Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information (ESI)

Spectroscopic and theoretical investigations of adenosine 5'-diphosphate and adenosine 5'-triphosphate dianions in the gas phase

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Fig. S1: Typical infrared laser intensity as used for the infrared multiphoton dissociation (IR-MPD) spectroscopy experiments.

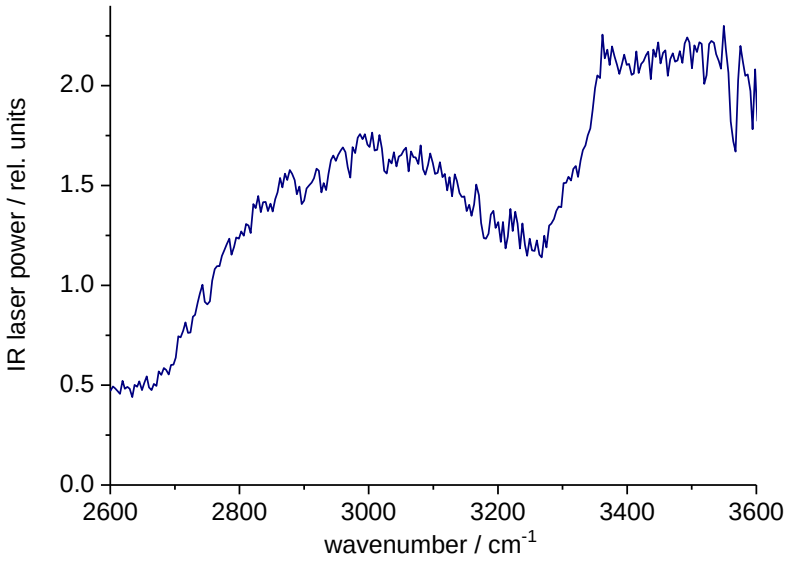

Fig. S2: Arrival time distribution of $[ADP\text{-}2H]^{2-}$.

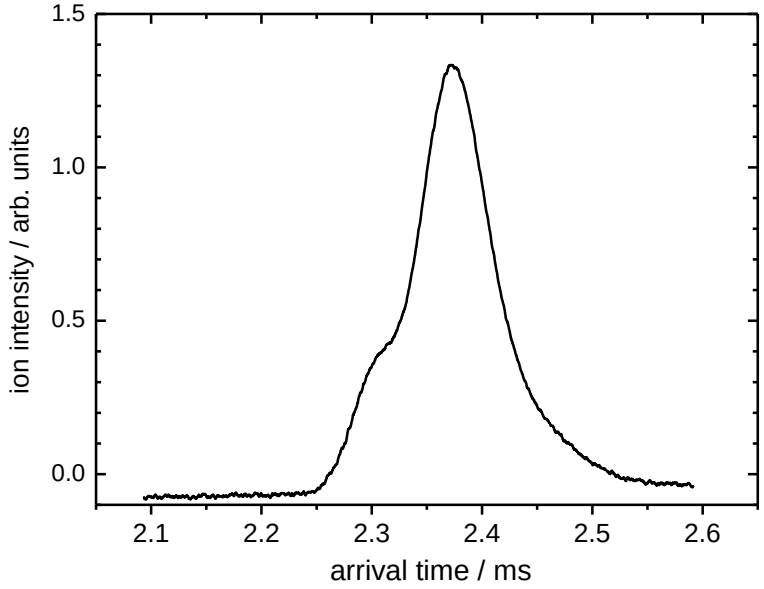

Table S1: Cartesian coordinates (in Å) of the B3-LYP/TZVPP geometry-optimized structure

