Table 2. Electron densities at BCP (a.u.) and sum of electron densities in the structures with optimized OH distances in O···O hydrogen bridge of 2.403(3) Å.

Positions of K^+	$\rho(r)_{OH(1)}$	$\rho(r)_{OH(2)}$	$\rho(r)_{C=O(1)}$	$\rho(r)_{C=O(2)}$	$\rho(r)_{C-O(1)}$	$\rho(r)_{C-O(2)}$	$\Sigma\rho(r)$
0	0.1522	0.2009	0.4021	0.3909	0.3601	0.3519	2.7163
1	0.1097	0.2789	0.3986	0.3928	0.3752	0.3488	2.7632
2	0.1134	0.2707	0.3973	0.3928	0.3765	0.3505	2.7590
3	0.1291	0.2374	0.4018	0.3921	0.3687	0.3518	2.7374
4	0.2634	0.1170	0.4039	0.3846	0.3404	0.3578	2.7257
5	0.2583	0.1192	0.4038	0.3850	0.3411	0.3577	2.7239
6	0.2847	0.1080	0.4041	0.3888	0.3369	0.3535	2.7347
1,2	0.1002	0.3054	0.3938	0.3941	0.3824	0.3488	2.7830
1,6	0.2039	0.1479	0.4010	0.3908	0.3473	0.3506	2.7016
2,3	0.1086	0.2825	0.3971	0.3936	0.3796	0.3511	2.7681
3,4	0.2485	0.1235	0.4038	0.3860	0.3437	0.3582	2.7212
4,5	0.2910	0.1059	0.4049	0.3790	0.3377	0.3603	2.7375
5,6	0.3055	0.1007	0.4050	0.3836	0.3351	0.3564	2.7449
1,2,3	0.0978	0.3129	0.3937	0.3947	0.3848	0.3500	2.7904
1,2,6	0.1181	0.2555	0.3990	0.3931	0.3730	0.3475	2.7461
2,3,6	0.2169	0.1397	0.3992	0.3916	0.3498	0.3535	2.7086
4,5,6	0.3235	0.0950	0.4059	0.3775	0.3337	0.3587	2.7522
1,2,3,4,5,6	0.2433	0.1234	0.3997	0.3839	0.3459	0.3579	2.7143

Table 3. Topological parameters in the structures with optimized OH distances in O···O hydrogen bridge of 2.403(3) Å: elipticity at BCP (ε(r)), distance of BCP to the centre of the OH bond (d(BCP) [Å]), electron kinetic energy density at BCP (G(r)), electron potential energy density at BCP (V(r)).

Positions of K^+	$\varepsilon(r)_1$	$\varepsilon(r)_2$	$d(BCP)_1$	$d(BCP)_2$	$G(r)_1$	$G(r)_2$	$V(r)_1$	$V(r)_2$
0	0.0206	0.0174	0.1683	0.0891	12.8313	13.6354	-32.7237	-51.6497
1	0.0269	0.0144	0.1590	0.0841	10.8768	14.0990	-19.5367	-89.4278
2	0.0221	0.0140	0.1613	0.0853	11.0007	13.9322	-20.5265	-85.5352
3	0.0218	0.0151	0.1651	0.0874	11.8193	13.5298	-25.1070	-68.3748
4	0.0144	0.0244	0.1776	0.0939	13.8205	11.1797	-81.7233	-21.5303
5	0.0146	0.0237	0.1774	0.0938	13.7210	11.2960	-79.0417	-22.1832
6	0.0144	0.0307	0.1775	0.0939	14.5289	10.7069	-93.0817	-19.0312
1,2	0.0258	0.0137	0.1548	0.0819	10.3428	15.4545	-17.0586	-104.0153
1,6	0.0177	0.0242	0.1738	0.0919	13.6308	12.5919	-53.5837	-31.4742
2,3	0.0214	0.0134	0.1596	0.0844	10.7314	14.3744	-19.2348	-91.9901
3,4	0.0110	0.0220	0.1772	0.0937	13.5879	11.5331	-74.0364	-23.4995
4,5	0.0138	0.0241	0.1774	0.0939	14.8364	10.6014	-96.6303	-18.5363
5,6	0.0139	0.0308	0.1760	0.0931	15.6580	10.3244	-104.4927	-17.1358
1,2,3	0.0251	0.0134	0.1534	0.0812	10.1913	15.9778	-16.4479	-108.3046
1,2,6	0.0231	0.0158	0.1635	0.0865	11.3052	13.5680	-22.1270	-78.1291
2,3,6	0.0142	0.0232	0.1756	0.0929	13.5451	12.3242	-59.2593	-28.7188
4,5,6	0.0139	0.0303	0.1733	0.0917	16.8300	10.0368	-114.1873	-15.7564
1,2,3,4,5,6	0.0133	0.0217	0.1793	0.0949	13.4502	11.5699	-72.6886	-23.8224

Table 4. Electron densities at BCP (a.u.) and sum of electron densities in the structures with optimized OHO hydrogen bond.

