## Supplementary Information to: Intramolecular proton bonding in aliphatic dicarboxylate anions: dynamic conformational landscapes and spectral signatures

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Fig. S1: Contour plot describing the electronic energy surface of the glutarate ion as a function of the two dihedral angles of its carbon backbone. The local energy wells for the low-energy proton-bonded configurations 5A and 5B and for the higher-energy linear chain configuration, 5L, are indicated. Computations are performed by iteratively scanning the dihedral angles  $\Omega_1 \equiv \Omega_{1234}$  and  $\Omega_2 \equiv \Omega_{2345}$  (see carbon numbering in the 5A structure) and computing electronic energies at the B3LYP-D3(BJ)/6-311++G(d,p) level.



Fig. S2: Low-energy conformations of the aliphatic dicarboxylate anions included in the present study. Zero-point energies at the MP2/aug-cc-pVTZ level are provided in kJ·mol<sup>-1</sup>. The point symmetry of the backbone is indicated  $(C_1, C_2 \text{ or } C_s)$ , along with the *anti-anti* (AA) or *anti-syn* (AS) type of proton bonding arrangement.



Fig. S3: Typical laser power curve reaching the ion trap in the region of absorbance of the diamond beam splitter incorporated to our mass spectrometer. The attenuation due to diamond absorbance induces a "W"-shaped modulation of the IRMPD signal in the  $1800-2300 \,\mathrm{cm}^{-1}$  spectral window.

**Table S1**: Structural parameters of the low-energy conformers of the aliphatic dicarboxylate anions represented in Fig. S2. The backbone adopts a configuration within a point symmetry  $C_2$  or  $C_1$  as indicated.  $\Omega_k$  (k=1-5) stands for the dihedral angles defined by the carbon atoms  $C_k$ - $C_{k+1}$ - $C_{k+2}$ - $C_{k+3}$  in the alkyl chain.  $\Theta$  denotes the relative angle between the planes of the two carboxylate groups. The proton bond is characterized by the two O–H distances r and R. Relative zero-point corrected electronic energies ( $E_{ZP}^{MP2}$ ) are given in kJ·mol<sup>-1</sup>, angles in degrees and distances in Å . All data obtained at the MP2/aug-cc-VTZ level. Relative energies at the B3LYP-D3(BJ)/6-311++G(d,p) level ( $E_{ZP}^{B3D3}$ ) are included for comparison.

Conformer	Energy		Backbone						Carboxylates		
	$\rm E_{ZP}^{B3D3}$	$\rm E_{ZP}^{MP2}$	$\Omega_1$	$\Omega_2$	$\Omega_3$	$\Omega_4$	$\Omega_5$	Θ	r	R	
Succinate											
$4A(C_2)$	0	0	80	-	-	-	-	27	1.12	1.30	
Glutarate											
$5A(C_2)$	0	0	58	55	-	-	-	55	1.10	1.34	
$5B(C_1)$	9.3	14.1	125	-64	_	—	-	31	1.04	1.46	
Adipate											
$6A(C_1)$	0	0	-67	-72	72	_	-	62	1.04	1.45	
$6B(C_2)$	7.4	5.9	98	-51	93	_	-	65	1.12	1.31	
$6C(C_2)$	11.5	11.3	65	-155	64	-	-	34	1.05	1.47	
6D ( $C_2$ )	12.1	11.4	-152	60	47	-	-	49	1.02	1.54	
$6E(C_2)$	14.5	12.4	152	-86	53	-	-	87	1.02	1.55	
Pimelate											
$7A(C_1)$	0	0	164	-65	-64	69	-	69	1.03	1.52	
7B $(C_1)$	4.4	3.4	174	-60	-50	84	-	84	1.02	1.54	
7C ( $C_1$ )	5.3	6.2	74	73	-146	63	-	63	1.03	1.50	
7D ( $C_1$ )	6.1	6.7	54	70	-84	91	-	76	1.06	1.42	
7E ( $C_1$ )	7.3	8.8	-87	70	-142	56	-	87	1.05	1.43	
$7F(C_1)$	8.3	9.5	66	90	-65	-59	-	62	1.02	1.51	
7G ( $C_1$ )	9.4	9.9	-171	98	-56	76	-	76	1.02	1.53	
$7 H(C_1)$	9.1	10.2	162	-92	76	-70	-	86	1.03	1.54	
Suberate											
$8A(C_2)$	0	0	-64	-73	153	-72	-60	76	1.09	1.36	
8B $(C_1)$	5.3	6.7	-178	65	65	-132	59	73	1.03	1.51	
8C $(C_1)$	7.9	9.5	-164	153	-62	-52	79	69	1.02	1.55	
8D ( $C_2$ )	9.6	10.8	-75	79	-154	81	-69	72	1.08	1.37	
$8 \mathbb{E}(C_1)$	9.8	11.9	-163	62	60	-85	-56	77	1.06	1.42	
8F $(C_1)$	11.3	13.7	-174	73	74	-120	70	76	1.04	1.50	
8G $(C_1)$	12.0	13.8	-81	-78	165	-91	56	61	1.05	1.46	
$8 { m H} (C_1)$	15.5	19.5	-69	-101	65	82	-62	66	1.04	1.48	

