Supplementary Material (ESI) for Organic and Biomolecular Chemistry

SUPPORTING INFORMATION

Structural and Theoretical Investigation of 2-Iminoimidazolines – Carbene Analogues of Iminophosphoranes

Matthias Tamm*, Dejan Petrovic, Sören Randoll,

Stephan Beer, Thomas Bannenberg, Peter G. Jones,

and Jörg Grunenberg

Contents:

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1. Electronic Structure Calculations

Structure of the dimer of 3a (atom, x-, y-, z-positions in Å):

N	-0.240765	0.408930	-1.589992
N	-0.511025	-0.058127	-3.900442
N	1.591686	-0.023805	-3.170938
C	0.262410	0.137039	-2.751910
C	0.331191	-0.324492	-4.979773
C	1.602498	-0.305025	-4.542236
C	-1.997449	0.052834	-3.950404
C	-2.618245	-0.995302	-3.008494
C	-2.481733	-0.219638	-5.382675
C	-2.415881	1.477952	-3.543464
C	2.797590	0.114360	-2.305098
C	4.059281	-0.130612	-3.149454
C	2.764883	-0.938297	-1.178932
H	0.470387	0.512035	-0.878257
H	-0.035194	-0.515601	-5.969956
H	2.505671	-0.476235	-5.095043
H	-2.281312	-0.833143	-1.986152
H	-2.330716	-2.004042	-3.318643
H	-3.709277	-0.924087	-3.042987
H	-2.085662	0.507989	-6.095802
H	-3.570655	-0.139303	-5.400605
H	-2.219454	-1.225924	-5.720167
H	-2.000191	2.210568	-4.241420
H	-2.060203	1.706974	-2.539882
H	-3.506046	1.564965	-3.566111
H	4.155447	0.591189	-3.964215
H	4.081873	-1.140727	-3.565716
H	4.933463	-0.019921	-2.504796
H	1.935990	-0.805519	-0.483779
H	3.690123	-0.879570	-0.598829
H	2.944833	2.271333	-2.559587
H	3.759771	1.652942	-1.112147
H	2.002314	1.808382	-1.141145
N	0.240765	-0.408930	1.589992
N	0.511025	0.058127	3.900442
N	-1.591686	0.023805	3.170938
C	-0.262410	-0.137039	2.751910
C	-0.331191	0.324492	4.979773
C	-1.602498	0.305025	4.542236
C	1.997449	-0.052834	3.950404
C	2.618245	0.995302	3.008494
C	2.481733	0.219638	5.382675
C	2.415881	-1.477952	3.543464
C	-2.797590	-0.114360	2.305098
C	-4.059281	0.130612	3.149454
C	-2.764883	0.938297	1.178932
C	-2.872784	-1.548430	1.742650
H	-0.470387	-0.512035	0.878257
H	0.035194	0.515601	5.969956
H	-2.505671	0.476235	5.095043
H	2.281312	0.833143	1.986152
H	2.330716	2.004042	3.318643
H	3.709277	0.924087	3.042987
H	2.085662	-0.507989	6.095802
H	3.570655	0.139303	5.400605
H	2.219454	1.225924	5.720167
H	2.000191	-2.210568	4.241420
H	2.060203	-1.706974	2.539882
H	3.506046	-1.564965	3.566111

H	-4.155447	-0.591189	3.964215
H	-4.081873	1.140727	3.565716
H	-4.933463	0.019921	2.504796
H	-1.935990	0.805519	0.483779
H	-3.690123	0.879570	0.598829
H	-2.695243	1.941899	1.606861
H	-2.944833	-2.271333	2.559587
H	-3.759771	-1.652942	1.112147
H	-2.002314	-1.808382	1.141145

Structure of 5 (atom, x-, y-, z-positions in Å):

