Electronic Supplementary Material (ESI) for Dalton Transactions.

On the comparison of Oxygen and Sulfur Transfer Reactivity in Phosphine and Phosphorene: the case of $R_3Sb(X)$ carriers (X = O, S)

Supporting Information

List of Coordinates and Energy parameters of Optimized Structures

Compound Me_3P
CARTESIAN COORDINATES

P	2.622179125770E+00	-2.918500162106E-01	4.811386818999E-01
C	3.113386681743E+00	1.493159421001E+00	3.069115240605E-01
H	3.091508379068E+00	1.981242759116E+00	1.280783468561E+00
H	4.109808682748E+00	1.621288035905E+00	-1.184036052970E-01
H	2.399598075984E+00	2.014114410628E+00	-3.304980217765E-01
C	3.022460747118E+00	-8.643738782265E-01	-1.242198136185E+00
H	2.302919146679E+00	-4.498343629051E-01	-1.947652189506E+00
H	4.023948484370E+00	-5.764014752030E-01	-1.565108294542E+00
H	2.942626575417E+00	-1.949420760220E+00	-1.300981774763E+00
C	4.142608330359E+00	-9.201485608405E-01	1.348014383744E+00
H	4.170247427719E+00	-5.425741175952E-01	2.369744257285E+00
H	4.113469855065E+00	-2.007755468631E+00	1.407281960405E+00
H	5.068401362234E+00	-6.287331285424E-01	8.497979280683E-01

Energy parameters

		AU	EV	KJ/MOL
Electronic Energy	:	-460.987483460195	-12544.107155036518	-1210322.46725937
Free Energy	:	-460.901692277723	-12541.772658277941	-1210097.22254154

Compound $Me_3P(O)$
CARTESIAN COORDINATES

P	3.342664684886E+00	2.195768599010E-02	2.512356080023E-02
C	4.000277586080E+00	7.973361351777E-02	-1.679604081297E+00
H	3.677071244909E+00	1.003643496861E+00	-2.155024045129E+00
H	5.088671986478E+00	2.808962914716E-02	-1.704338906389E+00
H	3.591662201476E+00	-7.537025220743E-01	-2.247517078038E+00
C	4.038291696608E+00	-1.505073884947E+00	7.504384556366E-01
H	3.629540784587E+00	-2.366700657807E+00	2.263657503743E-01
H	5.126061107591E+00	-1.533409169725E+00	6.883800783676E-01
H	3.739722493852E+00	-1.571570478885E+00	1.794731930632E+00
C	4.180569417345E+00	1.388759983873E+00	9.035220579293E-01
H	3.861302104986E+00	2.336527837585E+00	4.746491998566E-01
H	3.883931958040E+00	1.374298503884E+00	1.950405512445E+00
H	5.266207323377E+00	1.316536850044E+00	8.398025040093E-01
O	1.826725409788E+00	9.280911253509E-02	9.506506080280E-02

Energy parameters

		AU	EV	KJ/MOL
Electronic Energy	:	-536.240378145704	-14591.842524283718	-1407898.91441260
Free Energy	:	-536.151971345888	-14589.436852958781	-1407666.80239240

Compound $Me_3P(S)$
CARTESIAN COORDINATES

P	3.343173472502E+00	2.127320517556E-02	2.456446413703E-02
C	4.035836966957E+00	7.772643651731E-02	-1.673106513903E+00
H	3.722824254289E+00	1.000975736971E+00	-2.154902815693E+00
H	5.124490729705E+00	2.415666887213E-02	-1.667392129672E+00
H	3.636907083886E+00	-7.544530326812E-01	-2.248282585788E+00
C	4.073127194360E+00	-1.499425568101E+00	7.454811667455E-01
H	3.675912215907E+00	-2.366954886396E+00	2.238455378249E-01
H	5.160606743892E+00	-1.499950779376E+00	6.716146399574E-01
H	3.782739749704E+00	-1.572790396555E+00	1.790841029261E+00
C	4.211629132719E+00	1.380835087373E+00	8.977419299623E-01
H	3.901611810977E+00	2.332426789693E+00	4.724573235640E-01
H	3.924543861672E+00	1.371071152980E+00	1.946547589790E+00
H	5.294509984660E+00	1.285283434095E+00	8.185742924010E-01
S	1.364786798768E+00	1.117261514318E-01	1.140160714124E-01

