Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. *87* (7–8) S284–S294 (2022) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Theoretical study on the insertion reaction of the phosphenium cation and azirane

JINSONG GU, XIAODONG ZHAO, SHANKUI LIU and XIAOJUN TAN*

College of Biological Science and Technology, University of Jinan, Jinan, Shandong, 250022, People's Republic of China

J. Serb. Chem. Soc. *87* (7–8) (2022) 857–865

TABLE S-I. The Cartesian coordinates of the optimized specie (H_2P^+) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
P	0.000000	0.000000	0.117031
H	0.000000	1.028323	-0.877732
H	0.000000	-1.028323	-0.877732

TABLE S-II. The Cartesian coordinates of the optimized specie (Azirane) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	0.741742	-0.400099	0.023277
C	-0.743412	-0.397661	0.023314
H	1.250532	-0.564422	0.968543
H	1.281447	-0.749939	-0.849746
H	-1.252006	-0.559948	0.969008
H	-1.284617	-0.746014	-0.849376
N	0.001642	0.857569	-0.171807
H	0.003166	1.403901	0.684676

* Corresponding author. E-mail: chem.2001@163.com

TABLE S-III. The Cartesian coordinates of the optimized specie (Com) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	1.390212	-0.736451	-0.183067
C	1.390209	0.736453	-0.183066
H	1.077243	-1.264291	-1.075583
H	2.046946	-1.276269	0.487167
H	1.077238	1.264290	-1.075583
H	2.046941	1.276275	0.487166
P	-1.429443	0.000000	-0.201659
H	-1.876090	-1.041582	0.653840
H	-1.876091	1.041581	0.653840
N	0.273532	-0.000001	0.509470
H	0.348207	-0.000003	1.524545

TABLE S-IV. The Cartesian coordinates of the optimized specie (TS) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	1.415938	-0.442804	-0.271250
C	1.245202	0.960660	0.125210
H	1.525773	-0.626935	-1.339146
H	2.208595	-0.952693	0.282116
H	1.095917	1.769950	-0.581719
H	1.275264	1.202579	1.182388
P	-1.259765	0.200692	-0.141597
H	-2.272124	-0.753888	-0.411500
H	-1.719094	0.590118	1.137307
N	0.104851	-0.829833	0.249967
H	0.081342	-1.537811	0.980975

TABLE S-V. The Cartesian coordinates of the optimized specie (Pro) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.372724	-0.168360	-0.000024
C	-0.506694	1.143060	-0.000046
H	-1.985654	-0.275448	0.894407
H	-1.985767	-0.275432	-0.894378
H	-0.599089	1.760085	0.892044
H	-0.599005	1.759957	-0.892234
P	0.961782	0.051518	0.000070
H	1.825563	0.098572	1.115273
H	1.825871	0.098545	-1.114890
N	-0.203552	-1.097173	-0.000115
H	-0.207288	-2.107042	-0.000049

TABLE S-VI. The Cartesian coordinates of the optimized specie (^{F}Com) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.571281	0.847820	-0.368340
C	-1.962415	-0.520618	0.045588
H	-1.228251	1.020943	-1.382417
H	-1.991919	1.709705	0.136837
H	-1.900794	-1.331099	-0.672455
H	-2.667016	-0.665781	0.856368
P	1.025955	-0.609931	-0.273374
H	1.341834	-1.372098	0.923966
N	-0.602234	0.031351	0.487848
H	-0.533991	0.328042	1.463551
F	1.889846	0.808510	0.144038

TABLE S-VII. The Cartesian coordinates of the optimized specie (^{F}TS) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	1.645019	-0.681656	-0.296516
C	1.806735	0.772512	-0.130054
H	1.513614	-1.042014	-1.315123
H	2.405603	-1.269555	0.221424
H	1.683061	1.484090	-0.939373
H	2.103810	1.147085	0.843691
P	-0.789141	0.511332	0.032328
H	-1.178379	0.903212	1.335945
N	0.401782	-0.655585	0.482915
H	0.352927	1.228620	1.325750
F	-2.062946	-0.402247	-0.308691