## Table S2: Atomic coordinates ((in Å) of the conformers depicted in Fig. S2. Level of theory MP2/aug-cc-pVTZ.

								50			
4A	4 6704	0.0533	0.0744	SA	4 7046	0.0046	0.0740	28	4 94 63	0.0000	0.0477
C	1.6/21	0.0033	-0.0311	C	-1.7846	-0.2310	-0.0748	C	1.9163	-0.3093	-0.04//
C	0.6451	-1.0199	-0.3903	C	0.0203	1.5447	0.0198	C	-0.0164	1.29//	0.5685
C	-0.63/1	-0.9977	0.4526	C	-0.9140	0.7230	-0.8/92	C	1.4511	1.1418	0.2027
C	-1.6681	0.0432	0.0282	C	0.9584	0.7088	0.8988	C	-0.9660	0.8630	-0.5689
0	2.8/26	-0.2401	-0.0058	C	1.7812	-0.2746	0.0584	C	-1.9669	-0.1847	-0.1230
0	1.1863	1.2343	0.2151	0	2.9440	0.0260	-0.2508	0	1.0674	-1.2449	0.1628
0	-1.2039	1.2478	-0.1865	0	1.1611	-1.3509	-0.2970	0	3.0942	-0.4514	-0.4198
0	-2.8543	-0.2610	-0.0900	0	-1.2031	-1.3406	0.3212	0	-3.1780	-0.0180	-0.1932
н	1.1441	-1.9821	-0.2865	0	-2.9512	0.0486	0.1937	0	-1.4283	-1.2912	0.3590
н	0.3888	-0.8990	-1.4470	н	-1.5787	1.3944	-1.4212	н	1.6883	1.7173	-0.6958
н	-0.3756	-0.7994	1.4959	н	-0.3154	0.1550	-1.5918	н	2.0901	1.5386	0.9956
н	-1.1365	-1.9644	0.4143	н	-0.5876	2.1924	0.6575	н	-0.2253	2.3378	0.8300
н	-0.0988	1.2633	0.0035	н	0.6260	2.1940	-0.6176	н	-0.2178	0.7024	1.4598
				н	0.3704	0.1582	1.6347	н	-0.3729	0.4234	-1.3746
				Н	1.6459	1.3731	1.4215	н	-1.5246	1.7041	-0.9738
				н	-0.1348	-1.3543	0.0415	н	-0.3883	-1.2301	0.2998
6A				6B				6C			
С	-1.9588	-0.4428	0.1111	С	1.8483	-0.5576	0.0055	C	2.1759	-0.4656	0.0371
С	-1.0577	0.3604	1.0310	С	1.2554	0.4749	0.9762	C	1.8978	0.9599	-0.4900
C	1.7738	0.9311	-0.4598	С	-1.1707	0.4963	-0.9613	C	-1.8085	0.9769	0.4993
С	1.9307	-0.5067	0.0745	С	-1.8810	-0.4862	-0.0341	C	-2.2021	-0.4010	-0.0307
С	0.3774	1.3900	-0.8645	С	-0.6890	1.7406	-0.1867	С	-0.3266	1.2616	0.6625
С	-0.5653	1.6275	0.3167	C	0.7836	1.7342	0.2292	С	0.4243	1.2784	-0.6701
0	-1.3609	-1.2904	-0.7057	0	1.1119	-1.5677	-0.3158	0	1.1766	-1.2612	0.1283
0	-3.1729	-0.2753	0.1030	0	2.9889	-0.3391	-0.4285	0	3.3575	-0.7296	0.3202
0	2.8867	-0.7135	0.8428	0	-1.1981	-1.5084	0.4124	0	-1.2907	-1.3411	-0.1589
0	1.1046	-1.3855	-0.3588	0	-3.0509	-0.2706	0.2824	0	-3.3793	-0.6128	-0.2980
н	-0.2139	-0.2419	1.3640	н	2.0653	0.7484	1.6525	H	2.4396	1.0555	-1.4340
н	-1.6584	0.6468	1.8934	н	0.4401	0.0510	1.5643	н	2.3684	1.6598	0.2056
