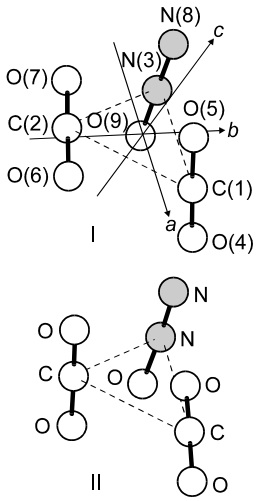
327 **$C_2N_2O_5$** **Carbon dioxide – dinitrogen monoxide (2/1)** **C_1**
MW (weakly bound complex) (large-amplitude motion)
$N_2O \cdot 2CO_2$

r_0	Å	
	I	II
C(1)–N(3)	3.638(8)	3.638(8)
C(2)–N(3)	3.427(9)	3.427(9)
C(1)–C(2)	3.521(9)	3.521(9)

θ_0	deg	
	I	II
C(1)–N(3)–C(2)	59.7(1)	59.7(1)
O(7)=C(2)–N(3)	62.6(39)	98.3(45)
O(4)=C(1)–C(2)	112.9(57)	116.7(57)
N(8)–N(3)–C(1)	123.2(4)	123.2(4)
O(7)=C(2)–N(3)–C(1) [a])	146.2(13)	121.0(4)
O(4)=C(1)–C(2)–N(3) [a])	–113.0(4)	–146.4(10)
N(8)–N(3)–C(1)–C(2) [a])	104.5(3)	104.5(3)

Atom	Structure	a_0 [Å]	b_0 [Å]	c_0 [Å]
C(1)		1.8813	0.8356	0.3372
C(2)		–0.2433	–1.9536	0.0200
N(3)		–1.6869	1.1380	–0.3049
O(4)	I	2.6517	0.9179	–0.5288
	II	2.9697	0.7107	–0.0502
O(5)	I	1.1109	0.7533	1.2032
	II	0.7929	0.9605	0.7246
O(6)	I	0.8451	–2.0785	–0.3674
	II	0.5271	–1.8713	–0.8460
O(7)	I	–1.3317	–1.8287	0.4074
	II	–1.0138	–2.0359	0.8860
N(8)		–2.4317	1.4431	0.4826
O(9)		–0.8992	0.8152	–1.1379
cm(N_2O) [b])		–1.6148	1.1084	–0.3812



Two possible structures I and II were derived. Both of them resemble a cylinder with three monomers roughly parallel to each other.

[a]) Dihedral angle.
[b]) Center of mass of N_2O.

Peebles, R.A., Peebles, S.A., Kuczkowski, R.L.: Mol. Phys. **96** (1999) 1355.