TABLE S-VIII. The Cartesian coordinates of the optimized specie (^{F}Pro) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	1.692775	-0.073138	-0.372355
C	0.848860	1.166327	0.095717
H	1.899693	-0.067830	-1.443888
H	2.616120	-0.203074	0.194102
H	0.589584	1.895141	-0.673536
H	1.203510	1.665706	0.998564
P	-0.579872	-0.042717	0.441952
H	-1.281020	-0.318798	1.650189
N	0.667036	-1.104494	0.013421
H	0.708850	-2.107238	-0.110688
F	-1.884191	0.105464	-0.630905

TABLE S-IX. The Cartesian coordinates of the optimized specie (^{CH3}Com) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.654878	0.829411	-0.451344
C	-2.016190	-0.463603	0.181458
H	-1.366702	0.844464	-1.496084
H	-2.060621	1.754853	-0.059354
H	-1.986423	-1.370308	-0.411686
H	-2.683469	-0.480972	1.035388
P	0.920773	-0.667524	-0.302207
H	1.116771	-1.521771	0.852501
N	-0.643475	0.140001	0.457957
H	-0.531379	0.562315	1.380599
C	2.159272	0.698945	0.160146
H	3.159677	0.299245	-0.038547
H	2.007987	1.564075	-0.488336
H	2.107667	0.992436	1.211362

TABLE S-X. The Cartesian coordinates of the optimized specie (^{CH3}TS) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.740183	0.701994	-0.292454
C	-1.899376	-0.738489	-0.064024
H	-1.668630	1.019353	-1.331189
H	-2.460311	1.318890	0.247740
H	-1.812362	-1.481483	-0.847727
H	-2.138566	-1.075702	0.938232
P	0.721672	-0.550098	-0.033755
H	0.901348	-1.177198	1.220726
N	-0.450676	0.692535	0.404181
H	-0.376153	1.254324	1.251116
C	2.303769	0.361036	-0.174695
H	2.455634	1.019880	0.685752
H	3.121379	-0.364766	-0.204313
H	2.322047	0.943178	-1.096241

TABLE S-XI. The Cartesian coordinates of the optimized specie (^{CH_3}Pro) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.787417	-0.122079	0.332778
C	-0.926324	1.159308	0.045537
H	-2.124577	-0.190537	1.369537
H	-2.645716	-0.208879	-0.338216
H	-0.690265	1.769372	0.917884
H	-1.271982	1.788543	-0.774460
P	0.522601	0.016415	-0.450546
H	0.849663	0.010278	-1.844452
N	-0.706425	-1.105898	0.016724
H	-0.758318	-2.112273	-0.014723
C	2.122124	0.022829	0.501442
H	2.691110	-0.883039	0.273904
H	2.705135	0.899811	0.203831
H	1.900623	0.061437	1.569286

TABLE S-XII. The Cartesian coordinates of the optimized specie (^{OH}Com) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.695852	0.763021	-0.471553
C	-1.971841	-0.509306	0.244245
H	-1.473340	0.735657	-1.532326
H	-2.113749	1.692326	-0.102057
H	-1.949100	-1.442866	-0.307205
H	-2.586103	-0.510032	1.137192
P	1.005391	-0.588565	-0.334955
H	1.148602	-1.461795	0.807123
N	-0.612040	0.157905	0.406718
H	-0.437178	0.636995	1.293815
O	2.021057	0.662487	0.322249
H	2.451984	1.250670	-0.333391

TABLE S-XIII. The Cartesian coordinates of the optimized specie (^{OH}TS) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	1.692162	-0.680690	-0.294859
C	1.826598	0.771648	-0.117195
H	1.587856	-1.036542	-1.317971
H	2.445899	-1.263996	0.236926
H	1.701297	1.485828	-0.922511
H	2.108074	1.144366	0.861184
P	-0.778849	0.502415	0.002067
H	-1.068812	0.997248	1.289859
N	0.431890	-0.670072	0.458816
H	0.387669	-1.221003	1.317023
O	-2.154086	-0.353768	-0.149948
H	-2.382341	-0.667218	-1.035320

