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APPENDICES

APPENDIX A

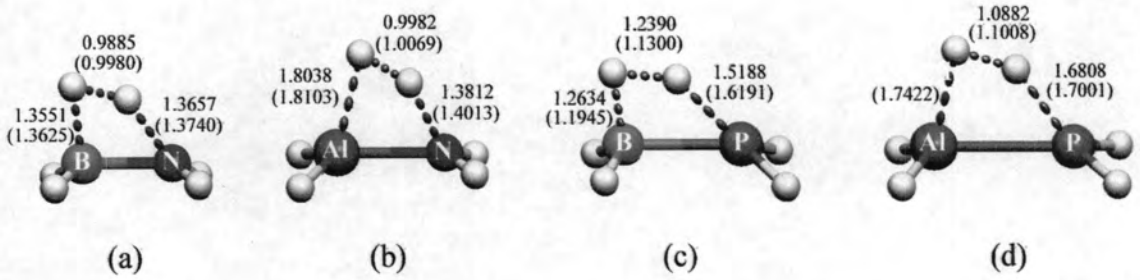


Figure A-1 The transition state structures of (a) tsba, (b) tsala, (c) tsbp and (d) tsalp were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

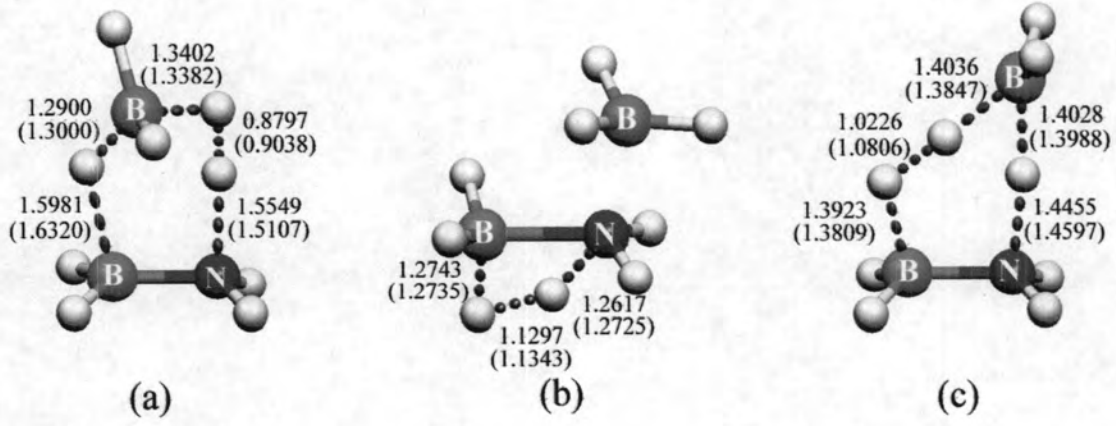


Figure A-2 The transition state structures of (a) tsba_BN, (b) tsba_BH_3 and (c) tsba_BB were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

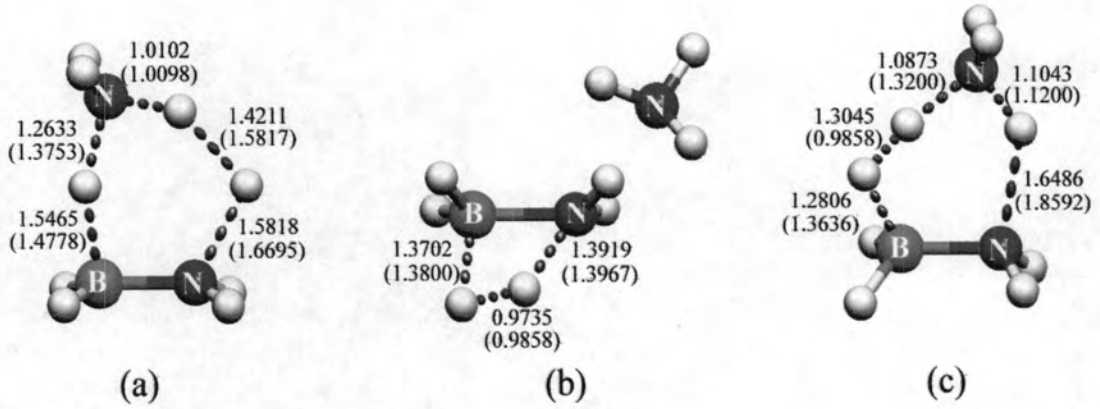


Figure A-3 The transition state structures of (a) tsba_NN, (b) tsba_NH_3 and (c) tsba_NB were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

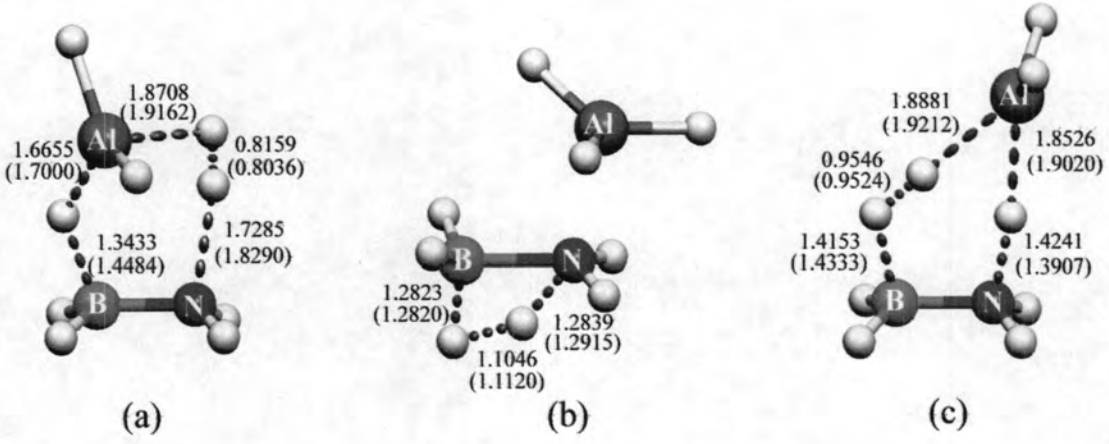


Figure A-4 The transition state structures of (a) tsba_AlN, (b) tsba_AlH_3 and (c) tsba_AlB were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

