

**U<sub>10</sub>Co<sub>51</sub>Si<sub>33</sub>** [1]

Structural features: Infinite columns of base-linked Si(U<sub>2</sub>Co<sub>4</sub>)Co<sub>2</sub> bicapped, Si(U<sub>2</sub>Co<sub>4</sub>)Co<sub>3</sub> and SiCo<sub>6</sub>Co<sub>3</sub> tricapped trigonal prisms share atoms to form a 3D-framework with 10-fold propeller-like columns containing three SiCo<sub>6</sub> prism columns shifted by  $c/2$  in channels.

Aksel'rud L.G. et al. (1980) [1]

Co<sub>51</sub>Si<sub>33</sub>U<sub>10</sub>

$a = 2.753$ ,  $c = 0.3678$  nm,  $c/a = 0.134$ ,  $V = 2.4141$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	6h	m..	0.005	0.365	$\frac{1}{4}$		11-vertex polyhedron Si <sub>4</sub> Co <sub>5</sub> U <sub>2</sub>
Co2	6h	m..	0.042	0.526	$\frac{1}{4}$		11-vertex polyhedron Si <sub>4</sub> Co <sub>5</sub> U <sub>2</sub>
Si3	6h	m..	0.044	0.135	$\frac{1}{4}$		tricapped trigonal prism Co <sub>7</sub> U <sub>2</sub>
Co4	6h	m..	0.074	0.07	$\frac{1}{4}$		10-vertex polyhedron Si <sub>3</sub> Co <sub>7</sub>
Si5	6h	m..	0.085	0.3	$\frac{1}{4}$		square prism (cube) Co <sub>6</sub> Si <sub>2</sub>
Si6	6h	m..	0.105	0.398	$\frac{1}{4}$		10-vertex polyhedron Co <sub>6</sub> Si <sub>2</sub> U <sub>2</sub>
Co7	6h	m..	0.11	0.233	$\frac{1}{4}$		11-vertex polyhedron Si <sub>4</sub> Co <sub>5</sub> U <sub>2</sub>
Si8	6h	m..	0.134	0.553	$\frac{1}{4}$		10-vertex polyhedron Co <sub>6</sub> Si <sub>2</sub> U <sub>2</sub>
Co9	6h	m..	0.154	0.054	$\frac{1}{4}$		cuboctahedron Si <sub>4</sub> Co <sub>5</sub> U <sub>3</sub>
Co10	6h	m..	0.166	0.489	$\frac{1}{4}$		cuboctahedron Si <sub>4</sub> Co <sub>6</sub> U <sub>2</sub>
Si11	6h	m..	0.19	0.383	$\frac{1}{4}$		10-vertex polyhedron Co <sub>6</sub> Si <sub>2</sub> U <sub>2</sub>
U12	6h	m..	0.1982	0.1841	$\frac{1}{4}$		23-vertex polyhedron Si <sub>9</sub> Co <sub>12</sub> U <sub>2</sub>
Co13	6h	m..	0.212	0.307	$\frac{1}{4}$		9-vertex polyhedron Si <sub>4</sub> Co <sub>5</sub>
Si14	6h	m..	0.233	0.632	$\frac{1}{4}$		square prism (cube) Co <sub>6</sub> Si <sub>2</sub>
Si15	6h	m..	0.244	0.072	$\frac{1}{4}$		tricapped trigonal prism Co <sub>7</sub> U <sub>2</sub>
Co16	6h	m..	0.249	0.472	$\frac{1}{4}$		cuboctahedron Si <sub>4</sub> Co <sub>6</sub> U <sub>2</sub>
Co17	6h	m..	0.27	0.573	$\frac{1}{4}$		cuboctahedron Si <sub>4</sub> Co <sub>6</sub> U <sub>2</sub>
Co18	6h	m..	0.28	0.017	$\frac{1}{4}$		11-vertex polyhedron Si <sub>4</sub> Co <sub>5</sub> U <sub>2</sub>
Si19	6h	m..	0.3	0.332	$\frac{1}{4}$		7-vertex polyhedron Co <sub>7</sub>
Co20	6h	m..	0.311	0.169	$\frac{1}{4}$		11-vertex polyhedron Si <sub>5</sub> Co <sub>6</sub>
Co21	6h	m..	0.334	0.275	$\frac{1}{4}$		11-vertex polyhedron Si <sub>5</sub> Co <sub>6</sub>
Si22	6h	m..	0.34	0.501	$\frac{1}{4}$		10-vertex polyhedron Co <sub>6</sub> Si <sub>2</sub> U <sub>2</sub>
Co23	6h	m..	0.372	0.43	$\frac{1}{4}$		cuboctahedron Si <sub>4</sub> Co <sub>5</sub> U <sub>3</sub>
U24	6h	m..	0.4045	0.1291	$\frac{1}{4}$		23-vertex polyhedron Si <sub>9</sub> Co <sub>12</sub> U <sub>2</sub>
Co25	6h	m..	0.419	0.255	$\frac{1}{4}$		11-vertex polyhedron Si <sub>5</sub> Co <sub>6</sub>
Si26	6h	m..	0.456	0.021	$\frac{1}{4}$		tricapped trigonal prism Co <sub>7</sub> U <sub>2</sub>
U27	6h	m..	0.4622	0.3909	$\frac{1}{4}$		23-vertex polyhedron Si <sub>9</sub> Co <sub>12</sub> U <sub>2</sub>
Si28	6h	m..	0.507	0.283	$\frac{1}{4}$		tricapped trigonal prism Co <sub>9</sub>
Co29	6h	m..	0.521	0.118	$\frac{1}{4}$		11-vertex polyhedron Si <sub>5</sub> Co <sub>6</sub>
Co30	6h	m..	0.543	0.222	$\frac{1}{4}$		11-vertex polyhedron Si <sub>5</sub> Co <sub>6</sub>
Co31	6h	m..	0.619	0.196	$\frac{1}{4}$		11-vertex polyhedron Si <sub>5</sub> Co <sub>6</sub>
U32	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		23-vertex polyhedron Co <sub>12</sub> Si <sub>9</sub> U <sub>2</sub>

Transformation from published data:  $y, x, -z$

Experimental: single crystal, diffractometer, X-rays, R = 0.127

References: [1] Aksel'rud L.G., Yarmolyuk Y.P., Gladyshevskii E.I. (1980), Dopov. Akad. Nauk Ukr. RSR, Ser. A 5, 79-81.