Energy parameters

		AU	EV	KJ/MOL
Electronic Energy	:	-859.043000032074	-23375.748430958974	-2255417.07873830
Free Energy	:	-858.956900075270	-23373.405532023658	-2255191.02333357

Compound Me_3Sb
CARTESIAN COORDINATES

Sb	-1.241281972613E+00	1.950678707781E-01	-2.542118692393E-01
C	-2.365857322454E+00	5.508818516254E-01	1.579916878023E+00
H	-2.218153455969E+00	1.574966611578E+00	1.916348674878E+00
H	-3.426879761611E+00	3.837375343386E-01	1.411111882832E+00
H	-2.022897698100E+00	-1.193428594692E-01	2.365449446852E+00
C	-2.242783057160E+00	-1.695195033952E+00	-6.773073233818E-01
H	-1.891703283491E+00	-2.465664496463E+00	5.901914868889E-03
H	-3.318647136658E+00	-1.586462275180E+00	-5.646428162741E-01
H	-2.024172743097E+00	-2.015037434888E+00	-1.693991895953E+00
C	-2.604140582277E+00	1.364056354552E+00	-1.491720585001E+00
H	-2.470795696538E+00	2.425750670834E+00	-1.294989732638E+00
H	-2.400773756767E+00	1.183907339722E+00	-2.545324122874E+00
H	-3.635143533263E+00	1.091962866524E+00	-1.279194452092E+00

Energy parameters

		AU	EV	KJ/MOL
Electronic Energy	:	-359.883597204997	-9792.930542916329	-944874.25130479
Free Energy	:	-359.805155132779	-9790.796025614520	-944668.30167320

Compound $Me_3Sb(O)$
CARTESIAN COORDINATES

Sb	-1.541105129724E+00	1.665203323776E-01	-2.409874149963E-01
C	-2.392366626724E+00	5.776782666045E-01	1.687594952666E+00
H	-2.160864083787E+00	1.601334257515E+00	1.968911525474E+00
H	-3.471401406571E+00	4.420236538433E-01	1.661609311785E+00
H	-1.958254496533E+00	-9.695033756629E-02	2.420428369260E+00
C	-2.260628017176E+00	-1.803104350723E+00	-7.057366455951E-01
H	-1.823867032067E+00	-2.515583934701E+00	-1.129025534104E-02
H	-3.345218863997E+00	-1.837535928957E+00	-6.291051070495E-01
H	-1.958637747568E+00	-2.064075458989E+00	-1.716321605693E+00
C	-2.648631238633E+00	1.440315262555E+00	-1.569134312784E+00
H	-2.421907947292E+00	2.477947881806E+00	-1.339859402952E+00
H	-2.351811663884E+00	1.231764339933E+00	-2.593357332672E+00
H	-3.716707848490E+00	1.267221162383E+00	-1.456763308408E+00
O	3.109011024482E-01	3.635448539180E-01	-3.351897736937E-01

Energy parameters

		AU	EV	KJ/MOL
Electronic Energy	:	-435.055480023541	-11838.461467191619	-1142238.00183128
Free Energy	:	-434.976491525990	-11836.312080900569	-1142030.61756019

Compound $Me_3Sb(S)$
CARTESIAN COORDINATES

Sb	-1.531881823336E+00	1.658992588578E-01	-2.407912977670E-01
C	-2.423419406440E+00	5.715986883935E-01	1.676895508808E+00
H	-2.216813805860E+00	1.602116903515E+00	1.951511315074E+00
H	-3.498074750330E+00	4.108942522992E-01	1.629666190042E+00
H	-1.983829237160E+00	-8.897906722802E-02	2.418685090000E+00
C	-2.294472554227E+00	-1.794268371289E+00	-7.025073810076E-01
H	-1.866460071815E+00	-2.513239892800E+00	-9.722579282889E-03
H	-3.378840425167E+00	-1.801261819012E+00	-6.187419987280E-01
H	-2.001170249041E+00	-2.057839820166E+00	-1.714701644227E+00
C	-2.676488069640E+00	1.428290748274E+00	-1.557160440388E+00
H	-2.458219455344E+00	2.467684096538E+00	-1.328652241851E+00
H	-2.388816633500E+00	1.221858751946E+00	-2.584186175545E+00
H	-3.739072095175E+00	1.236689665475E+00	-1.425695274426E+00
S	7.170575770357E-01	4.016566051952E-01	-3.538000707013E-01

