

# **Intramolecular double proton transfer - from 2-hydroxy-2-iminoacetic acid to 2-amino-2-oxoacetic acid**

## *Supplementary material*

by

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Table S1. QTAIM parameters of the species analyzed in this study (in au), the designations of atoms correspond to those of Scheme 1.

	O8H9			O4H9			N5H7			O3H7		
	$\rho(r)$	$V^2(r)$	$V(r)$	$\rho(r)$	$V^2(r)$	$V(r)$	$\rho(r)$	$V^2(r)$	$V(r)$	$\rho(r)$	$V^2(r)$	$V(r)$
I	0,027	0,109	-0,023	0,360	-2,883	-0,860	0,351	-1,970	-0,606	-	-	-
	0,026	0,101	-0,020	0,349	-2,467	-0,744	0,337	-1,719	-0,528	-	-	-
	0,027	0,105	-0,023	0,346	-2,466	-0,759	0,334	-1,776	-0,557	-	-	-
	0,027	0,117	-0,022	0,353	-2,620	-0,789	0,350	-2,033	-0,613	-	-	-
II	-	-	-	0,370	-2,954	-0,882	0,352	-1,957	-0,606	-	-	-
	-	-	-	0,358	-2,518	-0,760	0,338	-1,707	-0,528	-	-	-
	-	-	-	0,354	-2,505	-0,773	0,335	-1,752	-0,555	-	-	-
	-	-	-	0,363	-2,685	-0,809	0,351	-2,024	-0,613	-	-	-
III	0,363	-2,913	-0,868	-	-	-	0,025	0,096	-0,020	0,359	-2,887	-0,859
	0,351	-2,488	-0,750	-	-	-	0,025	0,092	-0,019	0,347	-2,466	-0,741
	0,348	-2,485	-0,764	-	-	-	0,026	0,096	-0,021	0,344	-2,459	-0,754
	0,356	-2,651	-0,798	-	-	-	0,025	0,100	-0,020	0,352	-2,625	-0,789
IV	-	-	-	-	-	-	-	-	-	-	-	-
	0,287	-1,819	-0,585	0,061	0,128	-0,058	0,333	-1,751	-0,526	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-
V	-	-	-	-	-	-	-	-	-	-	-	-
	0,365	-2,924	-0,875	-	-	-	-	-	-	0,370	-2,957	-0,882
	0,354	-2,496	-0,756	0,024	0,101	-0,019	-	-	-	0,358	-2,521	-0,760
	0,351	-2,497	-0,771	0,024	0,105	-0,021	-	-	-	0,353	-2,506	-0,772
VI	0,359	-2,661	-0,804	-	-	-	-	-	-	0,363	-2,689	-0,809
	0,371	-2,962	-0,885	-	-	-	-	-	-	0,370	-2,962	-0,883
	0,359	-2,524	-0,763	-	-	-	-	-	-	0,357	-2,519	-0,760
	0,355	-2,509	-0,775	-	-	-	-	-	-	0,353	-2,504	-0,772
VII	0,365	-2,695	-0,813	-	-	-	-	-	-	0,364	-2,701	-0,812
	0,369	-2,954	-0,884	-	-	-	-	-	-	0,369	-2,962	-0,882
	0,358	-2,528	-0,765	-	-	-	-	-	-	0,357	-2,522	-0,759
	0,355	-2,522	-0,780	-	-	-	-	-	-	0,352	-2,506	-0,770
VIII	0,362	-2,685	-0,811	-	-	-	-	-	-	0,363	-2,699	-0,810
	0,374	-2,962	-0,890	-	-	-	0,028	0,104	-0,023	0,361	-2,896	-0,866
	0,362	-2,526	-0,768	-	-	-	0,027	0,100	-0,021	0,350	-2,475	-0,748
	0,358	-2,512	-0,781	-	-	-	0,028	0,103	-0,024	0,347	-2,476	-0,763
IX	0,368	-2,694	-0,817	-	-	-	0,028	0,105	-0,022	0,355	-2,632	-0,795
	0,375	-2,964	-0,893	-	-	-	-	-	-	0,371	-2,957	-0,884
	0,363	-2,523	-0,770	-	-	-	-	-	-	0,359	-2,518	-0,761
	0,358	-2,506	-0,781	-	-	-	-	-	-	0,354	-2,502	-0,773
X	0,369	-2,695	-0,819	-	-	-	-	-	-	0,364	-2,689	-0,811
	0,369	-2,916	-0,874	-	-	-	0,331	-1,979	-0,592	0,031	0,115	-0,024
	0,357	-2,486	-0,754	-	-	-	0,319	-1,708	-0,513	0,029	0,107	-0,021
	0,355	-2,503	-0,773	-	-	-	0,313	-1,787	-0,544	0,032	0,115	-0,026
	0,362	-2,654	-0,803	-	-	-	0,329	-2,002	-0,592	0,031	0,122	-0,025

Table S2. Atoms' coordinates (Å) and absolute energies (a.u.).

