxo-urs-12-en-28-oic acid, $C_{30}H_{46}O_3 \cdot 1/6H_2O$

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Abstract

$C_{30}H_{46}O_3 \cdot 1/6H_2O$, monoclinic, $C2$ (no. 5), $a = 29.4307(4)$ Å, $b = 15.42797(17)$ Å, $c = 18.4667(2)$ Å, $\beta = 104.4652(12)^\circ$, $V = 8119.11(17)$ Å³, $Z = 12$, $R_{\text{gt}}(F) = 0.0432$, $wR_{\text{ref}}(F^2) = 0.1197$, $T = 293(2)$ K.

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One of three independent molecules of the title crystal structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	$0.29 \times 0.24 \times 0.20$ mm
Wavelength:	Cu K α radiation (1.54184 Å)
μ :	0.54 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max} , completeness:	66.8° , 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	34,354, 12,647, 0.029
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 11372
$N(\text{param})_{\text{refined}}$:	917
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], SUPERFLIP [3–5], SHELX [6]

Source of material

3-Oxo-urs-12-en-28-oic acid was synthesized by oxidation of ursolic acid (UA) with the Sarett reagent. Specifically, the Sarett reagent was added to a solution of UA in dichloromethane (DCM) at room temperature over a period till the brown color persisted. The resulting solution was stirred for further 6 h. The progress of the reaction was monitored by TLC. After completion of the reaction, isopropanol was added and stirred at r.t. for 30 min. The DCM was evaporated in vacuo to yield a black solid, which was purified using silica-gel column chromatography (petroleum ether:ethyl acetate = 20:1, v/v) to afford a white powder. Suitable crystals were obtained by recrystallization in ethyl acetate solution.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	U_{iso}^*/U_{eq}
O1	0.5867 (2)	0.0091 (5)	0.6690 (3)	0.206 (3)
O2	0.81273 (9)	0.5601 (2)	0.58312 (15)	0.0939 (8)
O3	0.82126 (8)	0.5673 (2)	0.70414 (13)	0.0832 (7)
H3	0.845625	0.541511	0.704072	0.125*
C1	0.64593 (16)	0.2046 (3)	0.7422 (2)	0.0847 (10)
H1A	0.617945	0.240355	0.729465	0.102*
H1B	0.663778	0.220992	0.791858	0.102*
C2	0.6315 (2)	0.1089 (3)	0.7428 (3)	0.1146 (17)
H2A	0.658852	0.075973	0.768576	0.137*
H2B	0.608486	0.104143	0.772169	0.137*
C3	0.61238 (15)	0.0684 (3)	0.6719 (3)	0.0934 (11)
C4	0.62633 (18)	0.0975 (3)	0.6011 (2)	0.0941 (12)
C5	0.64576 (12)	0.1921 (2)	0.60814 (18)	0.0678 (8)
H5	0.617630	0.228598	0.599046	0.081*
C6	0.66939 (15)	0.2177 (2)	0.5464 (2)	0.0802 (9)
H6A	0.700742	0.193304	0.557064	0.096*
H6B	0.651618	0.194471	0.498942	0.096*
C7	0.67217 (12)	0.3153 (2)	0.54113 (17)	0.0668 (7)
H7A	0.640574	0.338578	0.526466	0.080*
H7B	0.687709	0.329975	0.502202	0.080*
C8	0.69863 (9)	0.3591 (2)	0.61457 (15)	0.0566 (6)
C9	0.68082 (10)	0.3223 (2)	0.68112 (15)	0.0555 (6)
H9	0.648855	0.344946	0.673465	0.067*
C10	0.67558 (11)	0.2219 (2)	0.68597 (18)	0.0661 (7)
C11	0.70835 (14)	0.3634 (3)	0.75465 (18)	0.0828 (11)
H11E	0.689882	0.358446	0.791221	0.099*
H11F	0.737060	0.330730	0.773263	0.099*
C12	0.72067 (12)	0.4562 (2)	0.74834 (16)	0.0702 (8)
H12	0.735000	0.484809	0.792481	0.084*
C13	0.71313 (9)	0.5019 (2)	0.68574 (14)	0.0537 (6)
C14	0.68919 (9)	0.46032 (18)	0.61035 (14)	0.0508 (6)
C15	0.70782 (11)	0.5008 (2)	0.54577 (15)	0.0614 (7)
H15E	0.736816	0.471730	0.544320	0.074*
H15F	0.685220	0.488969	0.498742	0.074*
C16	0.71689 (10)	0.5977 (2)	0.55143 (15)	0.0601 (7)
H16E	0.687273	0.628033	0.544898	0.072*
H16F	0.730921	0.615634	0.511564	0.072*
C17	0.74956 (9)	0.6230 (2)	0.62708 (15)	0.0561 (6)
C18	0.72583 (9)	0.5979 (2)	0.68990 (15)	0.0549 (6)
H18	0.749599	0.605955	0.737117	0.066*
C19	0.68422 (11)	0.6589 (2)	0.69336 (18)	0.0664 (7)
H19	0.659969	0.652305	0.646483	0.080*
C20	0.70001 (13)	0.7542 (3)	0.6998 (2)	0.0784 (9)
H20	0.724955	0.760179	0.745886	0.094*
C21	0.72040 (14)	0.7786 (3)	0.6351 (2)	0.0824 (9)
H21E	0.730882	0.838343	0.640779	0.099*
H21F	0.696154	0.774052	0.588762	0.099*
C22	0.76128 (12)	0.7208 (2)	0.6307 (2)	0.0702 (8)
H22E	0.787027	0.731529	0.674103	0.084*
H22F	0.771793	0.736495	0.586657	0.084*
C23	0.5831 (3)	0.0931 (4)	0.5358 (4)	0.179 (4)
H23G	0.562858	0.141183	0.538260	0.268*
H23H	0.566652	0.039829	0.538243	0.268*
H23I	0.592488	0.095336	0.489651	0.268*
C24	0.6624 (3)	0.0291 (3)	0.5896 (4)	0.142 (2)

