

Beyond the Triple Bond: Unlocking Dinitrogen Activation with Tailored Superbase Phosphines

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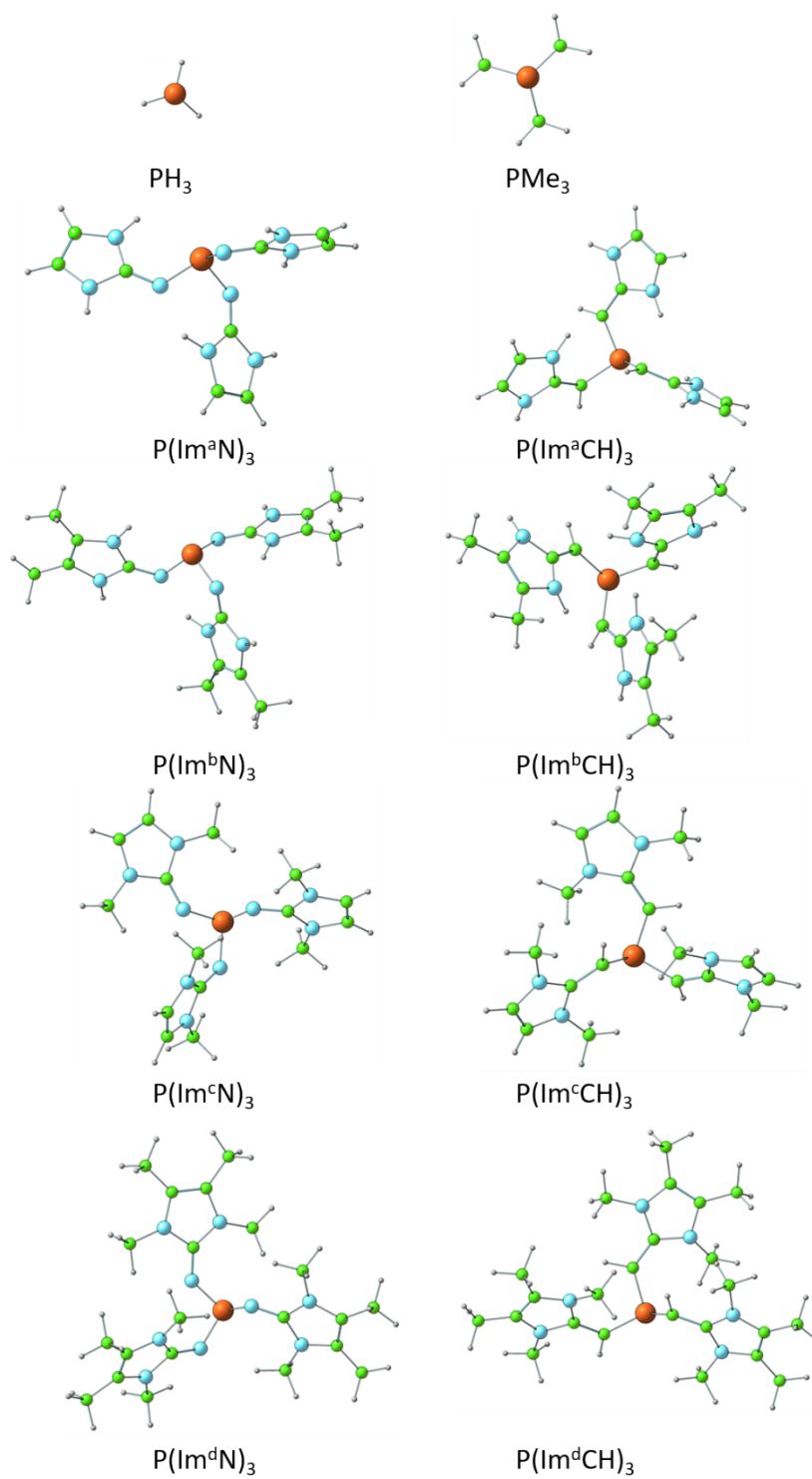


Figure S1: Optimized geometries of phosphine ligands at M06L/6-311++G(d,p) level DFT.

Table S1: Structural and energetic data of the mono-phosphine-N₂ van der Waals complexes at M06L/6-311++G(d,p) level DFT. Energy values in kcal/mol and the distance in Å.