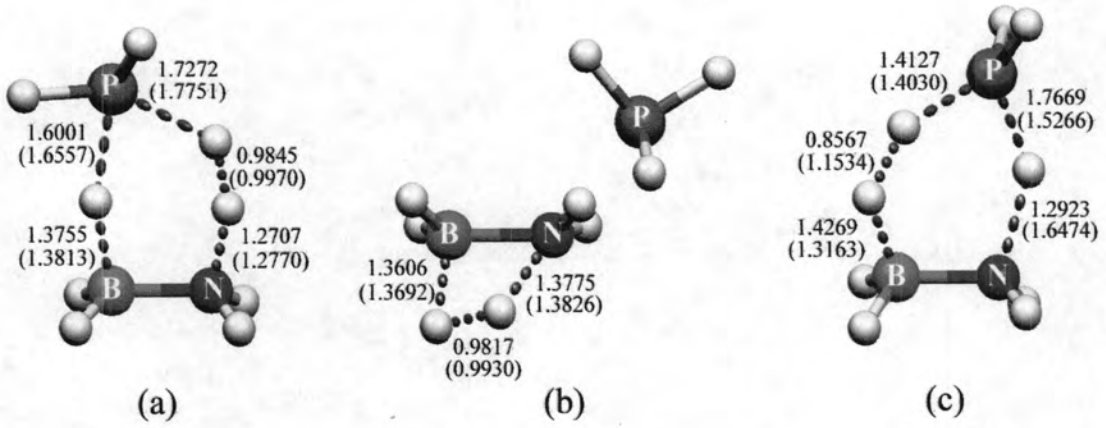


Figure A-5 The transition state structures of (a) tsba_PN, (b) tsba_PH_3 and (c) tsba_PB were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

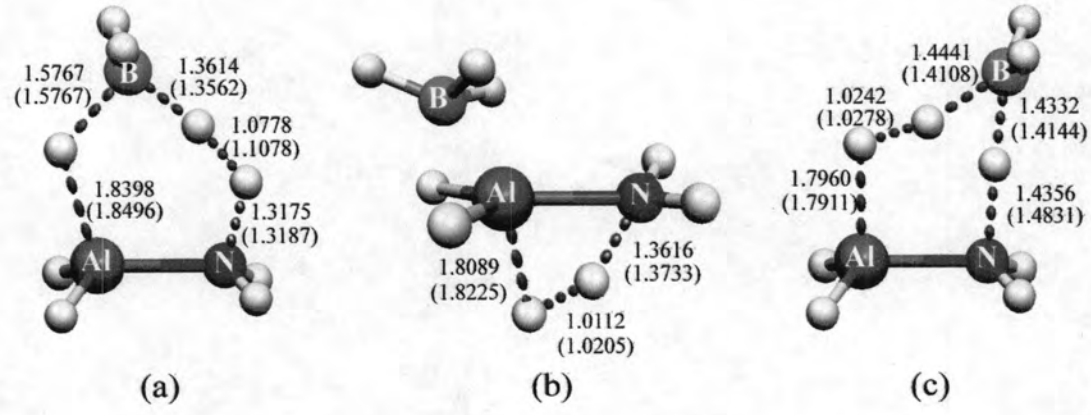


Figure A-6 The transition state structures of (a) tsala_BN, (b) tsala_BH_3 and (c) tsala_BAl were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

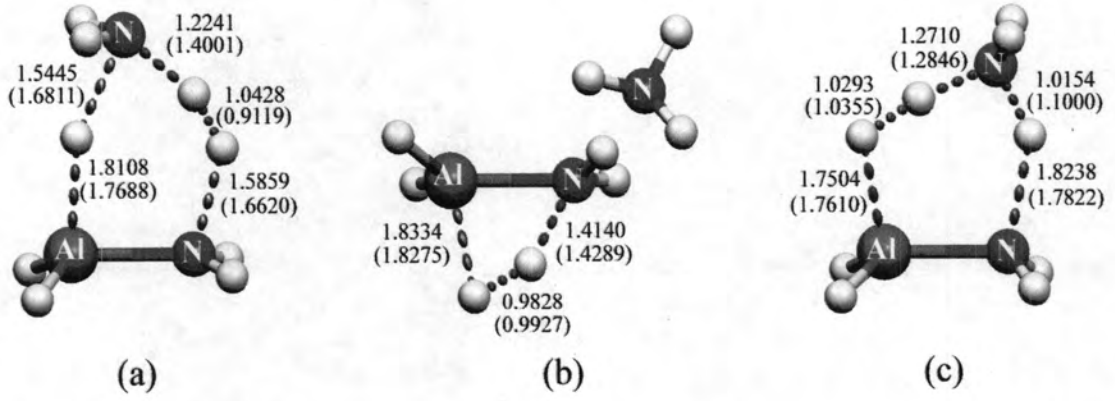


Figure A-7 The transition state structures of (a) tsala_NN, (b) tsala_NH_3 and (c) tsala_NAl were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

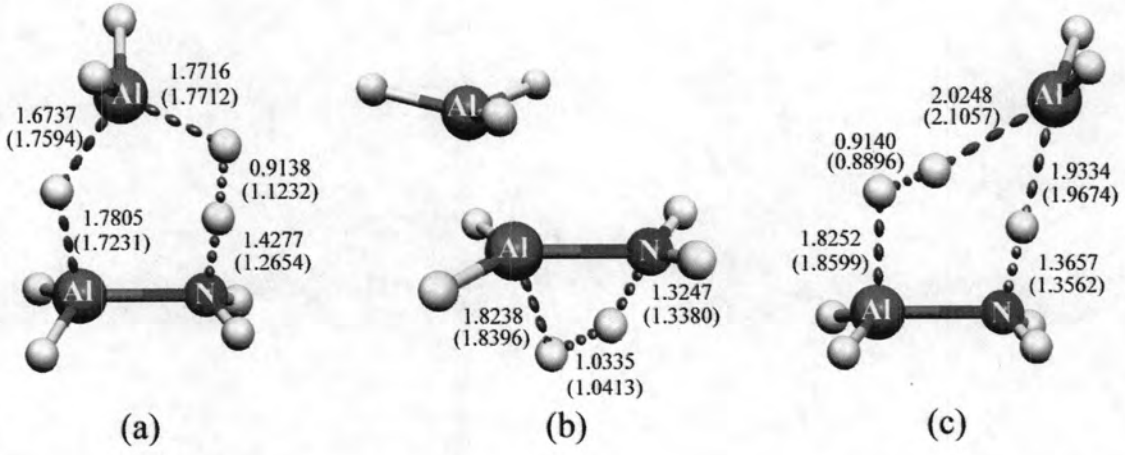


Figure A-8 The transition state structures of (a) tsala_AlN, (b) tsala_AlH_3 and (c) tsala_AlAl were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

