TABLE SM 1:
Force constants ,C_i, of O-C-O in dimensionless normal coordinates (in wavenumbers).[a]

i	i1	i2	i3	Cihla[b]	CCSD(T)[c]	DFT[c]
1	0	2	0	1198.888	1198.118	1179.435
2	2	0	0	677.165	675.922	661.126
3	1	2	0	-252.351	-251.682	-247.605
4	0	4	0	6.598	6.769	6.752
5	3	0	0	-43.019	-44.524	-43.672
6	2	2	0	19.428	20.653	20.814
7	1	4	0	?	-1.149	-0.879
8	0	6	0	0.068	0.012	?
9	4	0	0	1.407	1.770	1.778
10	3	2	0	4.119	-1.104	-0.880
11	2	4	0	-1.540	0.073	?
12	5	0	0	?	-0.047	-0.045
13	4	2	0	1.185	0.037	?
14	0	0	1	336.330	335.434	321.211
15	1	0	1	75.369	75.559	77.299
16	0	2	1	-28.165	-27.703	-27.348
17	2	0	1	-11.188	-11.763	-11.650
18	1	2	1	5.400	5.586	5.947
19	0	4	1	-0.187	-0.194	-0.173
20	3	0	1	0.665	0.823	0.894
21	2	2	1	0.397	-0.524	-0.471
22	1	4	1	?	0.026	?
23	4	0	1	-0.885	-0.031	-0.039
24	3	2	1	?	0.023	?
25	0	0	2	2.587	2.751	3.363
26	1	0	2	-1.052	-1.049	-0.864
27	0	2	2	0.313	0.283	?
28	2	0	2	0.097	0.129	?
29	1	2	2	?	-0.054	?
30	0	4	2	?	0.002	?
31	3	0	2	?	-0.008	?
32	2	2	2	?	0.004	?
33	0	0	3	?	-0.024	?
34	1	0	3	?	0.006	?
35	0	2	3	?	-0.001	?
36	2	0	3	?	-0.001	?

[a]

V = Sum_i {C_i*q_1^i1*q_2^i2*(q_3a^2+q_3b^2)^i3}

b

Cihla Z.,Chedin A.:J.Mol.Spectrosc.1971,40,337.

c

This study.

****
****

TABLE SM 2:

Valence force constants, C_i, of O-C-O-K+ in the curvilinear coordinates (in units providing V in wavenumbers)

a

i	i1	i2	i3	i4	i5	C_i	i	i1	i2	i3	i4	i5	C_i
1	2	0	0	0	0	414269.453	27	4	0	1	0	0	130235.298
2	1	1	0	0	0	52957.829	28	2	0	3	0	0	10067.144
3	1	0	1	0	0	-4526.592	29	0	5	0	0	0	-1104801.201
4	0	2	0	0	0	368708.055	30	0	0	0	2	0	17726.004
5	0	1	1	0	0	4906.581	31	1	0	0	2	0	-27082.049
6	0	0	2	0	0	5640.284	32	0	1	0	2	0	-26168.103
7	3	0	0	0	0	-970691.799	33	0	0	1	2	0	294.377

8	2	1	0	0	0	-59321.669	34	2	0	0	2	0	7362.284
9	1	2	0	0	0	-59637.498	35	1	1	0	2	0	54473.907
10	1	1	1	0	0	1171.050	36	0	2	0	2	0	11651.465
11	1	0	2	0	0	1693.935	37	0	0	0	4	0	1702.137
12	0	3	0	0	0	-855778.300	38	0	0	0	0	2	963.964
13	0	2	1	0	0	-4309.541	39	0	0	0	1	1	341.604
14	0	1	2	0	0	-4404.938	40	1	0	0	0	2	-954.761
15	0	0	3	0	0	-9179.636	41	1	0	0	1	1	-1671.797
16	4	0	0	0	0	1404577.839	42	0	1	0	0	2	-1808.878
17	3	1	0	0	0	57684.043	43	0	1	0	1	1	2374.504
18	3	0	1	0	0	-4933.214	44	0	0	1	0	2	-1096.799
19	2	1	1	0	0	6804.893	45	0	0	1	1	1	298.622
20	2	0	2	0	0	-2788.254	46	0	2	0	0	2	-2167.576
21	1	3	0	0	0	75954.068	47	0	1	1	0	2	343.576
22	1	0	3	0	0	-920.272	48	0	0	2	0	2	868.889
23	0	4	0	0	0	1224176.635	49	0	0	2	1	1	-804.083
24	0	1	3	0	0	3094.487	50	0	0	0	2	2	799.350
25	0	0	4	0	0	5999.940	51	0	0	0	0	4	213.241
26	5	0	0	0	0	-1420607.199							

==========

a

V = Sum_i {C_i*(R_OC-1.158123)^i1*(R_CO-1.181405)^i2*(R_OK-2.678163)^i3*
\gamma_x^i4*\chi_x^i5}