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H24G	0.671938	0.042124	0.544782	0.214*
H24H	0.648328	−0.027414	0.585423	0.214*
H24I	0.689323	0.030138	0.631619	0.214*
C25	0.72265 (17)	0.1732 (3)	0.7114 (3)	0.1086 (15)
H25G	0.737438	0.170223	0.670655	0.163*
H25H	0.717037	0.115634	0.726841	0.163*
H25I	0.742767	0.203515	0.752559	0.163*
C26	0.75182 (11)	0.3422 (3)	0.6267 (2)	0.0842 (10)
H26G	0.761864	0.362608	0.584149	0.126*
H26H	0.757866	0.281143	0.632920	0.126*
H26I	0.768729	0.372342	0.670717	0.126*
C27	0.63612 (9)	0.4818 (2)	0.59340 (17)	0.0617 (7)
H27G	0.624045	0.464180	0.634833	0.093*
H27H	0.619764	0.451455	0.549165	0.093*
H27I	0.631684	0.543072	0.585686	0.093*
C28	0.79677 (10)	0.5790 (2)	0.63502 (17)	0.0612 (7)
C29	0.6608 (2)	0.8166 (4)	0.7045 (4)	0.1164 (16)
H29G	0.634197	0.806733	0.663189	0.175*
H29H	0.671565	0.875160	0.702828	0.175*
H29I	0.652009	0.807346	0.750596	0.175*
C30	0.66287 (15)	0.6325 (3)	0.7575 (2)	0.0904 (11)
H30G	0.650918	0.574491	0.749372	0.136*
H30H	0.637762	0.671421	0.759515	0.136*
H30I	0.686531	0.635082	0.803846	0.136*
O1B	0.59041 (9)	0.9870 (2)	0.28189 (19)	0.1010 (9)
O2B	0.54190 (7)	0.33317 (19)	0.45594 (10)	0.0734 (6)
O3B	0.46502 (7)	0.33191 (19)	0.40640 (11)	0.0744 (6)
H3B	0.464788	0.331844	0.450717	0.112*
C1B	0.62096 (10)	0.7771 (2)	0.3542 (2)	0.0767 (10)
H1BA	0.647531	0.749705	0.388332	0.092*
H1BB	0.622085	0.762033	0.303707	0.092*
C2B	0.62565 (11)	0.8759 (3)	0.3637 (3)	0.0932 (12)
H2BA	0.629581	0.890400	0.416018	0.112*
H2BB	0.653561	0.894924	0.349259	0.112*
C3B	0.58429 (11)	0.9234 (2)	0.3182 (2)	0.0773 (9)
C4B	0.53508 (10)	0.8917 (2)	0.3183 (2)	0.0680 (8)
C5B	0.53382 (8)	0.79018 (17)	0.31693 (16)	0.0508 (6)
H5B	0.535805	0.775022	0.266279	0.061*
C6B	0.48726 (9)	0.7517 (2)	0.32311 (19)	0.0615 (7)
H6BA	0.461565	0.785991	0.293759	0.074*
H6BB	0.485475	0.753141	0.374840	0.074*
C7B	0.48276 (8)	0.65834 (19)	0.29499 (17)	0.0556 (6)
H7BA	0.481680	0.658359	0.242059	0.067*
H7BB	0.453267	0.634803	0.300602	0.067*
C8B	0.52298 (8)	0.59835 (17)	0.33584 (13)	0.0468 (5)
C9B	0.57078 (8)	0.64406 (18)	0.34279 (14)	0.0476 (5)
H9B	0.574751	0.645445	0.291673	0.057*
C10B	0.57543 (9)	0.74087 (19)	0.36895 (15)	0.0552 (6)
C11B	0.61063 (10)	0.5858 (2)	0.3860 (2)	0.0698 (8)
H11C	0.639428	0.602085	0.372967	0.084*
H11D	0.615063	0.596225	0.439121	0.084*
C12B	0.60226 (9)	0.4917 (2)	0.37120 (16)	0.0593 (7)
H12B	0.626584	0.454661	0.393829	0.071*
C13B	0.56415 (9)	0.45500 (18)	0.32950 (13)	0.0489 (6)
C14B	0.52257 (8)	0.51176 (16)	0.28929 (12)	0.0451 (5)
C15B	0.47503 (9)	0.46460 (18)	0.28050 (15)	0.0537 (6)