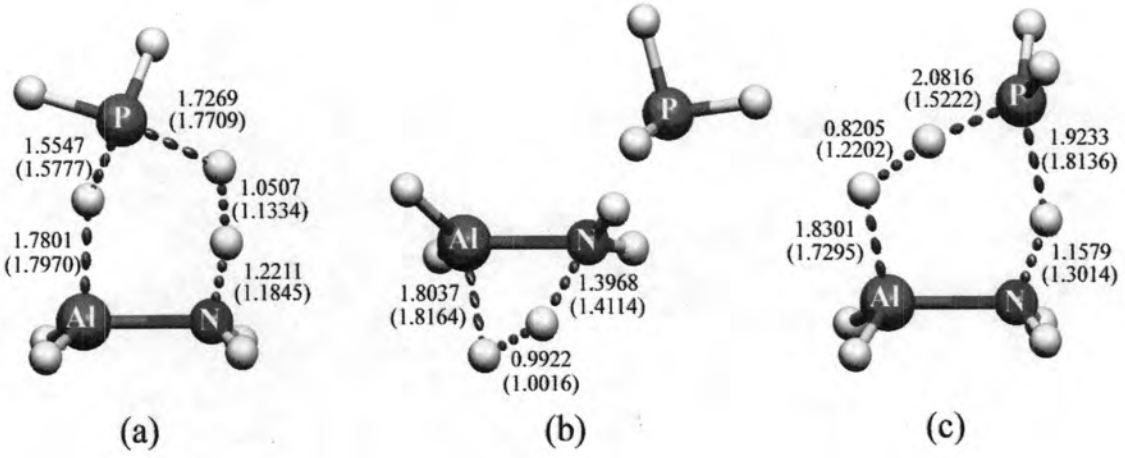


Figure A-9 The transition state structures of (a) tsala_PN, (b) tsala_PH_3 and (c) tsala_PAl were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

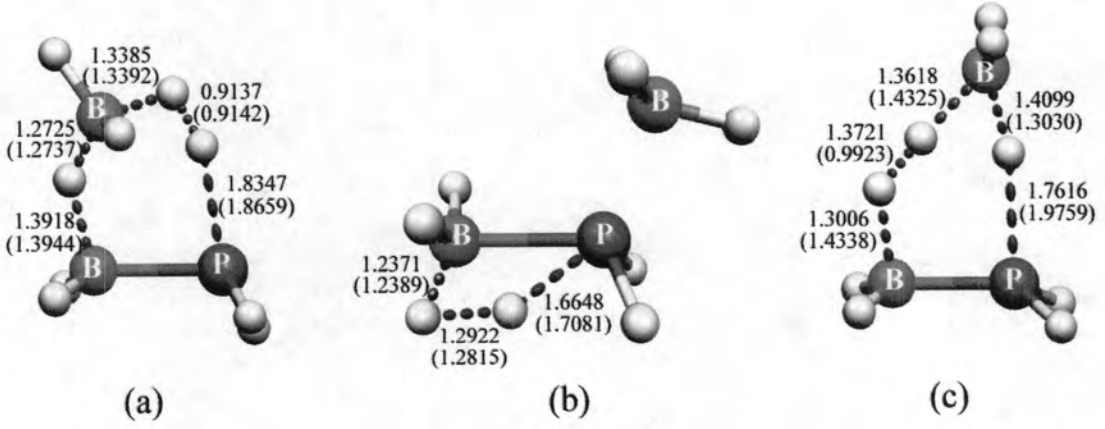


Figure A-10 The transition state structures of (a) tsbp_BP, (b) tsbp_BH_3 and (c) tsbp_BB were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

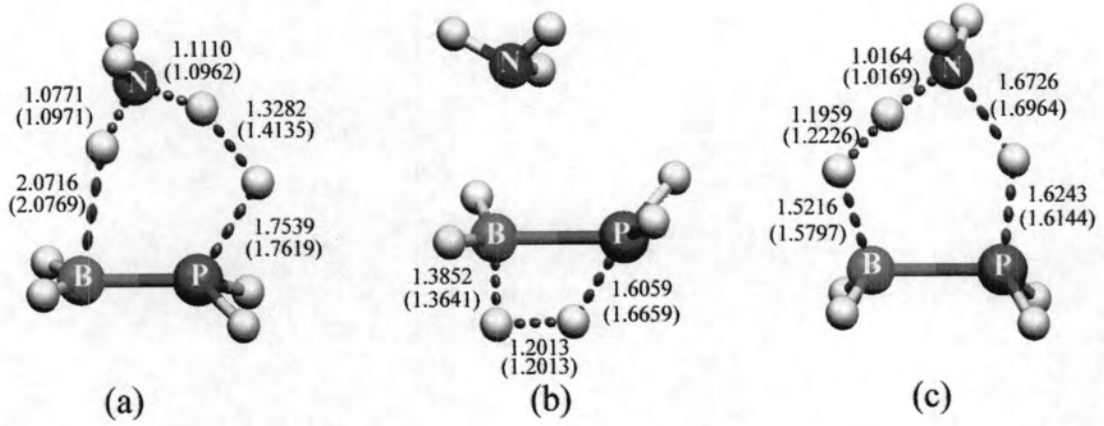


Figure A-11 The transition state structures of (a) tsbp_NP, (b) tsbp_NH_3 and (c) tsbp_NB were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

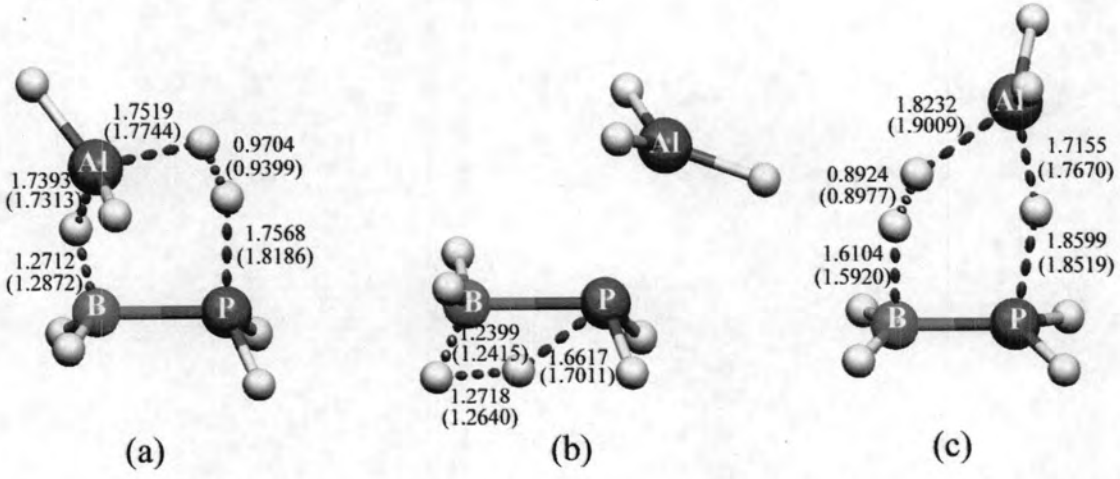


Figure A-12 The transition state structures of (a) tsbp_AlP, (b) tsbp_AlH_3 and (c) tsbp_AlB were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