$[ATP\text{-}2H]^{2-}$ ($\alpha\beta_1$)			
atom	x	y	z
P	5.7900714	0.2429197	4.9515798
P	5.5993199	-2.521778	6.2603827
O	6.9324621	0.6566599	4.0817111
O	4.7903196	-1.9278288	7.3741631
O	7.1097681	-2.855041	6.8095521
O	4.3800828	0.5697331	4.5771297
O	5.1678462	-3.7253601	5.5260259
C	7.912834	-1.8532915	7.4176158
C	9.2517961	-1.7598163	6.716359
C	10.6026253	-3.3716441	5.6646103
O	9.9687194	-3.0087651	6.8622685
O	11.5528212	-1.3671327	4.7337967
H	11.1734015	-0.4746488	4.6711253
H	9.8391015	-0.9626553	7.1832572
H	8.0668743	-2.1190861	8.4675541
H	7.4393472	-0.8700643	7.3818199
N	10.0459377	-4.6386575	5.1718606
C	8.7209194	-5.0308363	5.1052431
C	10.779634	-5.6624415	4.6350496
C	9.8410699	-6.6322661	4.2743179
C	10.3430134	-7.7929883	3.678719
N	8.5646925	-6.2220152	4.5751712
N	9.5152453	-8.8211189	3.3153439
N	11.662367	-7.9136947	3.482343
N	12.1040332	-5.7587305	4.46336
C	12.451056	-6.9041796	3.8872387
H	7.92851	-4.4011045	5.4878685
H	9.8822439	-9.4672674	2.637641
C	10.4212105	-2.2199356	4.6702449
H	11.6638109	-3.5643163	5.827392
H	10.2813107	-2.5969474	3.6525808
O	5.9813995	-1.3361259	5.1943962
C	9.180181	-1.4790232	5.2053404
H	8.5359416	-8.592701	3.2551691
H	13.5130118	-7.0475558	3.7131883
H	8.2708032	-1.9105049	4.7890859
O	9.2772294	-0.110051	4.9144552
H	8.3964428	0.2244518	4.5654049
P	5.0863747	1.4778832	7.5838216
O	6.0707985	0.8775135	6.4430659
O	3.7105637	1.6907526	6.8250725
O	5.6147463	2.6925707	8.219339
H	3.7492562	1.2702477	5.9131056
H	4.8381854	-0.6158273	8.1307021
O	4.917045	0.2901843	8.5960885

Table S2: Cartesian coordinates (in Å) of the B3-LYP/TZVPP geometry-optimized structure

$[ATP\text{-}2H]^{2-}$ ($\alpha\beta_2$)			
atom	x	y	z
P	5.8656375	0.0097779	4.844411
P	5.6144745	-2.3358493	6.7223929
O	7.0644755	0.5468674	5.6219744
O	5.273266	-1.3904595	7.8399694
O	7.213508	-2.6887429	6.8701644
O	5.8570736	0.0709461	3.3744042
O	4.919325	-3.617458	6.5067382
C	8.1114219	-1.8025418	7.5218957
C	9.4466118	-1.8049793	6.816054
C	10.7148656	-3.4584748	5.7376005
O	10.0870915	-3.1002592	6.9394511
O	11.7831578	-1.4519661	4.9591195
H	11.4536753	-0.5415176	4.9202451
H	10.0921385	-1.0547614	7.2843945
H	8.2442862	-2.1253174	8.5598684
H	7.7273548	-0.7822224	7.5195881
N	10.0661975	-4.6548045	5.1862414
C	8.7254473	-4.9905	5.2184296
C	10.6997087	-5.6526366	4.4963158
C	9.6883485	-6.5517329	4.1491844
C	10.0800445	-7.6726251	3.4109661
N	8.4657476	-6.1235623	4.6083825
N	9.1777448	-8.6324794	3.0418182
N	11.3693085	-7.8231328	3.0799432
N	11.9969949	-5.7806288	4.1913973
C	12.2369867	-6.8835324	3.4903623
H	8.0074616	-4.3589612	5.7252648
H	9.4525546	-9.2313708	2.2820414
C	10.6244191	-2.2567017	4.7903326
H	11.7577708	-3.7323479	5.9032225
H	10.527127	-2.5768169	3.7493258
O	5.5909712	-1.509805	5.30599
C	9.3877932	-1.5148331	5.3079648
H	8.2078321	-8.3653266	3.0942149
H	13.2706152	-7.0504364	3.2036054
H	8.4788895	-1.9526544	4.888617
O	9.4920888	-0.1508321	4.9992825
H	8.5882381	0.2435977	5.1605577
P	4.3003481	1.708356	6.7561107
O	4.5665411	0.8104974	5.4403413
O	3.8172437	0.6944834	7.8507794
O	3.3425582	2.7974103	6.5248175
H	4.3737592	-0.1600084	7.8763435
H	6.4413567	1.6650453	6.7065488
O	5.7528833	2.2186423	7.1650085

