Journal of the Serbian Chemical Society
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J. Serb. Chem. Soc. 85 (9) S426–S432 (2020) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Theoretical study on the reaction between phosphacyclopropenylidene and ethylene: An alternative approach to the formation of phosphorus-bearing heterocyclic compounds

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J. Serb. Chem. Soc. 85 (9) (2020) 1175–1184

TABLE S-I. Matrix of optimized structures

Species	Atom	Coordinates, Å		
R1 C_2PH	C	-0.84599500	-0.52455100	-0.00002800
	C	-0.83148400	0.85557600	0.00000700
	H	-1.52922400	-1.36434600	0.00009000
	P	0.77294000	-0.04145300	0.00000200
R2 C_2H_4	C	0.00000000	0.66439700	0.00000000
	H	0.92291200	1.23512400	0.00000000
	H	-0.92286400	1.23518300	0.00000000
	C	0.00000000	-0.66439700	0.00000000
	H	-0.92291200	-1.23512400	0.00000000
	H	0.92286400	-1.23518300	0.00000000
TSa	C	-0.75726700	0.91069200	-0.46026900
	C	-0.11006100	-0.29071500	-0.64851900
	H	-0.61406800	1.97131600	-0.62535900
	C	1.77670500	-0.63226300	-0.26616400
	H	1.61877500	-1.62117200	0.14852500
	H	2.14082700	-0.64052500	-1.28640400
	P	-1.71044700	-0.25634600	0.32098600
	C	2.11299800	0.41284900	0.56670200
	H	2.48856100	1.34937700	0.17158900
	H	1.88836500	0.38281400	1.62635600
IMa	C	0.31237900	0.08851000	-0.00000200
	C	-0.76901000	1.04760100	-0.00001700
	C	1.56497800	-0.13318700	-0.76921400
	H	2.02130300	0.71251200	-1.27602100
	H	1.71404700	-1.08645000	-1.26668900
	H	-0.90585300	2.12074000	-0.00003900
	P	-1.50698800	-0.43944400	0.00000800

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Species	Atom	Coordinates, Å		
	C	1.56498000	-0.13315000	0.76921900
	H	1.71405800	-1.08637800	1.26675600
	H	2.02130100	0.71258700	1.27596600
TS1	C	0.26341300	0.14705300	-0.03452600
	C	-0.51637400	1.13874200	-0.63418100
	C	1.51562400	-0.59883800	-0.51809600
	H	1.93349400	-0.24014300	-1.45102700
	H	1.48112000	-1.67452900	-0.39717100
	H	-1.90243000	0.42154700	1.22762400
	P	-1.49842600	-0.34595600	0.09161800
	C	1.60833400	0.25935000	0.68381900
	H	2.09922800	1.22264400	0.60798600
	H	1.63898800	-0.21802300	1.65622200
P1	C	-0.07451000	-0.56804900	-0.47702900
	C	0.08034300	0.88061200	-0.42609100
	C	1.32732400	-0.88486400	-0.03923100
	H	2.01943800	-1.01201400	-0.87583100
	H	1.46960200	-1.68016100	0.69498400
	P	-1.53400200	-0.08755300	0.19342400
	H	0.00383000	1.58168800	-1.24706600
	C	1.34921900	0.65113800	0.42460600
	H	2.23910200	1.21320200	0.12970300
	H	1.18379500	0.73755900	1.50332800
TS2a	C	0.28737600	0.13118100	-0.00380500
	C	-0.63739600	1.10826300	-0.53473900
	C	1.50373000	-0.45240600	-0.64543700
	H	1.93954600	0.09039300	-1.47744400
	H	1.58062100	-1.53186300	-0.71504000
	H	-1.62233600	1.03199200	0.60416300
	P	-1.47028600	-0.40078000	0.12156800
	C	1.57810700	0.17511000	0.74074600
	H	1.70105400	-0.49212200	1.58682200
	H	2.06449900	1.14040900	0.83739200
IM2	C	0.26341300	0.14705300	-0.03452600
	C	-0.51637400	1.13874200	-0.63418100
	C	1.51562400	-0.59883800	-0.51809600
	H	1.93349400	-0.24014300	-1.45102700
	H	1.48112000	-1.67452900	-0.39717100
	H	-1.90243000	0.42154700	1.22762400
	P	-1.49842600	-0.34595600	0.09161800
	C	1.60833400	0.25935000	0.68381900
	H	2.09922800	1.22264400	0.60798600
	H	1.63898800	-0.21802300	1.65622200
TS2b	C	-0.43969300	-0.26832200	-0.16085900
	C	0.61639700	-1.01250600	-0.61141300
	C	-1.46537800	0.81065000	-0.31387000
	H	-1.88605200	0.90291400	-1.30950400
	H	-1.32106700	1.74593500	0.21157000
	H	2.51609000	-0.54205100	0.75426300
	P	1.54797900	0.32215900	0.14491000