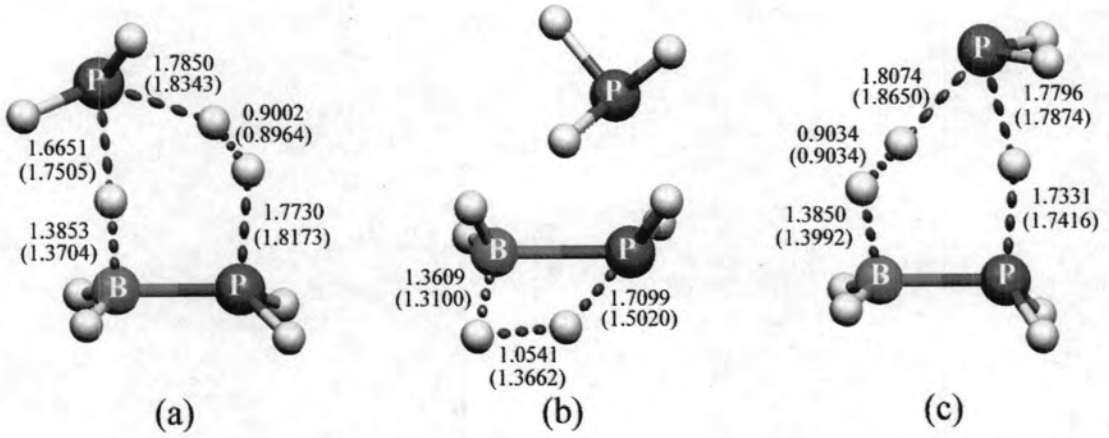


Figure A-13 The transition state structures of (a) tsbp_PP, (b) tsbp_PH_3 and (c) tsbp_PB were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

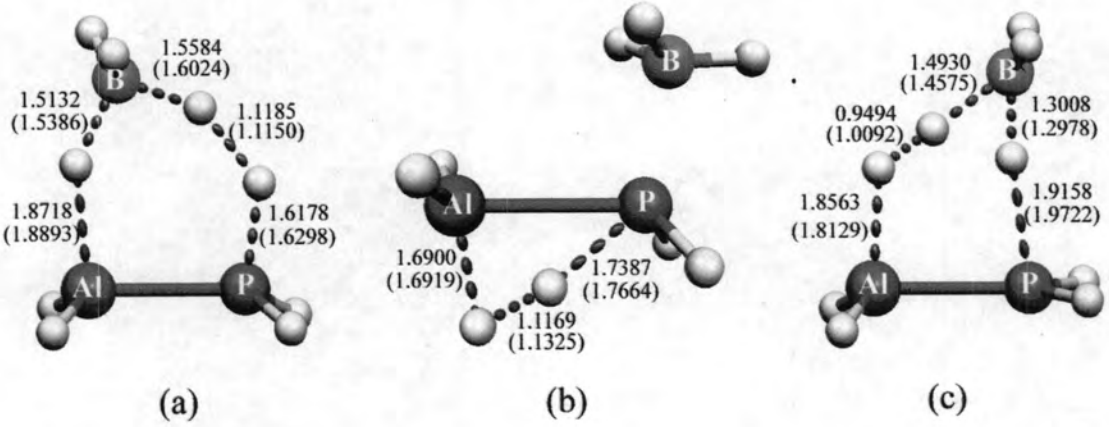
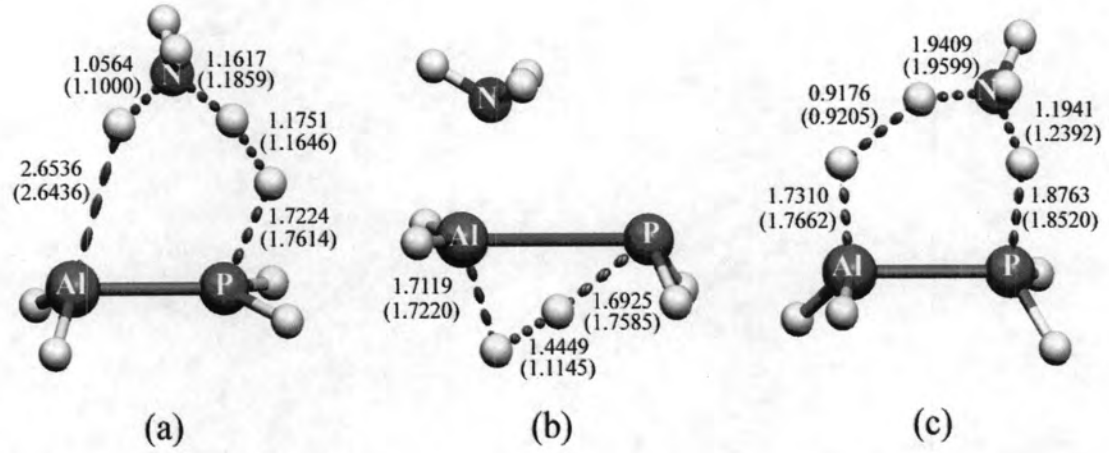
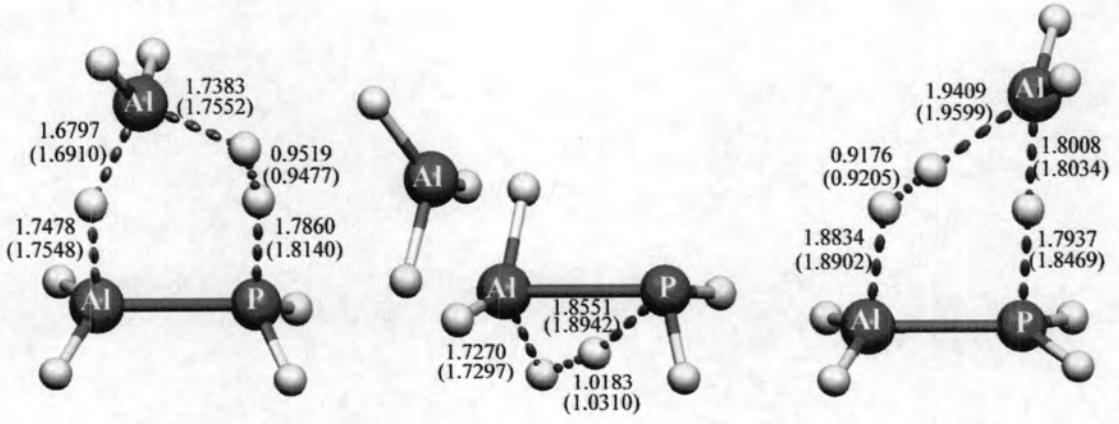