Complex	ΔE	ΔG	D_{P-N}
PH ₃ ⋯N ₂	-0.6	6.2	4.03
PMe ₃ ⋯N ₂	-1.4	4.5	3.44
P(Im ^a N) ₃ ⋯N ₂	-2.8	5.6	3.94
P(Im ^b N) ₃ ⋯N ₂	-7.1	0.5	4.37
P(Im ^c N) ₃ ⋯N ₂	-4.5	4.2	3.61
P(Im ^d N) ₃ ⋯N ₂	-5.0	3.6	4.32
P(Im ^a CH) ₃ ⋯N ₂	-2.2	3.2	3.83
P(Im ^b CH) ₃ ⋯N ₂	-3.0	4.7	4.25
P(Im ^c CH) ₃ ⋯N ₂	-3.4	3.4	3.86
P(Im ^d CH) ₃ ⋯N ₂	-4.2	4.2	4.43

Table S2: Structural and energetic data of the mono-phosphine-N₂ van der Waals complexes at M06L/6-311++G(d,p) level DFT. Energy values in kcal/mol and the distance in Å.

Complex	ΔE	ΔG	D_{P-N1}	D_{P-N2}	D_{N-N}
(Im ^c N) ₃ P-N ₂	70.1	83.5	1.72	1.82	1.29
(Im ^d N) ₃ P-N ₂	65.9	79.6	1.72	1.85	1.28

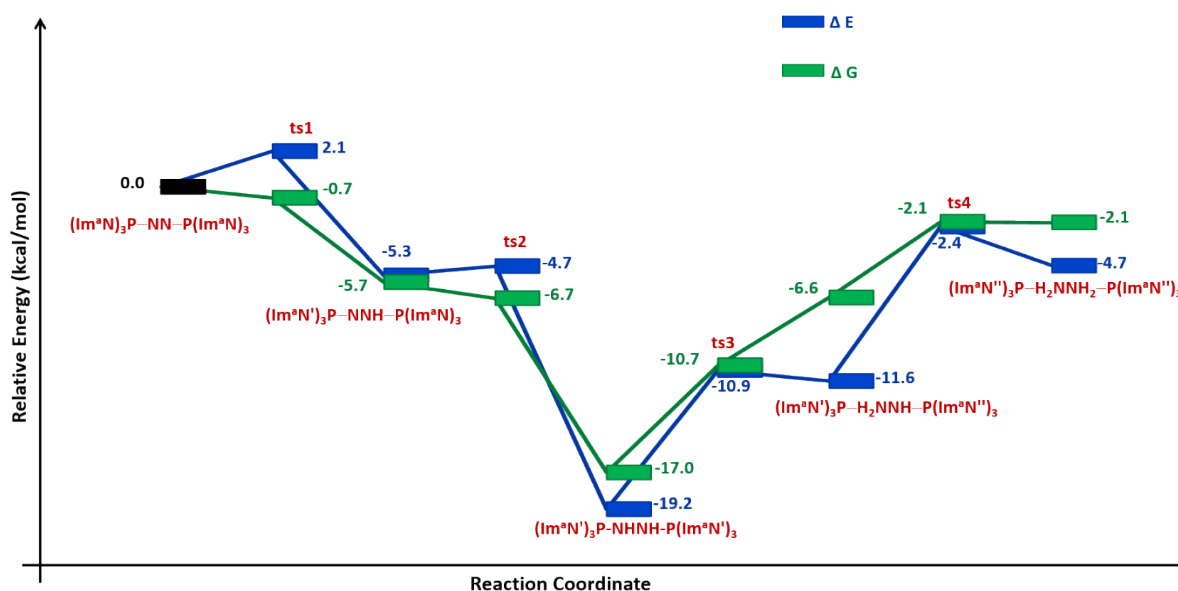


Figure S2: Energy profile diagram for the hydrogen transfer reactions takes place in the dinitrogen complex (without solvent).

Table S3: Cartesian coordinates of optimized geometries of phosphines at M06L/6-311++G(d,p) level DFT. Atomic number followed by X, Y, Z coordinates in Å.