Energy parameters

		AU	EV	KJ/MOL
Electronic Energy	:	-757.908760856828	-20623.745873894070	-1989889.17120336
Free Energy	:	-757.831456978054	-20621.642328410428	-1989686.20989824

Compound $[Me_3P\text{-}O\text{-}SbMe_3]_{TS}$
CARTESIAN COORDINATES

P	2.626730754270E+00	-2.731758741145E-01	4.527853926458E-01
C	3.107641092633E+00	1.504436796864E+00	3.158903091174E-01
H	3.050521686668E+00	1.979232020649E+00	1.294617328720E+00
H	4.120398489073E+00	1.635062201255E+00	-7.017877006614E-02
H	2.405994841122E+00	2.013481232640E+00	-3.395063281511E-01
C	3.016990510324E+00	-8.780325553710E-01	-1.248415802521E+00
H	2.318786486801E+00	-4.342171694484E-01	-1.953191304371E+00
H	4.036660087522E+00	-6.370562386394E-01	-1.554473824614E+00
H	2.892388850674E+00	-1.959241261877E+00	-1.294765518391E+00
C	4.156399833403E+00	-9.132225414525E-01	1.337978891276E+00
H	4.178767402140E+00	-5.359825718999E-01	2.359837969335E+00
H	4.125160676118E+00	-2.000898079925E+00	1.394145507353E+00
H	5.086722163527E+00	-6.216731004059E-01	8.441063316208E-01
Sb	-1.393772702934E+00	2.228012739230E-01	-2.404605260492E-01
C	-2.453783034243E+00	5.330863991299E-01	1.619065560981E+00
H	-2.312726872009E+00	1.556458030160E+00	1.957573364792E+00
H	-3.516993189726E+00	3.409141810127E-01	1.491930571143E+00
H	-2.048448022925E+00	-1.403853184026E-01	2.369272053793E+00
C	-2.231166257571E+00	-1.697956310307E+00	-7.832617101251E-01
H	-1.820727472717E+00	-2.458521565056E+00	-1.245347589037E-01
H	-3.315075520534E+00	-1.682848674641E+00	-6.914360957105E-01
H	-1.962465618110E+00	-1.942712649029E+00	-1.807914140982E+00
C	-2.646628092062E+00	1.485433875371E+00	-1.530988548662E+00
H	-2.498826065183E+00	2.532620799334E+00	-1.278906599763E+00
H	-2.378314688126E+00	1.330685585382E+00	-2.573163506827E+00
H	-3.692008286957E+00	1.220923341353E+00	-1.382721035604E+00
O	5.731729488213E-01	-1.701182650455E-02	2.007151899645E-01

Imaginary Frequency -371.2 cm^{-1}

Energy parameters

		AU	EV	KJ/MOL
Electronic Energy	:	-896.018768814362	-24381.910251803554	-2352496.94599516
Free Energy	:	-895.839768962245	-24377.039418199081	-2352026.98194966

Compound $[Me_3P\text{-}S\text{-}SbMe_3]_{TS}$
CARTESIAN COORDINATES

P	3.255985609709E+00	3.418925259029E-02	3.668512736757E-02
C	4.009952531775E+00	8.246805764840E-02	-1.649393950852E+00
H	3.728167485624E+00	1.008164188412E+00	-2.147328197417E+00
H	5.098438536583E+00	1.351303033877E-02	-1.624618775188E+00
H	3.618970942028E+00	-7.408039451208E-01	-2.244048695321E+00
C	4.050260629938E+00	-1.477639036890E+00	7.433393947409E-01
H	3.663148227066E+00	-2.360253477222E+00	2.370641864662E-01
H	5.136945268012E+00	-1.464638429250E+00	6.467822218682E-01