Figure A-14 The transition state structures of (a) tsalp_BP, (b) tsalp_BH_3 and (c) tsalp_BAl were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.



(a) (b) (c)

Figure A-15 The transition state structures of (a) tsalp_NP, (b) tsalp_NH_3 and (c) tsalp_NAl were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.



(a) (b) (c)

Figure A-16 The transition state structures of (a) tsalp_AlP, (b) tsalp_AlH_3 and (c) tsalp_AlAl were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

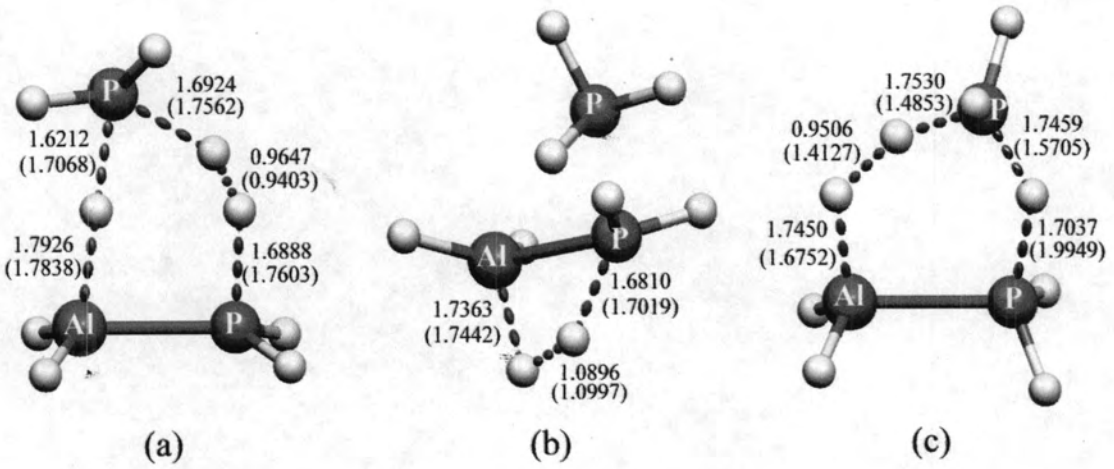


Figure A-17 The transition state structures of (a) tsalp_PP, (b) tsalp_PH_3 and (c) tsalp_PAl were optimized at MP2/6–311++G(d,p) and B3LYP/6–311++G(d,p) (in the parenthesis) levels of theory. Bond distances are in Å.

APPENDIX B

Table B-1 ΔE ,κ , $Q_{TS}/Q_{Complex}$ and A of hydrogen release from BH_3NH_3 without and with BH_3, NH_3, AlH_3 or PH_3 catalyst, computed at the B3LYP/6-311++G(d,p) (in the parenthesis) and MP2/6-311++G(d,p)

Reaction	Frequency,ν_i (cm^{-1})	κ	$Q_{TS}/Q_{Complex}$	A
BH_3NH_3 reactant:				
$BH_3+NH_3 \rightarrow BH_3NH_3$	-	-	-	-
	-	-	-	-
$BH_3NH_3 \rightarrow$ **tsba** $\rightarrow BH_2NH_2+H_2$	-	3.13	7.00	1.45×10^{-8}
	-	(3.02)	(6.84)	(4.72×10^{-7})
BH_3NH_3 and BH_3 reactants:				
$BH_3NH_3+BH_3 \rightarrow BH_3NH_3\cdots BH_3$	-	-	-	-
	-	-	-	-
$BH_3NH_3\cdots BH_3 \rightarrow$ **tsba-BN** $\rightarrow BH_2NH_2+H_2+BH_3$	-810.4003	1.64	4.82×10^{-1}	1.92×10^{-21}
	(-909.5569)	(1.80)	(3.28×10^{-1})	(3.40×10^{-17})
$BH_3NH_3\cdots BH_3 \rightarrow$ **tsba-BH_3** $\rightarrow NH_2BH_2BH_3$(ring)$+H_2$	-1203.9980	2.41	2.68	7.32×10^{-10}
	(-1188.2741)	(2.37)	(6.39×10^{-1})	(3.58×10^{-8})
$BH_3NH_3\cdots BH_3 \rightarrow$ **tsba-BB** $\rightarrow BH_2NH_2+H_2+BH_3$	-1411.0746	2.93	1.12	3.23×10^{-50}
	(-1537.0969)	(3.29)	(5.90×10^{-1})	(3.45×10^{-43})
BH_3NH_3 and NH_3 reactants:				
$BH_3NH_3+NH_3 \rightarrow BH_3NH_3\cdots NH_3$	-	-	-	-
	-	-	-	-
$BH_3NH_3\cdots NH_3 \rightarrow$ **tsba-NN** $\rightarrow BH_2NH_2+H_2+NH_3$	-1154.7513	2.29	4.47×10^{-2}	6.00×10^{-85}
	(-1801.6021)	(4.15)	(5.18×10^{-2})	(1.81×10^{-76})
$BH_3NH_3\cdots NH_3 \rightarrow$ **tsba-NH_3** $\rightarrow BH_2NH_2+H_2+NH_3$	-1465.3067	3.08	5.91	1.10×10^{-11}
	(-1435.3928)	(3.00)	(6.15)	(8.85×10^{-10})
$BH_3NH_3\cdots NH_3 \rightarrow$ **tsba-NB** $\rightarrow BH_2NH_2+H_2+NH_3$	-515.0212	1.26	3.80×10^{-2}	6.87×10^{-7}
	(-945.0833)	(1.87)	(6.45×10^{-2})	(1.21×10^{-6})
BH_3NH_3 and AlH_3 reactants:				
$BH_3NH_3+AlH_3 \rightarrow BH_3NH_3\cdots AlH_3$	-	-	-	-
	-	-	-	-
$BH_3NH_3\cdots AlH_3 \rightarrow$ **tsba-AlN** $\rightarrow NH_2BH_2AlH_3$(ring)$+H_2$	-338.1276	1.11	6.94×10^{-1}	5.64
	(-280.0881)	(1.08)	(7.61×10^{-1})	(6.18×10^{4})
$BH_3NH_3\cdots AlH_3 \rightarrow$ **tsba-AlH_3** $\rightarrow NH_2BH_2AlH_3$(ring)$+H_2$	-1296.6264	2.63	9.34×10^{-1}	8.61×10^{-10}
	(-1272.2278)	(2.57)	(1.47)	(5.39×10^{-9})
$BH_3NH_3\cdots AlH_3 \rightarrow$ **tsba-AlB** $\rightarrow BH_2NH_2+H_2+AlH_3$	-1355.0498	2.78	1.39	8.91×10^{-39}
	(-1469.2889)	(3.09)	(1.15)	(1.09×10^{-32})
BH_3NH_3 and PH_3 reactants:				
$BH_3NH_3+PH_3 \rightarrow BH_3NH_3\cdots PH_3$	-	-	-	-
	-	-	-	-
$BH_3NH_3\cdots PH_3 \rightarrow$ **tsba-PN** $\rightarrow BH_2NH_2+H_2+PH_3$	-1495.5276	3.17	8.94×10^{-3}	4.01×10^{-35}
	(-1469.4731)	(3.10)	(1.38×10^{-2})	(4.17×10^{-32})
$BH_3NH_3\cdots PH_3 \rightarrow$ **tsba-PH_3** $\rightarrow BH_2NH_2+H_2+PH_3$	-1475.2582	3.11	7.74	4.71×10^{-10}
	(-1438.1688)	(3.01)	(5.50×10^{1})	(1.36×10^{-8})
$BH_3NH_3\cdots PH_3 \rightarrow$ **tsba-PB** $\rightarrow BH_2NH_2+H_2+PH_3$	-1350.7780	2.77	4.78×10^{-2}	4.61×10^{-23}
	(-1215.0719)	(2.43)	(1.26×10^{-2})	(9.50×10^{-16})

