

• An  $r_m^{(1)}$  structure of ScC<sub>2</sub> determined experimentally

 Computationally determined geometries and molecular constants compared very well with highly accurate experimental structure

• CcCRE computational method can be used to predict geometries for starting experimental spectral surveys of other 3d-dicarbides

ScC <sub>2</sub>			
	CcCRE	Ехр.	% Diff.
В (мнг)	8401.348	8421.0934	0.235
C (MHz)	7214.709	7271.3857	0.782
r <sub>Sc-C</sub> (Å)	2.065	2.048	0.827
r <sub>c-c</sub> (Å)	1.2737	1.272	0.134
<b>∠</b> c–м–c	35.93	36.2	0.749