	B3LYP/6-311++G(d,p)			B3LYP/6-311++G(3df,3pd)			B3LYP/aug-cc-pVTZ			MP2/6-311++G(d,p)		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
<b>I</b>	E=-358.5904			E=-358.6171			E=-358.6233			E=-357.7000		
C1	-0.7261	-0.1929	0.0002	0.7247	-0.1905	-0.0004	0.7249	-0.1897	-0.0001	0.7236	-0.1911	-0.0040
C2	0.7686	0.2149	0.0002	-0.7677	0.2132	-0.0002	-0.7674	0.2133	0.0000	-0.7665	0.2102	-0.0002
O3	1.1412	1.3573	0.0000	-1.1439	1.3520	0.0000	-1.1458	1.3530	0.0000	-1.1449	1.3580	-0.0206
O4	1.5691	-0.8462	-0.0001	-1.5623	-0.8487	0.0004	-1.5622	-0.8508	0.0001	-1.5654	-0.8555	0.0188
N5	-1.5691	0.8504	-0.0001	1.5636	0.8517	0.0000	1.5638	0.8529	0.0000	1.5617	0.8614	0.0448
H6	-2.5650	0.6953	-0.0002	2.5577	0.7006	0.0002	2.5578	0.7027	0.0000	2.5526	0.7071	-0.0612
H7	-1.1952	1.7880	0.0000	1.1850	1.7848	0.0000	1.1851	1.7857	0.0000	1.1763	1.7892	-0.0530
O8	-1.0228	-1.3780	0.0000	1.0247	-1.3722	0.0000	1.0255	-1.3731	0.0000	1.0302	-1.3795	-0.0227
H9	0.9885	-1.6332	0.0001	-0.9774	-1.6316	0.0002	-0.9748	-1.6328	0.0001	-0.9634	-1.6236	0.0213
<b>II</b>	E=-358.5846			E=-358.6104			E=-358.6167			E=-357.6950		
C1	0.7595	-0.2241	-0.0005	-0.7593	-0.2227	-0.0003	0.7592	-0.2219	-0.0002	-0.7549	-0.2195	-0.0104
C2	-0.7402	0.1646	-0.0004	0.7394	0.1641	0.0000	-0.7389	0.1646	-0.0002	0.7378	0.1618	-0.0080
O3	-1.1251	1.3091	-0.0003	1.1237	1.3057	-0.0003	-1.1254	1.3071	-0.0001	1.1309	1.3073	-0.0964
O4	-1.5351	-0.9047	0.0005	1.5336	-0.9034	0.0003	-1.5330	-0.9055	0.0002	1.5237	-0.9135	0.0903
N5	1.5475	0.8772	0.0004	-1.5448	0.8752	0.0000	1.5451	0.8758	0.0002	-1.5410	0.8836	0.1210
H6	2.5485	0.7639	0.0010	-2.5436	0.7639	0.0003	2.5436	0.7648	0.0005	-2.5326	0.7696	-0.0240
H7	1.1353	1.7973	0.0006	-1.1296	1.7915	0.0001	1.1302	1.7918	0.0004	-1.1239	1.7930	-0.0100
O8	1.1376	-1.3740	-0.0002	-1.1377	-1.3702	0.0001	1.1382	-1.3709	-0.0002	-1.1407	-1.3712	-0.0903
H9	-2.4515	-0.5875	0.0009	2.4491	-0.5872	0.0004	-2.4492	-0.5893	0.0003	2.4344	-0.5833	0.0693
<b>III</b>	E=-358.5681			E=-358.5958			E=-358.6020			E=-357.6795		
C1	0.0000	0.7426	0.0000	0.0000	0.7417	0.0000	0.0000	0.7419	0.0000	0.0000	0.7401	0.0000