Table B-2 ΔE ,κ , $Q_{TS}/Q_{Complex}$ and A of hydrogen release from AlH_3NH_3 without and with BH_3, NH_3, AlH_3 or PH_3 catalyst, computed at the B3LYP/6-311++G(d,p) (in the parenthesis) and MP2/6-311++G(d,p)

Reaction	Frequency, ν_i (cm^{-1})	κ	$Q_{TS}/Q_{Complex}$	A
AlH_3NH_3 reactant:	-			
$AlH_3+NH_3 \rightarrow AlH_3NH_3$	-	-	-	-
	-	-	-	-
$AlH_3NH_3 \rightarrow$ **tsala** $\rightarrow AlH_2NH_2+H_2$	-	2.94	3.51	1.45×10^{-8}
		(2.76)	(3.26)	(4.72×10^{-7})
AlH_3NH_3 and BH_3 reactants:	-			
$AlH_3NH_3+BH_3 \rightarrow AlH_3NH_3\cdots BH_3$	-	-	-	-
	-	-	-	-
$AlH_3NH_3\cdots BH_3 \rightarrow$ **tsala-BN** $\rightarrow NH_2AlH_2BH_3$(ring)$+H_2$	-1164.2213	2.32	5.46×10^{-1}	1.92×10^{-21}
	(-1103.6687)	(2.18)	(6.60×10^{-1})	(3.40×10^{-17})
$AlH_3NH_3\cdots BH_3 \rightarrow$ **tsala-BH_3** $\rightarrow NH_2AlH_2BH_3+H_2$	-1443.8219	3.02	2.46×10^{-1}	7.32×10^{-10}
	(-1378.1680)	(2.84)	(3.64×10^{-1})	(3.58×10^{-8})
$AlH_3NH_3\cdots BH_3 \rightarrow$ **tsala-BAl** $\rightarrow AlH_2NH_2+H_2+BH_3$	-1616.7884	3.54	4.79×10^{-1}	3.23×10^{-50}
	(-1543.9723)	(3.31)	(6.47×10^{-1})	(3.45×10^{-43})
AlH_3NH_3 and NH_3 reactants:				
$AlH_3NH_3+NH_3 \rightarrow AlH_3NH_3\cdots NH_3$	-	-	-	-
	-	-	-	-
$AlH_3NH_3\cdots NH_3 \rightarrow$ **tsala-NN** $\rightarrow AlH_2NH_2+H_2+NH_3$	-1283.4826	2.60	6.86×10^{-2}	6.00×10^{-85}
	(-2126.8275)	(5.39)	(7.53×10^{-2})	(1.81×10^{-76})
$AlH_3NH_3\cdots NH_3 \rightarrow$ **tsala-NH_3** $\rightarrow AlH_2NH_2+H_2+NH_3$	-1392.8200	2.88	2.75	1.10×10^{-11}
	(-1325.4545)	(2.70)	(5.81)	(8.85×10^{-10})
$AlH_3NH_3\cdots NH_3 \rightarrow$ **tsala-NAl** $\rightarrow AlH_2NH_2+H_2+NH_3$	-980.2803	1.93	5.36×10^{-2}	6.87×10^{-7}
	(-1017.9322)	(2.01)	(4.08×10^{-2})	(1.21×10^{-6})
AlH_3NH_3 and AlH_3 reactants:				
$AlH_3NH_3+AlH_3 \rightarrow AlH_3NH_3\cdots AlH_3$	-	-	-	-
	-	-	-	-
$AlH_3NH_3\cdots AlH_3 \rightarrow$ **tsala-AlN** $\rightarrow NH_2AlH_2AlH_3$(ring)$+H_2$	-853.0479	1.71	3.46×10^{-1}	5.64
	(-869.4539)	(1.73)	(2.29×10^{-1})	(6.18×10^{4})
$AlH_3NH_3\cdots AlH_3 \rightarrow$ **tsala-AlH_3** $\rightarrow NH_2AlH_2AlH_3+H_2$	-1473.3575	3.11	3.42×10^{-1}	8.61×10^{-10}
	(-1410.6877)	(2.93)	(2.07×10^{-1})	(5.39×10^{-9})
$AlH_3NH_3\cdots AlH_3 \rightarrow$ **tsala-AlAl** $\rightarrow AlH_2NH_2+H_2+AlH_3$	-1440.9705	3.01	1.62	8.91×10^{-39}
	(-1365.6033)	(2.81)	(1.06)	(1.09×10^{-32})
AlH_3NH_3 and PH_3 reactants:				
$AlH_3NH_3+PH_3 \rightarrow AlH_3NH_3\cdots PH_3$	-	-	-	-
	-	-	-	-
$AlH_3NH_3\cdots PH_3 \rightarrow$ **tsala-PN** $\rightarrow AlH_2NH_2+H_2+PH_3$	-1427.9775	2.98	3.36×10^{-2}	4.01×10^{-35}
	(-1175.1997)	(2.34)	(1.15×10^{-3})	(4.17×10^{-32})
$AlH_3NH_3\cdots PH_3 \rightarrow$ **tsala-PH_3** $\rightarrow AlH_2NH_2+H_2+PH_3$	-1414.5688	2.94	1.88	4.71×10^{-10}
	(-1342.1498)	(2.75)	(1.29)	(1.36×10^{-8})
$AlH_3NH_3\cdots PH_3 \rightarrow$ **tsala-PAl** $\rightarrow AlH_2NH_2+H_2+PH_3$	-576.0863	1.32	3.18×10^{-2}	4.61×10^{-23}
	(-1157.3411)	(2.30)	(4.53×10^{-3})	(9.50×10^{-16})