Species	Atom	Coordinates, Å		
	C	-1.76543400	-0.43233100	0.50198700
	H	-1.79071400	-0.32224200	1.58032500
	H	-2.41329300	-1.20188900	0.09462900
P2	C	-0.75906700	-0.00079800	0.00836600
	C	0.52612900	-0.00185900	0.04545600
	C	-2.03227300	0.76020900	-0.00292000
	H	-2.29726900	1.27509000	-0.92096600
	H	-2.31476800	1.27547100	0.90961400
	H	2.45549700	-0.00031500	1.30006500
	P	2.17125400	0.00035700	-0.10420700
	C	-2.03389700	-0.75900000	-0.00315200
	H	-2.31753500	-1.27390300	0.90923100
	H	-2.30008400	-1.27301700	-0.92133900
TS3	C	-0.80243700	-0.12140800	-0.01940100
	C	0.24326100	0.10344400	-0.95049200
	C	-2.09561700	-0.87429600	-0.39501400
	H	-2.04633700	-1.48047600	-1.29139900
	H	-3.01270600	-0.31659800	-0.24797700
	H	0.45250800	1.62019100	1.13351800
	P	-0.45479900	1.67841400	0.03570900
	C	-1.30215100	-1.28505200	0.79563300
	H	-0.72069100	-2.19913200	0.73433600
	H	-1.68798500	-1.04570800	1.77958000
	C	2.22651200	-0.87719200	-0.52478100
	H	2.64903200	-0.55506700	-1.46597500
	H	1.78083200	-1.86442200	-0.51798900
	C	2.45433700	-0.20020400	0.61869200
	H	2.08403500	-0.55404500	1.57419100
	H	2.97986100	0.74730000	0.61825700
P3	C	-0.72954300	-0.05091900	0.00065300
	C	0.72952100	-0.05095300	0.00063400
	C	-1.77478900	-0.80085600	-0.75082900
	H	-1.48667900	-1.73479100	-1.22341300
	H	-2.53589000	-0.24213400	-1.28376700
	H	0.00044600	1.91232400	1.29202100
	P	0.00004000	1.65921700	-0.11401900
	C	-1.78941800	-0.75018100	0.77471500
	H	-1.51023500	-1.65024500	1.31425400
	H	-2.56212700	-0.16060200	1.25500800
	C	1.77473300	-0.80093700	-0.75084300
	H	2.53587200	-0.24227500	-1.28378900
	H	1.48654100	-1.73484700	-1.22342700
	C	1.78936500	-0.75026500	0.77470000
	H	1.51016500	-1.65031800	1.31424600
	H	2.56209800	-0.16070300	1.25497500
R1 C_2PF	C	-0.47594200	0.09500600	0.00001500
	C	0.24422600	1.26156100	-0.00003000
	P	1.13202600	-0.36488000	-0.00003400
	F	-1.73223200	-0.29624400	0.00006700