C2	-0.0193	-0.7820	0.0000	-0.0179	-0.7795	0.0000	-0.0177	-0.7792	0.0000	-0.0206	-0.7813	0.0000
O3	1.1803	-1.3442	0.0000	1.1798	-1.3403	0.0000	1.1821	-1.3401	0.0000	1.1802	-1.3455	0.0000
O4	-1.0649	-1.3824	0.0000	-1.0601	-1.3812	0.0000	-1.0605	-1.3829	0.0000	-1.0740	-1.3810	0.0000
N5	1.1229	1.3258	0.0000	1.1173	1.3297	0.0000	1.1174	1.3303	0.0000	1.1348	1.3236	0.0000
H6	1.0552	2.3428	0.0000	1.0448	2.3443	0.0000	1.0442	2.3447	0.0000	1.0420	2.3405	0.0000
H7	1.8323	-0.6141	0.0000	1.8313	-0.6114	0.0000	1.8324	-0.6092	0.0000	1.8137	-0.6014	0.0000
O8	-1.2111	1.3069	0.0000	-1.2109	1.2981	0.0000	-1.2129	1.2986	0.0000	-1.2095	1.3098	0.0000
H9	-1.8665	0.5855	0.0000	-1.8605	0.5726	0.0000	-1.8619	0.5717	0.0000	-1.8489	0.5767	0.0000
<b>IV</b>	E=-358.5620											
C1	0.0000	0.6839	0.0000									
C2	0.0554	-0.8857	0.0000									
O3	1.1719	-1.3881	0.0000									
O4	-1.1281	-1.2986	0.0000									
N5	1.0763	1.4171	0.0000									
H6	1.0614	2.4280	0.0000									
H7	1.9542	0.9072	0.0000									
O8	-1.1920	1.1508	0.0000									
H9	-1.6968	0.2429	0.0000									
<b>V</b>	E=-358.5615			E=-358.5887			E=-358.5951			E=-357.6729		
C1	-0.0496	-0.7733	0.0000	-0.0487	-0.7735	0.0000	-0.0487	-0.7736	0.0000	-0.0441	-0.7699	0.0000
C2	0.0000	0.7433	0.0000	0.0000	0.7414	0.0000	0.0000	0.7411	0.0000	0.0000	0.7439	0.0000
O3	-1.1883	1.3376	0.0000	-1.1863	1.3353	0.0000	-1.1887	1.3346	0.0000	-1.1963	1.3251	0.0000
O4	1.0628	1.3253	0.0000	1.0602	1.3226	0.0000	1.0609	1.3240	0.0000	1.0665	1.3317	0.0000
N5	-1.1416	-1.4045	0.0000	-1.1384	-1.4033	0.0000	-1.1385	-1.4037	0.0000	-1.1483	-1.4030	0.0000
H6	-0.9795	-2.4135	0.0000	-0.9826	-2.4109	0.0000	-0.9828	-2.4112	0.0000	-0.9560	-2.4088	0.0000
H7	-1.0365	2.2955	0.0000	-1.0351	2.2920	0.0000	-1.0387	2.2921	0.0000	-1.0317	2.2802	0.0000
O8	1.1843	-1.3220	0.0000	1.1825	-1.3172	0.0000	1.1846	-1.3174	0.0000	1.1886	-1.3205	0.0000
H9	1.8340	-0.5981	0.0000	1.8279	-0.5906	0.0000	1.8291	-0.5891	0.0000	1.8207	-0.5840	0.0000

<b>VI</b>	E=-358.5600			E=-358.5867			E=-358.5930			E=-357.6728		
C1	0.0000	0.7617	0.0000	0.0000	0.7616	0.0000	-0.0525	-0.7595	0.0000	0.0200	-0.0349	-0.0378
C2	-0.0552	-0.7612	0.0000	-0.0527	-0.7598	0.0000	0.0000	0.7612	0.0000	-0.6841	-1.2962	0.4284