Positions of K^+	$\rho(r)_{OH(1)}$	$\rho(r)_{OH(2)}$	$\rho(r)_{C=O(1)}$	$\rho(r)_{C=O(2)}$	$\rho(r)_{C-O(1)}$	$\rho(r)_{C-O(2)}$	$\Sigma\rho(r)$
0	0.1547	0.2143	0.4017	0.3909	0.3498	0.3518	2.7218
1	0.1004	0.2876	0.3986	0.3929	0.3580	0.3487	2.7447
2	0.1149	0.2721	0.3972	0.3928	0.3724	0.3506	2.7578
3	0.1373	0.2412	0.4016	0.3921	0.3600	0.3519	2.7407
4	0.2620	0.1184	0.4038	0.3846	0.3367	0.3578	2.7219
5	0.2560	0.1222	0.4037	0.3851	0.3376	0.3576	2.7210
6	0.2870	0.1044	0.4041	0.3887	0.3309	0.3537	2.7272
1,2	0.0875	0.3103	0.3940	0.3942	0.3740	0.3487	2.7659
1,6	0.1749	0.1768	0.4005	0.3911	0.3403	0.3496	2.6933
2,3	0.1103	0.2829	0.3971	0.3936	0.3791	0.3512	2.7698
3,4	0.2429	0.1308	0.4036	0.3861	0.3438	0.3580	2.7228
4,5	0.2930	0.1026	0.4049	0.3790	0.3354	0.3640	2.7375
5,6	0.3078	0.0953	0.4051	0.3836	0.3308	0.3566	2.7376
1,2,3	0.0864	0.3155	0.3939	0.3948	0.3800	0.3495	2.7757
1,2,6	0.1121	0.2613	0.3958	0.3932	0.3659	0.3474	2.7351
2,3,6	0.2052	0.1542	0.3997	0.3917	0.3564	0.3530	2.7185
4,5,6	0.3251	0.0875	0.4059	0.3774	0.3306	0.3589	2.7429
1,2,3,4,5,6	0.2485	0.1172	0.4000	0.3839	0.3515	0.3581	2.7193

Table 5. Topological parameters in the structures with optimized OHO hydrogen bridge: elipticity at BCP (ε(r)), distance of BCP to the centre of the OH bond (d(BCP) [Å]), electron kinetic energy density at BCP (G(*r*)), electron potential energy density at BCP (V(r)).

Positions of K^+	$\varepsilon(r)_1$	$\varepsilon(r)_2$	$d(BCP)_1$	$d(BCP)_2$	$G(r)_1$	$G(r)_2$	$V(r)_1$	$V(r)_2$
0	0.021	0.017	0.0879	0.0912	13.354	14.039	-33.552	-57.483
1	0.030	0.014	0.0841	0.0939	9.887	14.399	-16.988	-94.489
2	0.022	0.014	0.0855	0.0930	11.187	13.954	-20.965	-86.332
3	0.021	0.015	0.0866	0.0927	12.662	13.892	-27.680	-70.239
4	0.017	0.024	0.0938	0.0860	13.810	11.314	-80.976	-21.962
5	0.015	0.023	0.0936	0.0864	13.747	11.559	-77.768	-23.061
6	0.015	0.032	0.0937	0.0839	14.488	10.349	-94.019	-18.038
1,2	0.029	0.014	0.0822	0.0929	8.836	15.490	-13.861	-106.813
1,6	0.021	0.021	0.0902	0.0903	13.525	13.551	-41.432	-42.152
2,3	0.021	0.013	0.0843	0.0942	10.929	14.457	-19.695	-92.236
3,4	0.014	0.021	0.0933	0.0873	13.713	12.111	-71.348	-25.746
4,5	0.014	0.025	0.0938	0.0837	14.815	10.259	-97.525	-17.641
5,6	0.014	0.032	0.0928	0.0820	15.525	9.735	-105.247	-15.749
1,2,3	0.028	0.013	0.0816	0.0925	8.807	15.837	-13.615	-109.663
1,2,6	0.025	0.016	0.0864	0.0946	10.741	13.614	-20.358	-81.327
2,3,6	0.014	0.022	0.0919	0.0892	13.810	13.100	-54.103	-33.685
4,5,6	0.014	0.032	0.0912	0.0801	16.487	9.163	-114.254	-13.910
1,2,3,4,5,6	0.013	0.023	0.0954	0.0878	13.381	11.054	-75.472	-21.980

Table 6. Calculated electron densities at BCP (a.u.) and sum of electron densities in the structures with the solid state geometry of the OHO hydrogen bond.