Species	Atom	Coordinates, Å		
R1 C_2PCN	C	-0.07197400	0.21403800	0.00000200
	C	0.86299900	1.25000500	-0.00008000
	P	1.47501200	-0.47601300	-0.00008200
	C	-1.45358000	-0.01623700	0.00009000
	N	-2.59283600	-0.22094900	0.00016600
R1 C_2PCH_3	C	-0.41870100	0.12218200	-0.00161000
	C	0.39212600	1.24536700	0.00019400
	P	1.19889300	-0.39002600	0.00008700
	C	-1.85498300	-0.23941900	-0.00158600
	H	-2.36385500	0.28787800	-0.81460400
	H	-2.02061400	-1.31256400	-0.10156200
	H	-2.30957500	0.10629700	0.93287100
R1 C_2POH	C	-0.47531800	0.05393300	-0.00000100
	C	0.25351000	1.23297300	-0.00000500
	P	1.16262700	-0.34177400	0.00000300
	O	-1.72407300	-0.37396700	-0.00000900
	H	-2.31597300	0.39691300	0.00006900
R1 C_2POCH_3	C	0.05568400	-0.07780300	-0.00001700
	C	0.61093900	1.19753900	-0.00003600
	P	1.73921700	-0.22601900	0.00002200
	O	-1.10204300	-0.69024600	-0.00004500
	C	-2.26910700	0.17914200	0.00003000
	H	-2.26519500	0.80587700	-0.89201000
	H	-3.12523800	-0.49066300	-0.00138600
	H	-2.26656700	0.80376300	0.89356600
R1 C_2PNH_2	C	-0.46983900	0.07522100	-0.00000100
	C	0.33880200	1.22198000	0.00000400
	P	1.17678400	-0.36335700	0.00002300
	N	-1.76159500	-0.23492400	-0.00033100
	H	-2.45367100	0.50226200	0.00111200
	H	-2.08070100	-1.19064500	0.00084900
R1 C_2PNHCH_3	C	0.07945800	-0.08019500	-0.00009100
	C	0.68333700	1.19087100	-0.00015200
	P	1.78169600	-0.22411700	0.00010700
	N	-1.13704300	-0.60548700	-0.00034400
	H	-1.23529400	-1.60927900	0.00032700
	C	-2.35218200	0.21523100	0.00019000
	H	-2.38779900	0.85220700	-0.88580300
	H	-3.21742200	-0.44747000	-0.00166400
	H	-2.38930000	0.84926400	0.88826100

Species	Atom	Coordinates, Å		
R1 $C_2PN(CH_3)_2$	C	0.33770400	-0.18162100	-0.00010500
	C	1.22983400	-1.27082300	0.00006700
	P	1.96323300	0.35983800	0.00004800
	N	-0.96711900	0.04306500	-0.00053900
	C	-1.91188400	-1.07420200	0.00011500
	H	-1.35026100	-2.00663700	-0.00158400
	H	-2.54725000	-1.03292900	0.89066600
	H	-2.55021300	-1.03111900	-0.88814700
	C	-1.52603800	1.38805800	0.00012000
	H	-0.71471400	2.11415000	0.00000100
	H	-2.14735600	1.54472500	-0.88810600
	H	-2.14655300	1.54431300	0.88903900
TSa F	C	-0.77585600	0.50156500	-0.18921200
	C	0.09021200	-0.41312800	-0.73931700
	C	2.01253200	-0.53407400	-0.42594100
	H	2.04630900	-1.61414200	-0.34494600
	H	2.34466400	-0.15464900	-1.38421400
	P	-1.44663000	-0.96763600	0.26447800
	C	2.14980700	0.24443900	0.70055000
	H	2.32249600	1.31156300	0.62951600
	H	1.95730300	-0.15728100	1.68831200
	F	-0.87016700	1.81513800	-0.07025700
TSa CF_3	C	0.07454500	0.55495700	-0.21629400
	C	-1.20052900	0.49747500	-0.75061500
	C	-2.52881500	-0.89406600	-0.45326300
	H	-3.38252700	-0.22777300	-0.41728000
	H	-2.41716000	-1.41667700	-1.39534400
	P	-0.63207400	2.02276900	0.22157200
	C	-2.05810400	-1.47108100	0.70407300
	H	-1.35417300	-2.29379400	0.67711900
	H	-2.27462700	-1.04281700	1.67562400
	C	1.28607200	-0.30127100	-0.03963300
	F	1.32478500	-0.82105500	1.20569000
	F	1.30860200	-1.32784100	-0.91144900
	F	2.41890000	0.40705600	-0.21972200
TSa CN	C	0.69409100	0.23921900	-0.21501500
	C	-0.58089800	0.49254800	-0.73047800
	C	-2.15483600	-0.60336200	-0.43423400
	H	-2.85630500	0.22043900	-0.37154300
	H	-2.16610600	-1.11885100	-1.38684700
	P	0.30724100	1.81844200	0.26857100
	C	-1.79780200	-1.28840600	0.70503100
	H	-1.27471200	-2.23562700	0.65289700
	H	-1.91329900	-0.84508500	1.68720300
	C	1.62839600	-0.79984300	-0.09644100
	N	2.40972800	-1.64835000	0.00236300