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H15C	0.464744	0.472816	0.325997	0.064*
H15D	0.451987	0.491810	0.240058	0.064*
C16B	0.47576 (11)	0.3679 (2)	0.26465 (15)	0.0591 (7)
H16C	0.480601	0.359238	0.215088	0.071*
H16D	0.445574	0.343028	0.265228	0.071*
C17B	0.51444 (11)	0.32051 (19)	0.32204 (14)	0.0556 (6)
C18B	0.56276 (10)	0.35620 (18)	0.31921 (14)	0.0544 (6)
H18B	0.585265	0.332419	0.363030	0.065*
C19B	0.57919 (13)	0.3246 (2)	0.24972 (17)	0.0692 (8)
H19B	0.558515	0.350779	0.205165	0.083*
C20B	0.57500 (19)	0.2251 (2)	0.2412 (2)	0.0909 (13)
H20B	0.596529	0.199173	0.285020	0.109*
C21B	0.5265 (2)	0.1947 (2)	0.2400 (2)	0.0948 (13)
H21C	0.525310	0.132054	0.235467	0.114*
H21D	0.504577	0.218718	0.196451	0.114*
C22B	0.51171 (16)	0.2212 (2)	0.30996 (18)	0.0760 (9)
H22C	0.531876	0.192839	0.353045	0.091*
H22D	0.479796	0.201921	0.305877	0.091*
C23B	0.50085 (12)	0.9262 (2)	0.2475 (2)	0.0823 (10)
H23D	0.506217	0.896874	0.204512	0.123*
H23E	0.505710	0.987295	0.243032	0.123*
H23F	0.469205	0.915993	0.250516	0.123*
C24B	0.52183 (15)	0.9326 (3)	0.3865 (3)	0.0970 (13)
H24D	0.491303	0.912688	0.388685	0.145*
H24E	0.521457	0.994612	0.381799	0.145*
H24F	0.544481	0.916040	0.431404	0.145*
C25B	0.57787 (15)	0.7520 (3)	0.45288 (19)	0.0862 (10)
H25D	0.595310	0.803457	0.471237	0.129*
H25E	0.593148	0.702575	0.479977	0.129*
H25F	0.546674	0.756898	0.459642	0.129*
C26B	0.51576 (12)	0.5764 (2)	0.41406 (16)	0.0665 (8)
H26D	0.488777	0.539683	0.408583	0.100*
H26E	0.511025	0.628951	0.439025	0.100*
H26F	0.543010	0.546940	0.443041	0.100*
C27B	0.52876 (10)	0.52852 (19)	0.20915 (13)	0.0548 (6)
H27D	0.560363	0.546872	0.212276	0.082*
H27E	0.507323	0.572923	0.185388	0.082*
H27F	0.522416	0.476104	0.180376	0.082*
C28B	0.50774 (10)	0.33101 (19)	0.40069 (14)	0.0549 (6)
C29B	0.5894 (3)	0.1922 (3)	0.1712 (3)	0.131 (2)
H29D	0.569430	0.218049	0.127367	0.197*
H29E	0.586204	0.130332	0.168194	0.197*
H29F	0.621390	0.207911	0.174615	0.197*
C30B	0.62901 (15)	0.3562 (3)	0.2549 (2)	0.0923 (12)
H30D	0.629253	0.418355	0.252853	0.139*
H30E	0.639808	0.333010	0.213956	0.139*
H30F	0.649341	0.337082	0.301290	0.139*
O1C	0.6814 (2)	1.0565 (4)	0.0633 (3)	0.190 (3)
O2C	0.53260 (7)	0.39302 (18)	−0.06581 (10)	0.0709 (6)
H2C	0.507221	0.385396	−0.055970	0.106*
O3C	0.55522 (7)	0.40157 (18)	0.05711 (11)	0.0691 (6)
C1C	0.65497 (12)	0.8612 (2)	0.13312 (17)	0.0681 (8)
H1CA	0.651996	0.837028	0.180221	0.082*
H1CB	0.685728	0.845543	0.127055	0.082*
C2C	0.65174 (16)	0.9599 (3)	0.1368 (2)	0.0863 (10)
H2CA	0.622572	0.975939	0.148669	0.104*