Table S3: Cartesian coordinates (in Å) of the B3-LYP/TZVPP geometry-optimized structure $[ATP\text{-}2H]^{2-}$ ($\beta\gamma$)

atom	x	y	z
P	7.4850267	1.7944149	5.5482973
P	8.7311094	-0.40854	7.1517044
O	8.9386197	2.0093167	5.1456821
O	10.0276966	0.4330229	6.8357228
O	8.8188563	-1.7185387	6.2190455
O	6.7180463	2.8331494	6.2482785
O	8.5581642	-0.8432096	8.5405936
C	9.0538	-1.5835111	4.8045165
C	8.0525002	-2.404048	4.0288103
C	7.1889353	-4.4125929	4.8969924
O	8.2918878	-3.8205581	4.25565
O	4.9078335	-3.6390259	5.3917349
H	4.579839	-3.3216045	4.5344654
H	8.1909894	-2.195846	2.9676958
H	10.0660706	-1.9383482	4.5995952
H	8.9712826	-0.5479401	4.4801181
N	7.6719515	-5.2672322	5.9768133
C	8.3510545	-4.8607663	7.1049387
C	7.5824546	-6.6312629	6.0537946
C	8.2188029	-6.9708541	7.2521565
C	8.2417565	-8.3283748	7.5827146
N	8.6945873	-5.8500313	7.895431
N	8.864142	-8.777159	8.7188606
N	7.6688641	-9.2149912	6.7602596
N	7.0144236	-7.495673	5.2059117
C	7.1029247	-8.7490026	5.6334764
H	8.5650845	-3.8149136	7.2689859
H	8.5827633	-9.6874318	9.0417691
C	6.2691181	-3.2738881	5.3873831
H	6.6379972	-5.0703669	4.2218518
H	6.560386	-2.9774215	6.3938395
O	7.5307771	0.4331073	6.5463899
C	6.58838	-2.1430153	4.4025777
H	9.0465303	-8.0776708	9.4201507
H	6.6566745	-9.5037582	4.9935462
H	6.4712015	-1.1630285	4.8603511
O	5.7241433	-2.2892947	3.2960987
H	5.8380125	-1.43765	2.7757308
O	6.7015986	1.14732	4.3149245
O	6.3053202	-0.0574772	2.1299605
O	6.6524073	2.5143345	2.1328043
O	8.5800761	0.8835323	2.6383794
H	8.9987182	1.4325178	3.3292937
H	9.7951956	1.1437004	6.1434582
P	6.9763989	1.1726881	2.6616363

Table S4: Cartesian coordinates (in Å) of the B3-LYP/TZVPP geometry-optimized structure $[ATP\text{-}2H]^{2-}$ ($\alpha\gamma$)