Positions of K^+	$\rho(r)_{OH(1)}$	$\rho(r)_{OH(2)}$	$\rho(r)_{C=O(1)}$	$\rho(r)_{C=O(2)}$	$\rho(r)_{C-O(1)}$	$\rho(r)_{C-O(2)}$	$\Sigma\rho(r)$
0	0.1729	0.1768	0.4023	0.3906	0.3549	0.3528	2.7085
1	0.1689	0.1798	0.3992	0.3919	0.3552	0.3517	2.7048
2	0.1707	0.1785	0.398	0.3919	0.3581	0.3532	2.7086
3	0.1722	0.1774	0.4023	0.3915	0.3563	0.3537	2.7116
4	0.1747	0.1743	0.4034	0.3855	0.3547	0.355	2.7058
5	0.1745	0.1746	0.4033	0.3859	0.3548	0.3555	2.7068
6	0.176	0.1723	0.4035	0.3896	0.3532	0.3505	2.7032
1,2	0.167	0.1814	0.3946	0.393	0.3584	0.3522	2.7047
1,6	0.1718	0.1751	0.4007	0.3911	0.3537	0.3495	2.6999
2,3	0.17	0.1791	0.3979	0.3926	0.3593	0.3541	2.7112
3,4	0.174	0.1748	0.4033	0.3868	0.3561	0.3563	2.7095
4,5	0.1763	0.1722	0.4043	0.3803	0.3546	0.3578	2.7037
5,6	0.1776	0.1705	0.4044	0.3847	0.3532	0.3533	2.7018
1,2,3	0.1664	0.182	0.3946	0.3937	0.3596	0.3531	2.7075
1,2,6	0.1697	0.1767	0.3965	0.3924	0.3569	0.3501	2.7003
2,3,6	0.1729	0.1745	0.3995	0.392	0.3579	0.352	2.7069
4,5,6	0.1794	0.1685	0.4053	0.3788	0.3532	0.3554	2.6988
1,2,3,4,5,6	0.1722	0.1728	0.3992	0.3847	0.3579	0.3559	2.7007

Table 7. Topological parameters in the structures with the solid state geometry of the OHO hydrogen bond: elipticity at BCP (ε(r)), distance of BCP to the centre of the OH bond (d(BCP) [Å]), electron kinetic energy density at BCP (G(r)), electron potential energy density at BCP (V(r)).

Positions of K^+	$\varepsilon(r)_1$	$\varepsilon(r)_2$	$d(BCP)_1$	$d(BCP)_2$	$G(r)_1$	$G(r)_2$	$V(r)_1$	$V(r)_2$
0	0.0190	0.0193	0.0901	0.0904	13.42575	13.40586	-40.3439	-41.769
1	0.0194	0.0198	0.0896	0.0906	13.69503	13.10598	-39.4313	-42.5237
2	0.0163	0.0188	0.0901	0.0907	13.58181	13.22073	-39.9368	-42.2323
3	0.0178	0.0188	0.0901	0.0905	13.46859	13.34466	-40.2	-41.9199
4	0.0187	0.0171	0.0967	0.0845	13.2192	13.57875	-40.8424	-41.2916
5	0.0188	0.0171	0.0904	0.0905	13.23909	13.5558	-40.7862	-41.3478
6	0.0196	0.0209	0.0905	0.0899	13.0968	13.68891	-41.1653	-41.0112
1,2	0.0172	0.0197	0.0945	0.0907	13.84497	12.95757	-39.0347	-42.9098
1,6	0.0199	0.0212	0.0905	0.0907	13.34007	13.3569	-40.3053	-41.5163
2,3	0.0155	0.0184	0.0901	0.0908	13.62924	13.16106	-39.7859	-42.3727
3,4	0.0179	0.0167	0.0906	0.0907	13.25898	13.51908	-40.7125	-41.4531
4,5	0.0186	0.0154	0.0906	0.0904	13.05396	13.73328	-41.2495	-40.8529
5,6	0.0195	0.0192	0.0905	0.0897	12.94839	13.83732	-41.5373	-40.2843
1,2,3	0.0164	0.0191	0.0893	0.0907	13.89546	12.90861	-38.8978	-43.0326
1,2,6	0.0177	0.0208	0.0900	0.0911	13.48542	13.18095	-39.9087	-41.9691
2,3,6	0.0164	0.0199	0.0909	0.0907	13.28499	13.41657	-40.6388	-41.3689
4,5,6	0.0194	0.0178	0.0904	0.0892	12.79998	14.01021	-41.9129	-39.7964
1,2,3,4,5,6	0.0165	0.0166	0.0952	0.0915	13.16106	13.41504	-40.6985	-41.2881