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H2CB	0.677438	0.981642	0.176271	0.104*
C3C	0.6537 (2)	1.0003 (3)	0.0645 (3)	0.1052 (14)
C4C	0.62014 (19)	0.9665 (3)	−0.0066 (2)	0.0942 (12)
C5C	0.62088 (12)	0.8650 (2)	−0.00414 (16)	0.0638 (7)
H5C	0.652207	0.849611	−0.009347	0.077*
C6C	0.58735 (13)	0.8216 (2)	−0.07124 (17)	0.0741 (9)
H6CA	0.555715	0.822060	−0.064434	0.089*
H6CB	0.587265	0.853588	−0.116509	0.089*
C7C	0.60290 (12)	0.7286 (2)	−0.07864 (15)	0.0631 (7)
H7CA	0.633553	0.729433	−0.089271	0.076*
H7CB	0.581147	0.701801	−0.120931	0.076*
C8C	0.60562 (8)	0.67255 (18)	−0.00883 (13)	0.0481 (5)
C9C	0.63137 (8)	0.72287 (18)	0.06254 (13)	0.0481 (5)
H9C	0.664287	0.724597	0.060335	0.058*
C10C	0.61752 (9)	0.8205 (2)	0.06941 (15)	0.0554 (6)
C11C	0.63144 (12)	0.6691 (2)	0.13221 (15)	0.0636 (7)
H11A	0.656685	0.689191	0.173228	0.076*
H11B	0.602127	0.678748	0.145998	0.076*
C12C	0.63733 (9)	0.5737 (2)	0.12191 (14)	0.0548 (6)
H12C	0.640257	0.538955	0.163990	0.066*
C13C	0.63878 (8)	0.53371 (18)	0.05877 (13)	0.0466 (5)
C14C	0.63410 (8)	0.58604 (18)	−0.01343 (13)	0.0466 (5)
C15C	0.60845 (10)	0.53319 (19)	−0.08299 (14)	0.0528 (6)
H15A	0.574908	0.538001	−0.088342	0.063*
H15B	0.615247	0.559169	−0.126956	0.063*
C16C	0.62120 (10)	0.43798 (19)	−0.08125 (15)	0.0547 (6)
H16A	0.653508	0.432250	−0.084184	0.066*
H16B	0.601417	0.409439	−0.124604	0.066*
C17C	0.61534 (9)	0.39313 (18)	−0.01042 (14)	0.0528 (6)
C18C	0.64763 (9)	0.43686 (19)	0.05929 (15)	0.0523 (6)
H18C	0.638108	0.413759	0.102702	0.063*
C19C	0.70031 (10)	0.4120 (2)	0.07052 (18)	0.0688 (8)
H19C	0.711065	0.436300	0.028665	0.083*
C20C	0.70609 (13)	0.3134 (3)	0.0691 (2)	0.0835 (11)
H20C	0.695616	0.289301	0.111276	0.100*
C21C	0.67651 (14)	0.2738 (3)	−0.0016 (2)	0.0857 (11)
H21A	0.680729	0.211367	0.000406	0.103*
H21B	0.686904	0.295380	−0.044055	0.103*
C22C	0.62449 (13)	0.2948 (2)	−0.0123 (2)	0.0704 (8)
H22A	0.613190	0.266771	0.026899	0.084*
H22B	0.606956	0.271531	−0.059855	0.084*
C23C	0.6372 (3)	0.9963 (4)	−0.0741 (3)	0.146 (3)
H23A	0.664807	0.964324	−0.076263	0.220*
H23B	0.644382	1.057004	−0.069634	0.220*
H23C	0.613032	0.986147	−0.119016	0.220*
C24C	0.5720 (2)	1.0073 (4)	−0.0115 (4)	0.138 (2)
H24A	0.549252	0.982564	−0.052887	0.207*
H24B	0.573691	1.068719	−0.018592	0.207*
H24C	0.562760	0.996114	0.034001	0.207*
C25C	0.56941 (11)	0.8324 (3)	0.0877 (2)	0.0766 (9)
H25A	0.544909	0.829813	0.042354	0.115*
H25B	0.568552	0.887660	0.111262	0.115*
H25C	0.564902	0.787146	0.120911	0.115*
C26C	0.55512 (9)	0.6495 (2)	−0.00511 (19)	0.0658 (8)
H26A	0.556273	0.612664	0.037199	0.099*
H26B	0.539353	0.619882	−0.050088	0.099*