н	2.1978	1.6080	0.2851	н	-0.3393	0.0225	-1.4823	н	-2.2743	1.6981	-0.1762
н	2.4315	0.9810	-1.3335	н	-1.9184	0.8000	-1.6930	н	-2.3333	1.0756	1.4530
н	0.4692	2.3348	-1.4101	н	-0.8574	2.6294	-0.8008	н	-0.1982	2.2261	1.1627
н	-0.3270	-1.2810	-0.5686	н	-0.1320	-1.5108	0.0792	н	-0.2792	-1.1224	-0.0132
н	-1.4455	2.1815	-0.0222	н	0.9498	2.6140	0.8577	н	0.2930	2.2553	-1.1471
н	-0.0525	2.2603	1.0479	н	1.4203	1.8606	-0.6502	н	-0.0116	0.5397	-1.3455
н	-0.0615	0.6717	-1.5592	н	-1.3222	1.8587	0.6965	н	0.1178	0.5081	1.3133
6D				6E							
С	-2.1656	-0.2015	0.0415	С	2.0671	-0.1390	0.1212				
С	-1.1850	0.8731	0.4545	С	0.9169	0.6520	0.7023				
C	1.8642	0.6889	0.7445	С	-2.1961	0.5087	-0.4927				
С	1.8348	-0.7062	0.0941	C	-1.6460	-0.8184	0.0519				
С	1.1533	1.7020	-0.1647	С	-1.3047	1.6763	-0.0478				
С	-0.1939	1.1946	-0.6754	C	0.1733	1.4494	-0.3876				
0	-1.6406	-1.4123	-0.1052	0	1.7228	-1.2194	-0.5715				
0	-3.3520	0.0151	-0.1597	0	3.2374	0.1921	0.2505				
0	2.7233	-0.9631	-0.7401	0	-1.9776	-1.1481	1.2084				
0	0.8611	-1.4612	0.4460	0	-0.8261	-1.4235	-0.7231				
Н	-0.6325	0.4958	1.3143	н	1.3201	1.3311	1.4521				
Н	-1.7469	1.7585	0.7474	н	0.2270	-0.0352	1.1931				
Н	1.3821	0.6474	1.7216	н	-2.2096	0.4696	-1.5834				
Н	2.9007	0.9991	0.8827	н	-3.2104	0.6613	-0.1209				
н	1.0203	2.6506	0.3675	н	-1.6573	2.5939	-0.5282				
н	-0.6437	-1.4100	0.1113	н	0.7104	-1.3365	-0.5813				
Н	-0.0130	0.2946	-1.2649	н	0.6862	2.4040	-0.5269				
Н	-0.6435	1.9291	-1.3484	Н	0.2301	0.9095	-1.3348				
Н	1.7957	1.9009	-1.0259	н	-1.4119	1.8191	1.0314				

7A				7B				70			
С	1,4706	-1,1754	0.0213	С	-1,2990	-1.2709	0.0001	С	-2.0273	-0.7580	0.0862
c	2 4736	-0 0195	-0.1448	C	-2 3382	-0 1982	-0.3795	c	-2 3950	0 7358	-0.0496
c	1 2926	0.0155	0.2022	c	1 0027	0.7277	0.5755	č	1 7000	0.5363	0.0450
c	-1.2020	0.3000	-0.3923	c	2.2207	0.7577	0.0009	c	1.7009	0. 3202	0.0171
C	-2.2937	-0.1231	-0.1011	C	2.2297	-0.0201	0.1539	C	2.0904	-0.7004	0.0125
C	1.8465	1.2850	-0.6293	C	-2.0939	1.1004	0.4018	C	-1.21/4	1.6540	0.2387
C	-0.3178	1.1605	0.7836	С	0.2799	1.3643	-0.5908	C	1.3035	1.6771	-0.1186
C	0.9300	1.9575	0.3978	С	-1.0468	2.0281	-0.2250	C	-0.0677	1.4618	-0.7579
0	0.5964	-1.2661	-0.9134	0	-0.4717	-1.6147	-0.9120	0	-1.0356	-1.0047	0.8653