H	3.792755227833E+00	-1.565544952456E+00	1.797722609386E+00
C	4.202535267795E+00	1.372945958889E+00	8.938808387394E-01
H	3.917918412065E+00	2.340494654951E+00	4.839320368291E-01
H	3.949230444037E+00	1.377985970596E+00	1.952626757407E+00
H	5.282407180123E+00	1.253348786962E+00	7.924154877234E-01
S	6.635117234773E-01	3.925106944605E-02	4.618917702937E-02
Sb	-1.798897712294E+00	-1.656661631202E-02	-6.372970591939E-03
C	-2.803463147818E+00	-1.882681132266E+00	-4.791056741990E-01
H	-2.530690866337E+00	-2.636616085678E+00	2.547876635016E-01
H	-3.881783768811E+00	-1.740239113917E+00	-4.697066909842E-01
H	-2.491097816895E+00	-2.223174155096E+00	-1.462903066391E+00
C	-2.857383367561E+00	1.264347486476E+00	-1.404780080186E+00
H	-3.929962907245E+00	1.104992461907E+00	-1.320144962367E+00
H	-2.626981942712E+00	2.304356591621E+00	-1.188803672551E+00
H	-2.535417151606E+00	1.038021873547E+00	-2.417949545470E+00
C	-2.920243446480E+00	4.905444432039E-01	1.783706443888E+00
H	-2.653073022895E+00	-1.941686661651E-01	2.584672055815E+00
H	-2.672048453818E+00	1.503057991737E+00	2.091642724196E+00
H	-3.988183881593E+00	4.215437920485E-01	1.587909556562E+00

Imaginary Frequency -195.3 cm^{-1}

Energy parameters

		AU	EV	KJ/MOL
Electronic Energy	:	-1218.888856227799	-33167.651988802121	-3200192.24103721
Free Energy	:	-1218.706195438981	-33162.681536045435	-3199712.66520375

Phosphorene, P_{32}

Structural parameters

CELL	13.4084	9.4216	1.0000	90.0000	90.0000	89.9991
P	0.125013	0.048969	1.094710			
P	0.000010	0.207075	1.095071			
P	-0.000001	0.298943	-1.024535			
P	0.125020	0.456996	-1.026541			
P	-0.124987	0.048976	1.094446			
P	0.250008	0.207067	1.095007			
P	0.250057	0.298937	-1.024555			
P	-0.124981	0.457070	-1.024263			
P	0.125028	-0.451087	1.092936			
P	0.000066	-0.292970	1.094806			
P	0.000025	-0.201023	-1.024596			
P	0.125024	-0.042946	-1.024781			
P	-0.124970	-0.451024	1.095266			
P	0.250007	-0.292973	1.094843			
P	0.250017	-0.201025	-1.024568			
P	-0.124972	-0.042944	-1.025031			
P	-0.374984	0.048963	1.094489			
P	-0.499980	0.207047	1.094624			
P	-0.499977	0.298965	-1.024818			

P -0.374992 0.457073 -1.024374
P 0.375002 0.048964 1.094588
P -0.249989 0.207051 1.094600
P -0.249984 0.299004 -1.024791
P 0.375008 0.457062 -1.024300
P -0.374972 -0.451023 1.095121
P -0.499977 -0.292927 1.094740
P -0.499980 -0.201033 -1.024803
P -0.374976 -0.042947 -1.025002
P 0.375041 -0.451035 1.095242
P -0.249980 -0.292922 1.094636
P -0.249954 -0.201042 -1.024942
P 0.375030 -0.042941 -1.024923

Energy parameters

	AU/CELL	EV/CELL	KJ/MOL
Electronic Energy	: -10922.336784611631	-297211.893869990308	-28676591.18673322
Free Energy	: -10922.306010131868	-297211.056453822530	-28676510.38834799

Phosphorene oxide, $P_{32}O$
Structural parameters
CELL 13.4200 9.4427 1.0000 90.0000 90.0000 90.0002
P 0.125006 0.057845 0.952625
P -0.003659 0.210610 1.118689
P 0.000583 0.301095 -1.008276
P 0.125006 0.459896 -0.981918
P -0.126254 0.048749 1.109733
P 0.253677 0.210601 1.118796
P 0.249428 0.301095 -1.008153
P -0.125641 0.457071 -1.044007
P 0.125004 -0.449977 1.148880
P -0.001534 -0.293390 1.170889
P -0.000843 -0.202619 -0.959885
P 0.125007 -0.047218 -1.086366
P -0.125454 -0.452891 1.073908
P 0.251542 -0.293393 1.170844
P 0.250856 -0.202622 -0.959947
P -0.124638 -0.043326 -1.006863
P -0.374992 0.049160 1.093956
P -0.499459 0.207273 1.094330
P -0.499982 0.297867 -1.032191
P -0.374995 0.455688 -1.038690
P 0.376270 0.048740 1.109710
P -0.250527 0.207277 1.094331
P -0.250007 0.297869 -1.032202
P 0.375652 0.457069 -1.043901