O3	1.1929	-1.2796	0.0000	1.1895	-1.2821	0.0000	1.2772	1.1971	0.0000	0.0795	-2.3816	0.1623
O4	-1.0584	-1.4158	0.0000	-1.0557	-1.4109	0.0000	-0.9568	1.4808	0.0000	-1.7714	-1.3308	0.9471
N5	1.0401	1.4807	0.0000	1.0379	1.4782	0.0000	0.9337	-1.5467	0.0000	1.0541	0.0338	-0.7830
H6	1.8843	0.9130	0.0000	1.8821	0.9149	0.0000	1.8156	-1.0454	0.0000	1.3587	-0.9079	-1.0255
H7	1.1105	-2.2451	0.0000	1.0981	-2.2457	0.0000	1.2526	2.1649	0.0000	-0.4407	-3.1535	0.4282
O8	-1.2357	1.2850	0.0000	-1.2333	1.2839	0.0000	-1.3205	-1.1953	0.0000	-0.5976	1.0601	0.4320
H9	-1.1339	2.2483	0.0000	-1.1334	2.2462	0.0000	-1.2883	-2.1627	0.0000	-0.1019	1.8104	0.0738
<b>VII</b>	E=-358.5595			E=-358.5875			E=-358.5938			E=-357.6712		
C1	-0.0019	-0.7968	0.0000	-0.0040	-0.7966	0.0000	-0.0042	-0.7966	0.0000	0.0009	-0.7918	0.0000
C2	0.0000	0.7268	0.0000	0.0000	0.7244	0.0000	0.0000	0.7246	0.0000	0.0000	0.7286	0.0000
O3	-1.2292	1.2564	0.0000	-1.2232	1.2602	0.0000	-1.2249	1.2606	0.0000	-1.2352	1.2479	0.0000
O4	1.0227	1.3686	0.0000	1.0232	1.3610	0.0000	1.0244	1.3619	0.0000	1.0273	1.3746	0.0000
N5	-1.0182	-1.5455	0.0000	-1.0189	-1.5426	0.0000	-1.0189	-1.5433	0.0000	-1.0212	-1.5530	0.0000
H6	-1.8716	-0.9914	0.0000	-1.8729	-0.9940	0.0000	-1.8727	-0.9948	0.0000	-1.8575	-0.9693	0.0000
H7	-1.1446	2.2222	0.0000	-1.1300	2.2239	0.0000	-1.1323	2.2249	0.0000	-1.1366	2.2115	0.0000
O8	1.2421	-1.3036	0.0000	1.2370	-1.3009	0.0000	1.2379	-1.3017	0.0000	1.2431	-1.3024	0.0000
H9	1.8703	-0.5643	0.0000	1.8629	-0.5606	0.0000	1.8640	-0.5609	0.0000	1.8554	-0.5522	0.0000
<b>VIII</b>	E=-358.5562			E=-358.5838			E=-358.5902			E=-357.6682		
C1	0.0000	0.7215	0.0000	0.0000	0.7196	0.0000	0.0000	0.7197	0.0000	0.0000	0.7189	0.0000
C2	-0.0751	-0.8122	0.0000	-0.0740	-0.8118	0.0000	-0.0732	-0.8111	0.0000	-0.0731	-0.8085	0.0000
O3	1.1356	-1.3790	0.0000	1.1339	-1.3768	0.0000	1.1372	-1.3764	0.0000	1.1383	-1.3793	0.0000
O4	-1.1038	-1.4223	0.0000	-1.1004	-1.4219	0.0000	-1.1000	-1.4232	0.0000	-1.1103	-1.4190	0.0000
N5	1.1529	1.2515	0.0000	1.1481	1.2525	0.0000	1.1475	1.2541	0.0000	1.1622	1.2547	0.0000