TABLE S-XIV. The Cartesian coordinates of the optimized specie (^{OH}Pro) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	1.707575	0.014783	-0.379042
C	0.786996	1.169056	0.156139
H	1.917175	0.104814	-1.446714
H	2.637951	-0.091922	0.181078
H	0.460459	1.904437	-0.580542
H	1.124071	1.656822	1.070888
P	-0.564671	-0.125277	0.439795
H	-1.142846	-0.528675	1.681885
N	0.748829	-1.097490	-0.062340
H	0.848426	-2.081689	-0.267612
O	-1.865110	0.229451	-0.601463
H	-2.663523	-0.340835	-0.650405

TABLE S-XV. The Cartesian coordinates of the optimized specie (^{OCH_3}Com) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.873640	1.086102	-0.350917
C	-2.498523	-0.181116	0.109292
H	-1.581682	1.183915	-1.390361
H	-2.090556	2.013294	0.166738
H	-2.654169	-0.984232	-0.602569
H	-3.165381	-0.179826	0.963635
P	0.417048	-0.908645	-0.378200
H	0.232469	-1.975755	0.580613
N	-1.037731	0.092331	0.437031
H	-0.824842	0.350912	1.403660
O	1.666956	-0.130823	0.539836
C	2.588591	0.834682	-0.110134
H	3.351987	1.022333	0.642771
H	3.041797	0.399095	-1.003238
H	2.064571	1.762195	-0.355604

TABLE S-XVI. The Cartesian coordinates of the optimized specie (^{OCH_3}TS) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.903391	0.974604	-0.030631
C	-2.295116	-0.328828	-0.581776
H	-1.539492	1.712024	-0.743075
H	-2.644536	1.418816	0.635555
H	-2.115927	-0.619451	-1.609776
H	-2.826637	-1.019245	0.062866
P	0.256434	-0.753654	-0.088419
H	0.189468	-1.832447	0.818046
N	-0.837689	0.329805	0.749472
H	-0.890346	0.398644	1.766666
O	1.741692	-0.281282	0.336903
C	2.500409	0.732865	-0.376814
H	3.510074	0.678516	0.021305
H	2.510335	0.516959	-1.446734
H	2.079430	1.720765	-0.184775

TABLE S-XVII. The Cartesian coordinates of the optimized specie (^{OCH_3}Pro) at the B3LYP/6-311++G** level

Atoms	x	y	z
C	-2.143774	0.188350	-0.488199
C	-1.414850	-1.112924	-0.000728
H	-2.268121	0.219998	-1.572649
H	-3.102885	0.356365	0.004913
H	-1.113058	-1.814759	-0.779236
H	-1.888455	-1.635560	0.830555
P	0.048359	-0.029187	0.522437
H	0.526095	0.190643	1.854529
N	-1.097067	1.140550	0.010227
H	-1.067740	2.143923	-0.100942
O	1.420689	-0.439430	-0.388438
C	2.768215	0.188152	-0.239896
H	3.440278	-0.527337	-0.708845
H	2.782811	1.139612	-0.772583
H	3.022095	0.315037	0.816555

TABLE S-XV. The Cartesian coordinates of the optimized specie (^{NH_2}Com) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.723613	0.816451	-0.411983
C	-2.019364	-0.524470	0.157517
H	-1.431472	0.895187	-1.452950
H	-2.190809	1.697296	0.012567
H	-1.938832	-1.398925	-0.478796
H	-2.697714	-0.620162	0.997156
P	0.992646	-0.564238	-0.333020
H	1.137399	-1.470578	0.785332
N	-0.690912	0.142008	0.469879
H	-0.595095	0.531589	1.409286
N	2.147628	0.599330	0.189984
H	2.591006	0.605631	1.098890
H	2.496678	1.282277	-0.468429