0	1,5757	-1,9034	1,0250	0	-1.3197	-1.6666	1,1838	0	-2.7151	-1.5792	-0.5415
0	-3.4550	0.1233	0 1989	0	3.3648	0 3990	0.3241	0	3,2066	-0.7811	-0.4982
0	1 9202	1 3659	0.1710	0	2 0110	1 1701	0.1655	0	1 1079	1 6604	0.1070
Ň	-1.8393	-1.3038	-0.1712		2.0110	-1.1/91	-0.4000		1.1978	-1.0004	-0.12/9
н	3.2180	-0.3490	-0.8/63	н	-3.3205	-0.5913	-0.1095	н	-3.2148	0.9317	0.6484
н	2.9903	0.1251	0.8063	н	-2.3193	-0.0125	-1.4554	н	-2.7911	0.8925	-1.0551
н	-0.7136	0.6766	-1.2739	н	0.3372	0.0540	1.1360	н	0.8800	0.2899	1.4924
н	-1.8287	1.8889	-0.5899	н	1.3344	1.5146	1.2959	н	2.5814	0.8130	1.3922
н	-0.8468	-1.3951	-0.4435	н	1.0159	-1.3979	-0.5588	н	0.2907	-1.4265	0.2956
н	2.6413	1,9939	-0.8853	н	-3.0279	1,6647	0.4870	н	-1.5323	2.7031	0.2320
н	1,2980	1,0797	-1.5499	н	-1.8055	0.8234	1,4181	H H	-0.8631	1 4307	1.2455
	0.9457	1 6953	1 5051	ü	0.0304	2 1004	1 0450		1 2974	2 6109	0 4530
	-0.8457	1.0852	1.5851	н	0.9394	2.1094	-1.0459		1.28/4	2.0108	0.4530
н	-0.0257	0.1920	1.1889	н	0.0970	0.5894	-1.3354	н	2.0/8/	1.7806	-0.8820
н	0.6181	2.9342	0.0095	н	-0.8622	2.8650	0.4582	н	-0.1940	2.1476	-1.6008
н	1.5128	2.1544	1.3042	н	-1.4696	2.4611	-1.1381	н	-0.1111	0.4518	-1.1726
7D				7E				7F			
С	1.8309	-0.6938	-0.0392	C	-2.1383	-0.5635	-0.1693	C	-1.8339	-0.8852	0.1432
С	1,1225	-0.0238	1,1287	с	-1,9658	0.4113	1.0128	C	-1.9705	0.5258	0.7442
c	-1 5740	0 2606	-1 0308	C	1 6344	0 2159	-1 0674	C	1 /179	0 1382	0 9457
c	1.0740	0.2000	0.1150	c	2,0222	0.7109	0.0644	c	2 1112	0.4302	0.0104
C	-1.8344	-0.7298	0.1152	C	2.0323	-0.7198	0.0044	C	2.1115	-0.5137	-0.0124
C	1.0018	1.4841	0.8916	C	-0.5820	1.0441	1.1004	C	-1.585/	1.5//4	-0.2978
C	-1.1666	1.6666	-0.5729	C	1.2699	1.6341	-0.5915	C	0.9462	1.6910	0.1950
C	0.3413	1.9100	-0.4211	C	-0.1979	1.7795	-0.1912	C	-0.1608	1.4523	-0.8411
0	1.1433	-1.5668	-0.7484	0	-1.1135	-1.2574	-0.5136	0	-2.6276	-1.1836	-0.7668
0	2,9924	-0.4037	-0.3077	0	-3.2591	-0.6142	-0.7042	0	-0.8911	-1.6129	0.6208
0	-2.6622	-0.3954	0,9797	0	3,1459	-0.6392	0.5708	0	3,2380	-0.2828	-0.4310
0	-1 1702	-1 9265	0 0907	0	1 1442	-1 6110	0 1616	0	1 4257	-1 5992	-0 2907
	-1.1/92	-1.8305	0.0007		1.1442	-1.0110	1.0200		1.4557	-1.5882	-0.3897
н	1.7500	-0.1850	2.00//	н	-2.1803	-0.1480	1.9286	н	-1.3598	0.6210	1.6423