atom	x	y	z
P	7.9150986	1.5739375	6.345985
P	9.1995497	-0.8062894	7.6112339
O	9.3541083	2.1693706	6.5520095
O	10.4458251	0.010594	7.3957246
O	9.1236012	-1.9843016	6.4974178
O	6.8050929	2.4424732	6.7883271
O	8.8436833	-1.4336085	8.8958264
C	9.3866323	-1.7385294	5.1156872
C	8.3189187	-2.4121412	4.2814628
C	7.2813201	-4.3697734	5.0754654
O	8.4190488	-3.8534314	4.4251641
O	5.0666145	-3.4250883	5.5635704
H	4.781146	-3.0169145	4.7291778
H	8.4805848	-2.1662276	3.2306928
H	10.3679406	-2.1535299	4.8700242
H	9.385183	-0.6720208	4.889874
N	7.6986513	-5.2923718	6.1273818
C	8.334586	-4.9830347	7.3133243
C	7.5719919	-6.6561023	6.1053664
C	8.143121	-7.0955308	7.3033967
C	8.1154646	-8.4721027	7.539858
N	8.6145931	-6.0359695	8.0447685
N	8.675192	-9.0142457	8.6686509
N	7.5562119	-9.2842599	6.6348961
N	7.0185285	-7.4441702	5.176766
C	7.0531453	-8.7257979	5.5204132
H	8.56826	-3.9591908	7.5675543
H	8.3507681	-9.9328868	8.9195148
C	6.4540677	-3.177341	5.6000931
H	6.6765154	-4.9651889	4.3890807
H	6.7486256	-2.9436741	6.6212996
O	7.9407362	0.1679781	7.1125868
C	6.8837308	-2.0338385	4.6692638
H	8.8442452	-8.3667542	9.4215465
H	6.6142469	-9.4214706	4.8119307
H	6.8605086	-1.0774683	5.184271
O	6.0115266	-2.0263217	3.5585222
H	6.0853771	-1.1006226	3.1825703
O	7.7997135	1.1577499	4.8243088
O	6.5267521	0.3953875	2.7661476
O	7.1568688	2.8958706	3.0415803
O	5.3538963	1.7737108	4.5115697
H	5.5722456	2.2268373	5.3493896
H	9.9735457	1.4304743	6.8715103
P	6.6900387	1.6170524	3.616321

Table S5: Computed key parameters (B3LYP/TZVPP) of the hydrogen bonds OH…O (with OH groups labelled A-D, see main text for details) for the different tautomers of $[ATP\text{-}2H]^{2-}$.

	$[ATP\text{-}2H]^{2-}$	$\alpha\beta_1$	$\alpha\beta_2$	$\alpha\gamma$	$\beta\gamma$
A	bond length / pm	151.1	152.5	158.6	157.4
	bond angle / °	176	176	160	160
B	bond length / pm	160.1	162.1	161.4	159.4
	bond angle / °	175	166	167	177
C	bond length / pm	163.5	167.8	190.7	190.7
	bond angle / °	159	158	148	146
D	bond length / pm	194.6	200.2	196.6	197.7
	bond angle / °	123	121	123	122

Table S6: Relevant transitions from TDDFT calculations for $\alpha\beta[ATP\text{-}2H]^-$, from structures $\alpha\beta_1$ and $\alpha\beta_2$. Contributions of 25% or more (or greatest contribution present) are included for each transition.

$[ATP\text{-}2H]^-$ ($\alpha\beta_1$)			$[ATP\text{-}2H]^-$ ($\alpha\beta_2$)		
Transition and contribution	%	Excitation energy (eV)	Transition and contribution	%	Excitation energy (eV)
129a → 130a	85	0.970	126a → 130a 129a → 130a	51 32	0.851
126a → 130a 128a → 130a	42 25	1.004	129a → 130a	65	0.987
126a → 130a	39	1.126	125a → 130a	65	1.099
128a → 130a 127a → 130a	50 36	1.190	127a → 130a	38	1.159
125a → 130a	88	1.307	124a → 130a 127a → 130a	44 31	1.292
124a → 130a 123a → 130a	52 42	1.350	123a → 130a	24	1.327
122a → 130a	94	1.461	122a → 130a 123a → 130a	59 31	1.391
			121a → 130a	99	1.447