Table B-3 ΔE ,κ , $Q_{TS}/Q_{Complex}$ and A of hydrogen release from BH_3PH_3 without and with BH_3, NH_3, AlH_3 or PH_3 catalyst, computed at the B3LYP/6-311++G(d,p) (in the parenthesis) and MP2/6-311++G(d,p)

Reaction	Frequency,ν_i (cm^{-1})	κ	$Q_{TS}/Q_{Complex}$	A
BH_3PH_3 reactant:	-			
$BH_3+PH_3 \rightarrow BH_3PH_3$	-	-	-	-
	-	-	-	-
$BH_3PH_3 \rightarrow$ **tsbp** $\rightarrow BH_2PH_2+H_2$	-	2.47	18.94	1.45×10^{-8}
		(2.37)	(13.50)	(4.72×10^{-7})
BH_3PH_3 and BH_3 reactants:	-			
$BH_3PH_3+BH_3 \rightarrow BH_3PH_3\cdots BH_3$	-	-	-	-
	-	-	-	-
$BH_3PH_3\cdots BH_3 \rightarrow$ **tsbp-BP** $\rightarrow PH_2BH_2BH_3$(ring)$+H_2$	-822.2809	1.66	6.95×10^{-1}	1.92×10^{-21}
	(-692.3240)	(1.47)	(5.03×10^{-1})	(3.40×10^{-17})
$BH_3PH_3\cdots BH_3\rightarrow$ **tsbp-BH_3** $\rightarrow PH_2BH_2BH_3+H_2$	-657.8321	1.42	1.37	7.32×10^{-10}
	(-673.3205)	(1.44)	(8.03×10^{-1})	(3.58×10^{-8})
$BH_3PH_3\cdots BH_3\rightarrow$ **tsbp-BB** $\rightarrow BH_2PH_2+H_2+BH_3$	-1179.9359	2.35	2.64	3.23×10^{-50}
	(-1160.3256)	(2.31)	(2.59)	(3.45×10^{-43})
BH_3PH_3 and NH_3 reactants:				
$BH_3PH_3+NH_3 \rightarrow BH_3PH_3\cdots NH_3$	-	-	-	-
	-	-	-	-
$BH_3PH_3\cdots NH_3 \rightarrow$ **tsbp-NP** $\rightarrow BH_2PH_2+H_2+NH_3$	-1105.8613	2.19	2.57×10^{-2}	6.00×10^{-85}
	(-1043.7944)	(2.06)	(1.31×10^{-3})	(1.81×10^{-76})
$BH_3PH_3\cdots NH_3 \rightarrow$ **tsbp-NH_3** $\rightarrow BH_2PH_2+H_2+NH_3$	-1535.4245	3.29	1.43×10^{-1}	1.10×10^{-11}
	(-1444.5900)	(3.02)	(5.57×10^{-2})	(8.85×10^{-10})
$BH_3PH_3\cdots NH_3\rightarrow$ **tsbp-NB** $\rightarrow PH_2BH_2NH_3+H_2$	-1216.6776	2.44	1.25×10^{-2}	6.87×10^{-7}
	(-1274.6289)	(2.58)	(1.24×10^{-3})	(1.21×10^{-6})
BH_3PH_3 and AlH_3 reactants:				
$BH_3PH_3+AlH_3 \rightarrow BH_3NH_3\cdots AlH_3$	-	-	-	-
	-	-	-	-
$BH_3PH_3\cdots AlH_3 \rightarrow$ **tsbp-AlP** $\rightarrow PH_2BH_2AlH_3$(ring)$+H_2$	-837.8021	1.68	1.85×10^{-1}	5.64
	(-597.4072)	(1.35)	(2.45×10^{-1})	(6.18×10^{4})
$BH_3PH_3\cdots AlH_3 \rightarrow$ **tsbp-AlH_3** $\rightarrow BH_2PH_2+H_2+AlH_3$	-660.2306	1.42	1.33	8.61×10^{-10}
	(-672.5255)	(1.44)	(8.81×10^{-1})	(5.39×10^{-9})
$BH_3PH_3\cdots AlH_3 \rightarrow$ **tsbp-AlB** $\rightarrow BH_2PH_2+H_2+AlH_3$	-897.3370	1.78	3.66×10^{-1}	8.91×10^{-39}
	(-937.4236)	(1.85)	(4.09×10^{-1})	(1.09×10^{-32})
BH_3PH_3 and PH_3 reactants:				
$BH_3PH_3+PH_3 \rightarrow BH_3NH_3\cdots PH_3$	-	-	-	-
	-	-	-	-
$BH_3PH_3\cdots PH_3 \rightarrow$ **tsbp-PP** $\rightarrow BH_2PH_2+H_2+PH_3$	-1134.6073	2.25	4.06×10^{-3}	4.01×10^{-35}
	(-1142.7990)	(2.27)	(7.40×10^{-5})	(4.17×10^{-32})
$BH_3PH_3\cdots PH_3 \rightarrow$ **tsbp-PH_3** $\rightarrow BH_2PH_2+H_2+PH_3$	-1291.3383	2.62	4.89×10^{-1}	4.71×10^{-10}
	(-1117.5357)	(2.21)	(3.59×10^{-1})	(1.36×10^{-8})
$BH_3PH_3\cdots PH_3 \rightarrow$ **tsbp-PB** $\rightarrow BH_2PH_2+H_2+PH_3$	-1389.9844	2.87	1.58×10^{-2}	4.61×10^{-23}
	(-1290.8626)	(2.62)	(1.80×10^{-4})	(9.50×10^{-16})