н	0.1559	-0.4/86	1.3214	н	-2.7409	1.1/33	0.9136	н	-3.0155	0.6//1	1.0240
н	-0.8364	-0.1409	-1.7270	н	2.5146	0.2767	-1.7079	н	0.5882	-0.0653	1.4353
Н	-2.5260	0.3321	-1.5631	н	0.8031	-0.2012	-1.6361	н	2.1626	0.7303	1.6875
н	0.1422	-1.6803	-0.4068	н	0.1907	-1.4281	0.0565	н	0.4944	-1.6078	0.0146
н	0.4521	1,9271	1.7275	н	-0.5457	1.7413	1,9431	н	-2.2862	1,4835	-1.1305
н	2,0114	1,9017	0.9065	н	0.1454	0.2678	1.3229	н	-1.7113	2,5815	0.1244
	1 5210	2 2052	1 2125		1 0202	1 0176	0 2224		0 5095	2.3013	0.0227
	-1.5519	2.3052	-1.5125		1.9505	1.9170	1 4112		1.0221	2.4314	0.9255
н	-1.6882	1.8884	0.3624	н	1.4/63	2.32/8	-1.4113	н	1.8231	2.1184	-0.29/3
н	0.8707	1.4396	-1.2565	н	-0.4428	2.8417	-0.0950	н	-0.0458	2.1853	-1.6447
н	0.5164	2.9860	-0.5233	н	-0.8078	1.3952	-1.0131	н	-0.0340	0.4705	-1.3062
7G				7H							
С	-1.2936	-1.2577	0.0002	C	-2.2229	-0.0764	-0.0885				
С	-2.1482	-0.2019	-0.7319	C	-1.0529	0.6285	-0.7442				
С	1.1264	0.8343	-0.5980	С	2.3787	-0.2369	-0.2768				
c	2.2705	-0.0076	-0.0733	c	1.2704	-1.2780	-0.0431				
c	2.2705	1 0036	0.0601	č	0 2669	1 5771	0.0401				
C	-2.2039	1.0920	0.0091	C	-0.5008	1.5//1	0.2300				
C	0.2451	1.3333	0.5565	C	2.1817	1.1119	0.4066				
C	-1.0501	1.9981	0.0615	С	1.0556	1.9956	-0.1478				
0	-0.3540	-1.7906	-0.6874	0	-1.9143	-1.0330	0.7767				
0	-1.5800	-1.4881	1.1905	0	-3.3854	0.2346	-0.3128				
0	3.3694	0.4717	0.1739	0	1.0864	-2.1251	-0.9385				
0	2,0073	-1,2897	0.1414	0	0.6216	-1,1616	1.0543				
н	-3 1/1/	-0 6400	-0.8617	ц	-1 /389	1 1034	-1 5922				
	1 7260	0.0409	1 7252		0 2527	0 1104	1 1171				
н	-1./369	-0.0122	-1./253	H	-0.353/	-0.1184	-1.11/1				
Н	1.5549	1.6899	-1.1205	н	3.3082	-0.6883	0.0851				
н	0.5262	0.2423	-1.2867	Н	2.4937	-0.1138	-1.3562				
Н	1.0528	-1.5339	-0.1378	Н	-0.8997	-1.1671	0.8542				
Н	-3.1329	1.6733	-0.3113	Н	-0.9966	2.4656	0.3469				
н	-2.5201	0.8108	1.0984	н	-0.3217	1.0999	1.2290				
Н	-0.0037	0.5034	1,2208	н	1,9994	0,9396	1,4698				
н	0.8338	2.0111	1,1406	н	3,1174	1,6763	0.3252				
Ц	-1 2721	2 0701	0 6940	Ц	1 2275	2 0110	0.3233				
н	-1.2/21	2.8/01	0.0840	н	1.22/5	5.0118	0.2209				
н	-0.88/0	2.3809	-0.9525	Н	1.1348	2.0501	-1.2399				

<b>8</b> A				8B				8C			
С	2.0163	-0.9496	0.1857	С	-2.4606	-0.1865	0.0559	C	1.0728	-1.4058	0.2814