P -0.374995 -0.452014 1.080886
P 0.499999 -0.294774 1.090544
P 0.499983 -0.200840 -1.021443
P -0.374993 -0.043093 -1.023194
P 0.375465 -0.452889 1.074001
P -0.249986 -0.294777 1.090533
P -0.249970 -0.200839 -1.021435
P 0.374652 -0.043328 -1.006903
O 0.124999 -0.047114 2.112919

Energy parameters

		AU/CELL	EV/CELL	KJ/MOL
Electronic Energy	:	-10997.555842865309	-299258.708503118076	-28874078.79634720
Free Energy	:	-10997.522772082795	-299257.808601375727	-28873991.96901995

Phosphorene sulphide, $P_{32}S$
Structural parameters

CELL 13.4160 9.4970 1.0000 90.0000 90.0000 89.9994
P 0.125008 0.063633 1.096371
P -0.004873 0.214700 1.082940
P 0.000263 0.299619 -1.057731
P 0.125001 0.457683 -1.028091
P -0.126018 0.051148 1.111413
P 0.254886 0.214698 1.083006
P 0.249745 0.299623 -1.057643
P -0.126172 0.455002 -1.090449
P 0.125007 -0.455128 1.112246
P -0.002364 -0.300690 1.167911
P -0.000177 -0.202293 -0.926360
P 0.125007 -0.047231 -0.930963
P -0.126628 -0.457300 1.035578
P 0.252369 -0.300695 1.167570
P 0.250194 -0.202292 -0.926645
P -0.124230 -0.044420 -0.990305
P -0.374993 0.049570 1.076067
P -0.499017 0.207500 1.064251
P -0.499610 0.296407 -1.070725
P -0.374996 0.453946 -1.075950
P 0.376032 0.051145 1.111372
P -0.250972 0.207503 1.064265
P -0.250378 0.296410 -1.070721
P 0.376181 0.454999 -1.090370
P -0.374994 -0.454119 1.047129
P 0.499953 -0.298043 1.071284
P 0.499572 -0.201186 -1.025515
P -0.374992 -0.044704 -1.030349
P 0.376644 -0.457297 1.035670

P -0.249940 -0.298049 1.071289
P -0.249555 -0.201187 -1.025488
P 0.374245 -0.044417 -0.990372
S 0.125001 -0.041531 2.808914

Energy parameters

		AU/CELL	EV/CELL	KJ/MOL
Electronic Energy	:	-11320.356692462023	-308042.566183339979	-29721592.30752706
Free Energy	:	-11320.326542904517	-308041.745772171358	-29721513.14987499

Transition State $[P_{32}\text{-O-SbMe}_3]_{TS}$

Structural parameters

CELL 13.4163 9.4247 1.0000 90.0000 90.0000 90.0033
P 0.115609 0.172802 1.092018
P -0.012498 0.326947 1.317213
P -0.012388 0.427398 -1.050339
P 0.111266 -0.416092 -1.068149
P -0.140411 0.172907 1.078547
P 0.237811 0.334237 1.080639
P 0.236778 0.426657 -1.041338
P -0.136042 -0.415996 -1.070073
P 0.112597 -0.323878 1.061752
P -0.012518 -0.166523 1.058702
P -0.012309 -0.071598 -1.055454
P 0.112438 0.086805 -1.040195
P -0.137461 -0.324211 1.060098
P 0.237238 -0.165358 1.071354
P 0.237455 -0.072307 -1.045412
P -0.137206 0.086599 -1.049898
P -0.387944 0.177300 1.074109
P 0.487616 0.335380 1.073406
P 0.487572 0.427115 -1.041650
P -0.386962 -0.415539 -1.043188
P 0.363182 0.177300 1.075116
P -0.262570 0.334200 1.076134
P -0.261679 0.426885 -1.044382
P 0.362027 -0.415682 -1.041977
P -0.387329 -0.323075 1.071217
P 0.487535 -0.165307 1.070906
P 0.487549 -0.073297 -1.044970
P -0.387621 0.084909 -1.041746
P 0.362377 -0.323067 1.071979
P -0.262018 -0.165637 1.068639
P -0.262318 -0.072469 -1.047680
P 0.362785 0.085027 -1.041271
O -0.012676 0.314167 3.046212
Sb -0.017341 0.155554 4.556365
C 0.090084 -0.015028 4.766952