Table B-4 ΔE ,κ , $Q_{TS}/Q_{Complex}$ and A of hydrogen release from AlH_3PH_3 without and with BH_3, NH_3, AlH_3 or PH_3 catalyst, computed at the B3LYP/6-311++G(d,p) (in the parenthesis) and MP2/6-311++G(d,p)

Reaction	Frequency,ν_i (cm^{-1})	κ	$Q_{TS}/Q_{Complex}$	A
AlH_3PH_3 reactant:	-			
$AlH_3+PH_3 \rightarrow AlH_3PH_3$	-	-	-	-
	-	-	-	-
$AlH_3PH_3 \rightarrow$ **tsalp** $\rightarrow AlH_2PH_2+H_2$	-	2.89	6.08	1.45×10^{-8}
		(2.56)	(6.66)	(4.72×10^{-7})
AlH_3PH_3 and BH_3 reactants:	-			
$AlH_3PH_3+BH_3 \rightarrow AlH_3PH_3\cdots BH_3$	-	-	-	-
	-	-	-	-
$AlH_3PH_3\cdots BH_3 \rightarrow$ **tsalp-BP** $\rightarrow PH_2AlH_2BH_3$(ring)$+H_2$	-1234.2069	2.48	1.77×10^{-1}	1.92×10^{-21}
	(-1207.5788)	(2.41)	(5.10×10^{-1})	(3.40×10^{-17})
$AlH_3PH_3\cdots BH_3\rightarrow$ **tsalp-BH_3** $\rightarrow PH_2AlH_2BH_3$(ring)$+H_2$	-1238.7948	2.49	1.03	7.32×10^{-10}
	(-1140.3262)	(2.26)	(3.50×10^{-1})	(3.58×10^{-8})
$AlH_3PH_3\cdots BH_3\rightarrow$ **tsalp-BAl** $\rightarrow AlH_2PH_2+H_2+BH_3$	-1041.3033	2.05	2.53×10^{-1}	3.23×10^{-50}
	(-1049.7214)	(2.07)	(5.77×10^{-1})	(3.45×10^{-43})
AlH_3PH_3 and NH_3 reactants:				
$AlH_3PH_3+NH_3 \rightarrow AlH_3PH_3\cdots NH_3$	-	-	-	-
	-	-	-	-
$AlH_3PH_3\cdots NH_3 \rightarrow$ **tsalp-NP** $\rightarrow AlH_2PH_2+H_2+NH_3$	-1596.5302	3.47	9.03×10^{-2}	6.00×10^{-85}
	(-1759.7693)	(4.00)	(1.93×10^{-2})	(1.81×10^{-76})
$AlH_3PH_3\cdots NH_3 \rightarrow$ **tsalp-NH_3** $\rightarrow AlH_2PH_2+H_2+NH_3$	-1191.7264	2.38	4.04×10^{-2}	1.10×10^{-11}
	(-1116.0203)	(2.21)	(2.90×10^{-2})	(8.85×10^{-10})
$AlH_3PH_3\cdots NH_3 \rightarrow$ **tsalp-NAl** $\rightarrow AlH_2PH_2+H_2+NH_3$	-954.6652	1.88	3.53×10^{-2}	6.87×10^{-7}
	(-1055.3080)	(2.08)	(1.45×10^{-2})	(1.21×10^{-6})
AlH_3PH_3 and AlH_3 reactants:				
$AlH_3PH_3+AlH_3 \rightarrow AlH_3PH_3\cdots AlH_3$	-	-	-	-
	-	-	-	-
$AlH_3PH_3\cdots AlH_3 \rightarrow$ **tsalp-AlP** $\rightarrow PH_2AlH_2AlH_3$(ring)$+H_2$	-810.3551	1.61	1.48×10^{-1}	5.64
	(-606.9124)	(1.36)	(3.17×10^{-1})	(6.18×10^{4})
$AlH_3PH_3\cdots AlH_3 \rightarrow$ **tsalp-AlH_3** $\rightarrow PH_2AlH_2AlH_3+H_2$	-1173.2073	2.34	2.15×10^{-1}	8.61×10^{-10}
	(-1093.9242)	(2.16)	(1.46×10^{-1})	(5.39×10^{-9})
$AlH_3PH_3\cdots AlH_3 \rightarrow$ **tsalp-AlAl** $\rightarrow AlH_2PH_2+H_2+AlH_3$	-810.3551	1.64	6.43×10^{-1}	8.91×10^{-39}
	(-935.7940)	(1.85)	(4.15×10^{-1})	(1.09×10^{-32})
AlH_3PH_3 and PH_3 reactants:				
$AlH_3PH_3+PH_3 \rightarrow AlH_3PH_3\cdots PH_3$	-	-	-	-
	-	-	-	-
$AlH_3PH_3\cdots PH_3 \rightarrow$ **tsalp-PP** $\rightarrow AlH_2PH_2+H_2+PH_3$	-1313.3022	2.67	2.77×10^{-3}	4.01×10^{-35}
	(-1211.6389)	(2.42)	(5.51×10^{-5})	(4.17×10^{-32})
$AlH_3PH_3\cdots PH_3 \rightarrow$ **tsalp-PH_3** $\rightarrow AlH_2PH_2+H_2+PH_3$	-1398.9487	2.90	4.00×10^{1}	4.71×10^{-10}
	(-1271.6496)	(2.57)	(1.03)	(1.36×10^{-8})
$AlH_3PH_3\cdots PH_3 \rightarrow$ **tsalp-PAl** $\rightarrow AlH_2PH_2+H_2+PH_3$	-1381.9840	2.85	3.18×10^{-2}	4.61×10^{-23}
	(-866.1488)	(1.73)	(2.52×10^{-4})	(9.50×10^{-16})

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