С	1.8548	-0.0820	-1.0693	C	-1.3345	0.6491	0.6298	C	2.4599	-0.8413	-0.0873
C	-1./894	-0.0048	1.0654	C	-0.66/8	1.4/63	-0.4/51	C	-1.4881	0.6405	0.7617
c	-1 7483	1 4733	0 6579	C	1 6983	1 1549	0.0208	C	-0 1128	1 35/3	-0.0023
c	1.8849	1.3968	-0.6662	c	2.3691	0.6346	-0.6063	c	2,4053	0.4038	-0.9755
С	-0.6222	1.7654	-0.3328	С	2.5869	-0.8267	-0.2038	С	0.8491	1.6271	0.6695
С	0.7660	1.7489	0.3129	C	1.2287	-1.4539	0.1364	С	2.0917	1.7007	-0.2185
0	3.1245	-0.9517	0.7439	0	-2.1001	-1.2801	-0.5965	0	0.8352	-1.6629	1.4801
0	0.9677	-1.5743	0.6026	0	-3.6355	0.1443	0.1606	0	0.2783	-1.5520	-0.7089
0	-1.1336	-1.5812	-0.6569	0	0.4114	-1.4984	-0.8486	0	-2.2292	-1.0479	-0.7810
U U	-3.2252	-0.8058	-0.0045	U L	-0 6007	-1./885	1 1022	Ц	2 0916	-1 6256	-0.1415
н	2,6937	-0.2900	-1.7355	н	-1.7641	1.3114	1.3821	н	3.0144	-0.6445	0.8328
н	-2.5948	-0.1601	1.7844	Н	-1.4158	2.1469	-0.9080	н	-1.9493	1.3315	1.4666
н	-0.8480	-0.3170	1.5152	Н	-0.3402	0.7987	-1.2648	н	-0.9850	-0.1583	1.3125
н	-0.1993	-1.5292	-0.0999	н	0.1796	2.9516	0.8404	н	-1.2439	-1.2924	-0.6449
н	2.8537	1.5942	-0.2028	н	0.8605	2.9599	-0.7793	н	1.6624	0.2219	-1.7537
н	1.8073	2.0306	-1.5567	н	1.3547	0.7751	1.2943	н	3.3663	0.5364	-1.4831
н	-1.0211	1 0254	1.5501	н	1 7270	2.1104	-1 4960	н	0.0012	2.2807	1 4010
н	-0.7847	2.7388	-0.8052	н	3.3197	1.0955	-0.8906	н	0.7522	2,5581	1.2374
н	0.9573	2.7268	0.7654	н	3.0391	-1.3747	-1.0336	н	1.9832	2.5180	-0.9408
н	0.7888	1.0218	1.1281	н	3.2391	-0.8949	0.6682	н	2.9532	1,9529	0.4097
н	-2.7142	1.7260	0.2151	н	-1.0746	-1.4119	-0.6078	н	-0.2173	0.7128	-0.9557
8D				8E				8F			
C	-2.0243	-0.7339	-0.2977	C	2.3343	-0.5435	-0.0209	C	2.5099	-0.1247	-0.1148
С	-1.8629	-0.1445	1.0969	С	1.4786	0.4753	-0.7478	С	1.4833	0.9320	-0.4736
С	1.9549	-0.2961	-1.0722	С	1.0704	1.5867	0.2286	С	0.5562	1.2409	0.7069
С	1.9254	-0.8259	0.3677	C	-0.0981	2.4271	-0.2802	С	-0.5636	2.2021	0.3042
С	1.6605	1.2064	-1.1584	C	-1.4136	1.6715	-0.4891	С	-1.6415	1.5584	-0.5727
C	-1.5104	1.3501	1.0855	C	-2.0047	1.0074	0.7608	С	-2.5809	0.6052	0.1950
C	0.2112	1.5552	-0.8093	C	-1.4583	-0.3869	0 1101	C	-2.5541	-0.8373	-0.3253
0	-3.0167	-0.4616	-0.9679	0	1.7142	-1.6308	0.3956	0	2.0912	-1.3770	-0.1351
0	-1.0738	-1.5315	-0.7361	ō	3.5183	-0.3281	0.2141	0	3,6584	0.1729	0.1934