H6	1.1702	2.2707	0.0000	1.1601	2.2698	0.0000	1.1576	2.2712	0.0000	1.1483	2.2758	0.0000
H7	1.7928	-0.6562	0.0000	1.7903	-0.6549	0.0000	1.7927	-0.6527	0.0000	1.7795	-0.6454	0.0000
O8	-1.2127	1.2907	0.0000	-1.2098	1.2886	0.0000	-1.2130	1.2872	0.0000	-1.2166	1.2834	0.0000
H9	-1.1356	2.2537	0.0000	-1.1325	2.2504	0.0000	-1.1366	2.2497	0.0000	-1.1164	2.2438	0.0000
<b>IX</b>	E=-358.5512			E=-358.5784			E=-358.5848			E=-357.6642		
C1	0.0000	0.7521	0.0000	0.0000	0.7196	0.0000	0.0000	0.7507	0.0000	-0.0008	0.7514	-0.0658
C2	0.0079	-0.7721	0.0000	-0.0740	-0.8118	0.0000	0.0074	-0.7712	0.0000	-0.0345	-0.7216	-0.4226
O3	-1.2332	-1.2793	0.0000	1.1339	-1.3768	0.0000	-1.2326	-1.2804	0.0000	-1.1677	-1.3033	0.0024
O4	1.0121	-1.4320	0.0000	-1.1004	-1.4219	0.0000	1.0111	-1.4300	0.0000	0.8512	-1.2827	-1.0235
N5	-1.0891	1.3936	0.0000	1.1481	1.2525	0.0000	-1.0856	1.3929	0.0000	-1.0878	1.4092	0.0460
H6	-0.9561	2.4074	0.0000	1.1601	2.2698	0.0000	-0.9580	2.4044	0.0000	-0.9064	2.3947	0.2574
H7	-1.1412	-2.2443	0.0000	1.7903	-0.6549	0.0000	-1.1375	-2.2443	0.0000	-1.1216	-2.2210	-0.3041
O8	1.2718	1.2141	0.0000	-1.2098	1.2886	0.0000	1.2700	1.2146	0.0000	1.2827	1.1656	0.0505
H9	1.2679	2.1796	0.0000	-1.1325	2.2504	0.0000	1.2630	2.1793	0.0000	1.2811	2.1162	0.2177
<b>X</b>	E=-358.5331			E=-358.5611			E=-358.5675			E=-357.6391		
C1	-0.6673	-0.0480	-0.0002	-0.6643	-0.0457	0.0000	-0.6637	-0.0446	0.0000	0.6591	-0.0480	-0.0038
C2	0.9593	-0.0462	-0.0001	0.9495	-0.0486	0.0000	0.9484	-0.0494	0.0000	-0.9414	-0.0480	-0.0013
O3	1.3504	1.1313	-0.0003	1.3487	1.1251	0.0000	1.3501	1.1258	-0.0005	-1.3428	1.1352	-0.0221
O4	1.4555	-1.1587	0.0004	1.4472	-1.1592	-0.0001	1.4460	-1.1622	0.0004	-1.4425	-1.1682	0.0211
N5	-1.2146	1.1336	0.0003	-1.2037	1.1340	0.0002	-1.2024	1.1358	0.0003	1.1995	1.1387	0.0258
H6	-2.2055	1.3425	0.0006	-2.1919	1.3418	0.0002	-2.1899	1.3456	0.0004	2.1871	1.3566	-0.0003
H7	-0.4930	1.8671	0.0003	-0.4781	1.8609	0.0003	-0.4747	1.8608	0.0006	0.4537	1.8500	0.0088
O8	-1.3371	-1.1638	-0.0003	-1.3355	-1.1573	-0.0001	-1.3370	-1.1576	-0.0002	1.3313	-1.1653	-0.0180
H9	-2.3011	-1.0492	-0.0002	-2.2981	-1.0438	-0.0001	-2.2999	-1.0413	-0.0002	2.2882	-1.0156	-0.0066