TABLE S-XVI. The Cartesian coordinates of the optimized specie (^{NH_2}TS) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	1.710735	-0.690565	-0.287556
C	1.911635	0.745586	-0.069940
H	1.616525	-1.013806	-1.322520
H	2.429086	-1.319169	0.242482
H	1.818443	1.485114	-0.856297
H	2.180080	1.082357	0.924569
P	-0.759200	0.511430	-0.042677
H	-1.018858	1.117213	1.205301
N	0.434414	-0.673560	0.442253
H	0.348943	-1.275734	1.262683
N	-2.191729	-0.339102	-0.172709
H	-2.940078	-0.262809	0.503537
H	-2.479151	-0.726108	-1.061439

TABLE S-XVII. The Cartesian coordinates of the optimized specie (^{NH_2}Pro) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.775432	-0.100882	0.302593
C	-0.901995	1.158938	-0.011682
H	-2.124990	-0.136896	1.336756
H	-2.623395	-0.203915	-0.377976
H	-0.689952	1.812706	0.835544
H	-1.211652	1.751119	-0.873638
P	0.558127	-0.007588	-0.404628
H	1.048259	-0.103510	-1.739038
N	-0.701248	-1.105180	0.023541
H	-0.756590	-2.112333	0.065506
N	2.006609	0.059340	0.483108
H	2.902338	-0.112083	0.044132
H	2.011112	0.191279	1.486125

TABLE S-XVIII. The Cartesian coordinates of the optimized specie (^{NHCH3}Com) at the B3LYP/6-311++G** level

Atoms	x	y	z
C	-1.892170	1.137037	-0.206584
C	-2.545124	-0.191151	-0.065733
H	-1.452606	1.411128	-1.158817
H	-2.216227	1.963719	0.414769
H	-2.569210	-0.861745	-0.917703
H	-3.338725	-0.330295	0.658950
P	0.426751	-0.867474	-0.377522
H	0.250910	-2.001483	0.504899
N	-1.159155	0.025662	0.515934
H	-1.111892	0.118153	1.532046
N	1.788858	-0.199328	0.427825
H	2.081794	-0.550901	1.332029
C	2.614210	0.887424	-0.135677
H	2.490447	1.815654	0.431475
H	3.668046	0.596552	-0.118527
H	2.326789	1.067133	-1.174634

TABLE S-XIX. The Cartesian coordinates of the optimized specie (^{NHCH3}TS) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-1.934062	0.970953	-0.009008
C	-2.413656	-0.314598	-0.522559
H	-1.590538	1.688653	-0.751337
H	-2.621087	1.449088	0.691755
H	-2.284910	-0.627085	-1.551756
H	-2.923802	-0.984227	0.159633
P	0.237707	-0.739795	-0.143335
H	0.153834	-1.889625	0.672519
N	-0.839505	0.326912	0.737620
H	-0.824018	0.449380	1.751720
N	1.779940	-0.280490	0.305571
H	2.297778	-0.865615	0.949493
C	2.571057	0.755911	-0.372834
H	2.939006	1.485174	0.351271
H	3.419283	0.314733	-0.900672
H	1.945777	1.277902	-1.098544

TABLE S-XX. The Cartesian coordinates of the optimized specie (^{NHCH_3}Pro) at the B3LYP/6-311++G** level

Atoms	*x*	*y*	*z*
C	-2.275046	0.143762	-0.294408
C	-1.442024	-1.131860	0.058020
H	-2.632665	0.152604	-1.326677
H	-3.114264	0.298697	0.387417
H	-1.265501	-1.826137	-0.764994
H	-1.760468	-1.678805	0.946249
P	0.068649	-0.008026	0.385198
H	0.582534	0.155809	1.704254
N	-1.168302	1.120204	-0.056285
H	-1.193140	2.125805	-0.142115
N	1.506309	-0.229079	-0.500661
H	1.419218	-0.485880	-1.477926
C	2.870556	0.094833	-0.019267
H	2.863691	0.226537	1.066309
H	3.537650	-0.737383	-0.254543
H	3.246247	1.010851	-0.483389