0	0.9137	-1.5497	0.7085	0	-2.7682	-1.4451	-0.5960	0	-1.0314	-1.8449	1.1955
0	2.8643	-0.5065	1.1150	0	-0.5726	-1.9446	-0.5215	0	-0.3231	-1.4476	-0.9154
н	-0.1980	-1.5452	-0.0986	н	0.6004	-0.0147	-1.1623	н	0.8897	0.5771	-1.3151
н	-1.1056	-0.6894	1.6601	Н	2.0654	0.9061	-1.5598	н	2.0255	1.8340	-0.7596
н	-2.8326	-0.2709	1.5810	Н	1.9381	2.2250	0.4102	н	1.1537	1.6862	1.5070
н	2 9622	-0.8378	-1.6952	н	0.8078	2 9973	1.1936	н	-0.1352	3,0533	-0 2244
н	1.8718	1.5387	-2.1794	н	-0.2775	3,2431	0.4286	н	-1.0416	2.6078	1.2021
н	2.3486	1.7411	-0.4968	н	-1.3067	0.9159	-1.2708	н	-1.1624	1.0049	-1.3830
н	-1.6890	1.7388	2.0921	н	-2.1424	2.3914	-0.8735	н	-2.2315	2.3509	-1.0414
н	-2.1968	1.8752	0.4141	н	-1.8690	1.6719	1.6227	н	-2.3014	0.5774	1.2520
н	-0.0577	2.5185	-1.2541	н	-3.0786	0.8917	0.6058	н	-3.6043	0.9885	0.1525
н	-0.4405	0.8161	-1.2774	н	-0.4173	-0.3641	1.3977	н	-3.3376	-1.4152	0.1674
н	0.2295	2.6248	1.0498	н	-2.0380	-0.8021	1.9128	н	-2.7167	-0.8490	-1.4045
н	0.5831	0.9244	1.2312	н	0./168	-1.7099	0.0345	н	1.0927	-1.4502	-0.4110
8G				8H							
С	-1.5566	-1.2553	-0.0586	С	-1.5423	-1.2889	0.0278				
С	-2.7393	-0.3690	-0.4548	С	-2.5942	-0.3058	-0.4933				
С	1.7775	0.7228	-0.8111	С	-2.0053	1.0876	-0.7256				
С	2.4078	-0.4505	-0.0742	C	-1.4600	1.7453	0.5476				
C	1.2548	1.7691	0.1853	C	1.5585	0.6225	-0.9191				
c	-2.5779	1.0245	0.1039	C	1 0523	1 7452	-0.1121				
c	-1.2472	1.6903	-0.2087	c	-0.0505	1.3298	0.9851				
0	-1.5767	-1.7918	1.0630	0	-0.5868	-1.5133	-0.8027				
0	-0.5977	-1.2897	-0.9159	0	-1.6564	-1.7428	1.1797				
0	1.7012	-1.5538	0.0521	0	1.7457	-1.5578	0.1421				
0	3.5380	-0.3442	0.3919	0	3.4660	-0.1523	0.2925				
н	-3.6630	-0.8248	-0.0952	н	-2.9837	-0.6899	-1.4392				
н	-2.//8/	-0.2/58	-1.5415	н	-3.4120	-0.2405	0.2205				
н	0.9726	0.3833	-1.4157	н	-1.2218	1.0234	-1.4837				
н	0.7327	-1.4798	-0.3409	н	-2.1585	1.5408	1.3655				
н	-3.4128	1.6526	-0.1589	н	-1.4509	2.8325	0.4077				
Н	-2.6480	0.9365	1.2540	н	2.2620	1.0432	-1.6394				
н	1.1706	2.7368	-0.3210	Н	0.7330	0.1471	-1.4432				
Н	-0.1154	0.3506	1.0665	Н	0.7724	-1.5952	-0.2238				
Н	-0.2854	1.9788	1.6855	н	0.6841	2.5681	-0.6264				
н	-0.9580	1.3/07	-0.20/1	н	0.1425	1,8113	1.9476				
н	2.0011	1.8886	0.9743	н	-0.0121	0.2568	1.1762				