H	0.082873	-0.085214	3.911886
H	0.074854	-0.072034	5.691467
H	0.164726	0.029458	4.789278
C	-0.006614	0.258962	6.482119
H	-0.061152	0.344028	6.530605
H	0.067585	0.303414	6.600240
H	-0.020856	0.182691	7.276491
C	-0.157500	0.044388	4.752718
H	-0.217820	0.121294	4.747892
H	-0.157970	-0.014903	5.686910
H	-0.166358	-0.026808	3.907458

Imaginary Frequency -292.27 cm^{-1}

Energy parameters

		AU/CELL	EV/CELL	KJ/MOL
Electronic Energy	:	-11357.384904620314	-309050.155060995778	-29818809.86484822
Free Energy	:	-11357.261168689063	-309046.788035130186	-29818484.99620650

Transition State $[P_{32}\text{-}S\text{-}SbMe_3]_{TS}$

Structural parameters

CELL	13.4088	9.4565	1.0000	90.0000	90.0000	89.9379
P	0.127855	0.025732	0.934897			
P	0.000401	0.179771	0.908897			
P	0.002787	0.267071	-1.227822			
P	0.127313	0.425555	-1.222741			
P	-0.122913	0.018772	0.909165			
P	0.254859	0.180695	0.901209			
P	0.252651	0.268294	-1.232732			
P	-0.122919	0.424129	-1.261963			
P	0.127414	-0.482483	0.896691			
P	0.000847	-0.326987	0.903461			
P	0.002589	-0.231374	-1.201439			
P	0.127463	-0.074704	-1.170177			
P	-0.123137	-0.485062	0.853924			
P	0.253298	-0.325876	0.907171			
P	0.252447	-0.231391	-1.200108			
P	-0.122206	-0.073467	-1.209013			
P	-0.372450	0.018818	0.884423			
P	-0.497181	0.176658	0.880676			
P	-0.497452	0.267384	-1.245670			
P	-0.372544	0.424826	-1.252357			
P	0.377889	0.019389	0.907669			
P	-0.247838	0.176456	0.875753			
P	-0.247829	0.266565	-1.250651			
P	0.377883	0.425770	-1.254009			
P	-0.372550	-0.483024	0.866488			

P	-0.497544	-0.325594	0.878720
P	-0.497800	-0.231157	-1.227878
P	-0.372544	-0.074122	-1.227901
P	0.377994	-0.483711	0.864868
P	-0.247376	-0.326320	0.878002
P	-0.247126	-0.231212	-1.227118
P	0.377078	-0.073454	-1.208401
S	0.115912	-0.058645	3.092399
Sb	0.070128	-0.147240	5.488037
C	-0.014429	-0.022165	6.916064
H	0.032294	0.061388	7.320037
H	-0.040034	-0.089716	7.726221
H	-0.078379	0.024936	6.418171
C	-0.035487	-0.317475	5.224486
H	-0.000498	-0.402277	4.659505
H	-0.099167	-0.278616	4.660885
H	-0.060197	-0.357538	6.188427
C	0.169831	-0.251330	6.895234
H	0.212830	-0.331841	6.376028
H	0.126512	-0.300227	7.689795
H	0.220729	-0.174201	7.322376

Imaginary Frequency -191.7 and -26.5 cm^{-1}

Energy parameters

		AU/CELL	EV/CELL	KJ/MOL
Electronic Energy	:	-11680.229129153166	-317835.193033234915	-30666437.25690686
Free Energy	:	-11680.101829475991	-317831.729032912583	-30666103.03165153