Species	Atom	Coordinates, Å		
TSa CH_3	C	-0.81504600	0.43302600	-0.19537600
	C	0.09382300	-0.48332300	-0.70002600
	C	2.01686800	-0.48449400	-0.42964200
	H	2.10010200	-1.55855200	-0.30871900
	H	2.32025300	-0.13567700	-1.40937100
	P	-1.36308200	-1.11256400	0.26327800
	C	2.18949700	0.33825600	0.66482400
	H	2.34667800	1.40422400	0.54887900
	H	2.03963800	-0.02853700	1.67350000
	C	-1.01939100	1.89455600	-0.06971200
	H	-0.44310400	2.25361500	0.79063100
	H	-0.64371100	2.41502400	-0.95463900
	H	-2.06812600	2.15023400	0.09014400
TSa OH	C	-0.78633700	0.52909200	-0.16763900
	C	0.05370900	-0.43338300	-0.70882200
	C	1.94316500	-0.61983700	-0.39655500
	H	1.90192900	-1.68562000	-0.20131700
	H	2.31784000	-0.38189800	-1.38479300
	P	-1.45002800	-0.96930100	0.25809900
	C	2.19116800	0.25027300	0.64874500
	H	2.49735600	1.27502300	0.46965500
	H	1.96321100	-0.01911900	1.67283400
	O	-0.90096900	1.84042700	-0.03104800
	H	-0.13239600	2.27084000	-0.43385300
TSa OCH_3	C	-0.69007300	0.47566000	0.01521400
	C	0.50807100	0.38818800	0.71994200
	C	1.98177900	-0.84210100	0.50161700
	H	2.74866500	-0.08895300	0.64072500
	H	1.82965200	-1.46391700	1.37602000
	P	0.08140600	1.98034400	-0.13678100
	C	1.78754200	-1.38564900	-0.75428800
	H	1.23374000	-2.30667300	-0.89311000
	H	2.06128300	-0.84251300	-1.65078200
	O	-1.75035500	-0.21993600	-0.32183200
	C	-1.83439000	-1.56631900	0.21084900
	H	-2.80050200	-1.94634400	-0.11261800
	H	-1.02860200	-2.17788000	-0.19399100
	H	-1.78005100	-1.53807300	1.30013000
TSa NH_2	C	-0.80884700	0.50277200	-0.17325700
	C	0.06423100	-0.45891500	-0.69881600
	C	1.96558500	-0.54418600	-0.40382700
	H	1.98466400	-1.61433500	-0.22965800
	H	2.31402300	-0.26837200	-1.39200500
	P	-1.37885800	-1.05458700	0.25648300
	C	2.19592800	0.31512400	0.65517500
	H	2.43666700	1.35960900	0.49234600
	H	1.99514800	0.01505300	1.67666200
	N	-0.94177800	1.82324100	-0.08621900
	H	-0.23356400	2.43596900	-0.46176400
	H	-1.72300800	2.23942800	0.39505100

Species	Atom	Coordinates, Å		
TSa $NHCH_3$	C	0.49707100	0.16063400	-0.31070100
	C	-0.80003900	0.55309500	-0.67604500
	C	-2.42050000	-0.41196700	-0.28467000
	H	-2.97363100	0.46480200	0.03382400
	H	-2.68237300	-0.73904200	-1.28391900
	P	0.20084700	1.74851300	0.27613200
	C	-2.05628400	-1.35675200	0.65809100
	H	-1.74015100	-2.35210600	0.36648200
	H	-1.92929500	-1.09054800	1.70063500
	N	1.31512300	-0.87905000	-0.39283200
	H	0.94465700	-1.73261700	-0.78798200
	C	2.64479800	-0.92037900	0.20198900
	H	3.30414300	-1.53427300	-0.41429800
	H	3.04612900	0.09226600	0.24438900
	H	2.62167500	-1.33062400	1.21673600
TSa $N(CH_3)_2$	C	0.31673500	0.44751400	-0.21987600
	C	-0.99879000	0.43595100	-0.71863100
	C	-2.41976400	-0.77190300	-0.23581900
	H	-3.17958200	0.00007400	-0.18844300
	H	-2.47775000	-1.36593200	-1.14059200
	P	-0.41141100	1.98659200	0.03636600
	C	-1.99704900	-1.37363900	0.93673800
	H	-1.44607500	-2.30685800	0.92650000
	H	-2.06103900	-0.85550500	1.88618000
	N	1.36454500	-0.34958100	-0.07729200
	C	2.60520400	0.11441000	0.52975000
	H	3.43972400	-0.00478300	-0.16933200
	H	2.50488200	1.16609700	0.79238400
	H	2.82692600	-0.45815000	1.43655400
	C	1.33304300	-1.73210200	-0.54800600
	H	1.43269600	-2.42813500	0.29085200
	H	0.38746500	-1.91212900	-1.05452700
	H	2.15583200	-1.90786900	-1.24896800