H	-2.671886	0.788728	0.964581
H	2.771556	0.489146	1.066747
C	2.464977	0.301349	0.032107
C	0.688547	-1.517311	0.000275
C	-0.660500	-1.530740	0.005453
H	2.525901	1.240122	-0.517955
C	-2.463673	0.260553	0.027380
N	1.104161	-0.188917	-0.039055
N	-1.095796	-0.202035	-0.024658
N	0.083936	1.943231	-0.005994
C	0.002606	0.655879	-0.024025
H	-3.131705	-0.597490	-0.043682
H	-2.678160	0.934067	-0.808237
H	3.137425	-0.431647	-0.416440
H	1.390345	-2.333233	0.000736
H	-1.350510	-2.356591	0.007678
H	-0.830830	2.382565	-0.012616

Structure of 5-H (atom, x-, y-, z-positions in Å):

H	-2.697268	0.817041	0.898841
H	3.136961	-0.616145	-0.040537
C	2.478672	0.248826	-0.007659
C	0.674181	-1.560431	0.003113
C	-0.674251	-1.560434	0.003176
H	2.697029	0.817343	0.898692
C	-2.478694	0.248966	-0.007721
N	1.093292	-0.227208	0.005815
N	-1.093337	-0.227170	0.005928
N	0.000117	1.907544	-0.036826
C	-0.000009	0.559330	0.007829
H	-3.137057	-0.615959	-0.040932
H	-2.661198	0.860387	-0.893430
H	2.661407	0.859967	-0.893533
H	1.379662	-2.372745	0.003117
H	-1.379819	-2.372670	0.003142
H	-0.854737	2.416666	0.123867
H	0.855122	2.416410	0.123931

Structure of 6 (atom, x-, y-, z-positions in Å):

H	-2.647916	0.419668	1.123046
H	3.154107	-0.210322	0.595349
C	2.447191	0.372930	-0.000126
C	0.766238	-1.496087	-0.123304
C	-0.745890	-1.503467	0.107121
H	2.485221	1.415206	0.311507
C	-2.443692	0.333086	0.044874
N	1.103061	-0.122232	0.215845
N	-1.099860	-0.128096	-0.233452
N	0.086522	1.981848	-0.000066
C	0.006009	0.703367	-0.006593
H	-3.160403	-0.366152	-0.390940
H	-2.611868	1.306055	-0.419741
H	2.742384	0.313462	-1.058537
H	1.296719	-2.207016	0.514538
H	-0.980866	-1.729256	1.159187
H	1.006237	-1.723078	-1.174636
H	-1.272209	-2.218237	-0.529632
H	-0.818606	2.420045	-0.138261

Structure of 6-H (atom, x-, y-, z-positions in Å):

H	-2.697268	0.817041	0.898841
H	3.136961	-0.616145	-0.040537
C	2.478672	0.248826	-0.007659
C	0.674181	-1.560431	0.003113
C	-0.674251	-1.560434	0.003176
H	2.697029	0.817343	0.898692
C	-2.478694	0.248966	-0.007721
N	1.093292	-0.227208	0.005815
N	-1.093337	-0.227170	0.005928
N	0.000117	1.907544	-0.036826
C	-0.000009	0.559330	0.007829
H	-3.137057	-0.615959	-0.040932
H	-2.661198	0.860387	-0.893430
H	2.661407	0.859967	-0.893533
H	1.379662	-2.372745	0.003117
H	-1.379819	-2.372670	0.003142
H	-0.854737	2.416666	0.123867
H	0.855122	2.416410	0.123931

Structure of 7 (atom, x-, y-, z-positions in Å):