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H26C	0.538385	0.701687	−0.000139	0.099*
C27C	0.68417 (9)	0.6046 (2)	−0.02168 (16)	0.0578 (6)
H27A	0.702940	0.627728	0.024378	0.087*
H27B	0.682677	0.645765	−0.061160	0.087*
H27C	0.697998	0.551687	−0.033379	0.087*
C28C	0.56441 (9)	0.39821 (18)	−0.00600 (14)	0.0493 (5)
C29C	0.75723 (18)	0.2862 (5)	0.0781 (4)	0.130 (2)
H29A	0.768697	0.310667	0.038248	0.195*
H29B	0.759133	0.224177	0.076484	0.195*
H29C	0.775937	0.306812	0.125222	0.195*
C30C	0.72983 (12)	0.4517 (3)	0.1424 (2)	0.0923 (12)
H30A	0.727594	0.513758	0.139260	0.138*
H30B	0.761986	0.434576	0.149252	0.138*
H30C	0.718545	0.431914	0.183993	0.138*

Experimental details

All hydrogen atoms were placed in idealized positions with the carrier atom–H distances = 0.93 Å for alkene, 0.96 Å for methyl, 0.97 Å for methylene and 0.98 Å for methine. The *U*_{iso} values of the hydrogen atoms of methyl groups were set to 1.5 *U*_{eq} and the *U*_{iso} values of all other hydrogen atoms were set to 1.2 *U*_{eq}(C). The absolute configuration was derived from the synthesis. The solvent molecule was presumed to be two water molecule on the basis of the 43 Å³ voids.

Comment

Ursolic acid (UA), a pentacyclic triterpenoid compound, is widely distributed in food products such as apples, basil, as well as in more than 120 plant species, many of which are applied as medicinal plants in traditional formulations [7]. UA has been reported to have multiple pharmacological activities like anti-inflammatory [8], antitumor [9], antioxidative [10], antiviral [11]. The pentacyclic triterpene system of title compound molecule consists of condensed six-membered rings with a ketone functional group at C-3 and a carboxyl moiety at C-28. It has been reported that 3-oxo-ursolic acid derivatives exhibit significant activity in inhibiting the production of nitric oxide induced by interferon-γ in mouse macrophages [12, 13]. And other study also showed that its derivatives more potently inhibit the growth of MCF-7 and THP-1 cancer cell lines [14]. Accordingly, the title compound was synthesized according to reported procedures [15]. In the molecule of the title

compound, bond lengths and angles within the six-membered rings are similar to those given in the literature for tetracyclic triterpeneoids [16–18].

Single-crystal structure analysis indicated that there are three molecules in the asymmetric unit of the title crystal structure. All cyclohexane rings are in the usually observed chair conformation, cyclohexene is in a conformation intermediate between sofa and half-chair: the C8 and C9 atoms deviate in different directions with respect to the planar C11–C12=C13–C14 fragment by 0.66 and 0.12 Å, respectively, in one molecule, by 0.70 and 0.84 Å in the second molecule and by 0.66 and 0.13 Å in the third molecule.

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