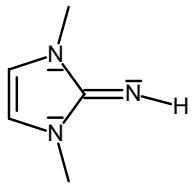
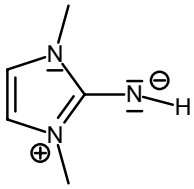
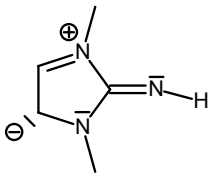
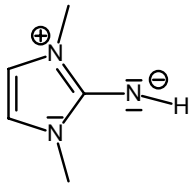
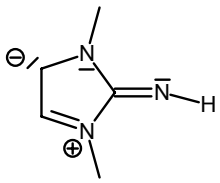
H	-2.316391	0.997152	1.215914
H	2.719650	0.990192	0.851225
C	2.429705	0.538196	-0.107048
H	2.320236	1.340579	-0.833509
C	-2.418695	0.439041	0.284328
N	1.183396	-0.212207	-0.008856
N	-1.167960	-0.225298	-0.041945
N	0.076440	1.816388	0.202196
C	0.009702	0.541291	0.055867
H	-3.193338	-0.318733	0.423689
H	-2.761751	1.128163	-0.504854
H	3.220169	-0.144090	-0.430945
H	-0.828350	2.258056	0.065584
C	-1.289987	-1.176250	-1.147753
H	-0.316283	-1.590980	-1.396372
H	-1.961605	-1.992133	-0.865039
H	-1.696945	-0.692978	-2.049224
C	1.297967	-1.416519	0.812127
H	0.330879	-1.902270	0.916365
H	1.997673	-2.116287	0.346386
H	1.672103	-1.177392	1.819140

Structure of 7-H (atom, x-, y-, z-positions in Å):

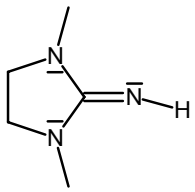
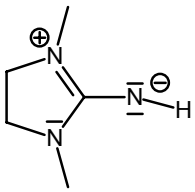
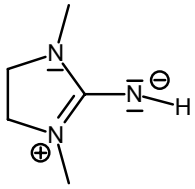
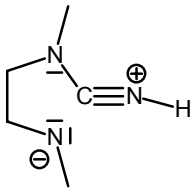
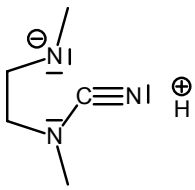
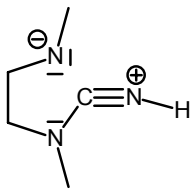
H	-2.321034	1.223824	0.970231
H	3.139033	-0.268854	-0.540771
C	2.447567	0.493023	-0.180031
H	2.887753	0.963563	0.705449
C	-2.449151	0.484835	0.180821
N	1.166923	-0.157743	0.132146
N	-1.166412	-0.161303	-0.132363
N	-0.002958	1.842096	0.001446
C	-0.000802	0.494456	0.000416
H	-3.138218	-0.279870	0.540161
H	-2.890760	0.955512	-0.703878
H	2.317010	1.232984	-0.968128
H	-0.772873	2.364644	-0.384643
H	0.765097	2.366510	0.388712
C	-1.267831	-1.453279	-0.830158
H	-0.322318	-1.705416	-1.303087
H	-1.560334	-2.251627	-0.144824
H	-2.028257	-1.364859	-1.609103
C	1.272519	-1.450531	0.827814
H	0.327830	-1.706492	1.300339
H	1.567582	-2.246809	0.141172
H	2.032674	-1.360936	1.606889

2. NRT (Natural Resonance Theory) Analysis

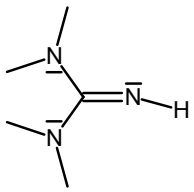
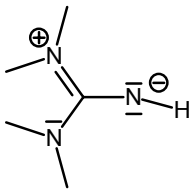
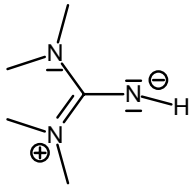
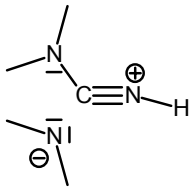
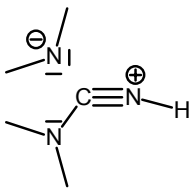
Most important resonance structures of compound 5.

weight-%	resonance structures
48.97	
12.27	
8.96	
8.34	
4.35	

Most important resonance structures of compound 6.

weight-%	resonance structures
62.01	
9.11	
7.56	
2.87	
1.47	
1.24	

Most important resonance structures of compound 7.

weight-%	resonance structures
64.90	
7.36	
6.74	
2.27	
1.41	
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