PH₃				PMe₃			
15	-0.000044000	0.000128000	-0.129701000	15	-0.000058000	-0.000015000	-0.611832000
1	0.253718000	-1.157637000	0.647618000	6	-1.552395000	-0.446479000	0.281520000
1	0.876324000	0.797204000	0.648859000	1	-1.868863000	-1.453558000	0.000716000
1	-1.129389000	0.358508000	0.649030000	1	-2.355858000	0.237982000	0.000102000
				1	-1.431860000	-0.411294000	1.369547000
				6	1.162910000	-1.121158000	0.281480000
				1	1.072025000	-1.034533000	1.369500000
				1	2.193294000	-0.891264000	0.000951000
				1	0.972244000	-2.159142000	-0.000274000
				6	0.389568000	1.567625000	0.281445000
				1	0.358811000	1.445928000	1.369484000
				1	-0.323832000	2.345502000	0.000029000
				1	1.384413000	1.920685000	0.000743000
P(Im^aN)₃				P(Im^bN)₃			
15	-0.287865000	0.682155000	-0.648227000	15	-0.361319000	-0.851729000	-0.640124000
7	0.710112000	1.336270000	0.575360000	7	0.613396000	-1.424519000	0.642747000
7	2.772503000	1.110467000	-0.703466000	7	2.676585000	-1.416033000	-0.651518000
7	2.832670000	2.232122000	1.157862000	7	2.700208000	-2.342451000	1.310738000
7	-1.504674000	-0.005829000	0.391482000	6	1.856637000	-1.689755000	0.430988000
7	-3.831376000	-0.051133000	0.881398000	6	3.994995000	-1.800931000	-0.395312000
7	-3.256007000	1.249829000	-0.749769000	6	4.009832000	-2.388771000	0.825477000
6	1.962744000	1.526875000	0.343751000	1	2.349074000	-0.757041000	-1.352252000
6	4.089884000	1.493268000	-0.492548000	1	2.388947000	-2.636154000	2.220504000
1	4.877437000	1.257159000	-1.187255000	6	5.099257000	-3.032754000	1.590115000
6	4.126972000	2.199141000	0.656929000	1	6.043796000	-2.960744000	1.049480000
1	4.946901000	2.693568000	1.147847000	1	5.246083000	-2.563973000	2.570105000
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6	-4.630218000	1.364723000	-0.602780000	1	5.202748000	-0.526875000	-1.627362000
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6	0.587720000	-3.407976000	1.050803000	6	2.265174000	4.920782000	-0.693888000
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6	1.400265000	-3.864343000	0.073313000	1	3.346059000	4.737913000	-0.698975000
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				1	-6.478994000	2.572928000	-0.120961000
				1	-5.189306000	3.769260000	-0.204820000
				6	4.959505000	3.720316000	0.098609000
				1	5.652680000	3.581924000	0.929380000
				1	5.502075000	3.484829000	-0.824443000
				1	4.707761000	4.785975000	0.054414000
				6	4.166575000	1.550306000	2.452491000
				1	3.622541000	1.778530000	3.376274000
				1	4.355078000	0.470150000	2.457327000
				1	5.133074000	2.053024000	2.511014000
P(Im ^a CH) ₃				P(Im ^b CH) ₃			
15	-0.036429000	0.401671000	1.226458000	15	0.094318000	-0.107056000	-2.751889000
6	0.797415000	0.760012000	-0.349595000	6	0.311876000	1.555123000	-2.066662000
7	2.917921000	1.336409000	0.768355000	7	-0.929506000	1.467092000	0.074309000
7	2.809877000	1.835876000	-1.348193000	7	-0.483608000	3.449924000	-0.672553000
6	-0.722664000	-1.265742000	0.947245000	6	-0.333775000	2.107433000	-0.982101000
7	-0.298730000	-3.663292000	0.439456000	6	-1.454551000	2.373538000	0.992590000
7	1.202487000	-2.238244000	-0.253259000	6	-1.201137000	3.616606000	0.520446000
6	2.064486000	1.280790000	-0.318084000	1	-0.890786000	0.461189000	0.213743000
6	4.078530000	2.029096000	0.448749000	1	-0.332491000	4.174558000	-1.353014000
1	4.865170000	2.186038000	1.166215000	6	-1.525112000	4.957477000	1.051497000
6	4.016196000	2.343734000	-0.858523000	1	-2.078386000	4.874351000	1.987817000
1	4.736428000	2.821044000	-1.499801000	1	-0.624825000	5.549801000	1.251816000
6	0.002115000	-2.306205000	0.432629000	1	-2.143552000	5.539330000	0.357740000
6	0.587489000	-4.358015000	-0.384653000	6	-2.133724000	1.895495000	2.215884000
1	0.518144000	-5.422551000	-0.526781000	1	-2.975971000	1.237325000	1.973344000
6	1.510425000	-3.474635000	-0.810389000	1	-1.456408000	1.319703000	2.858280000
1	2.396087000	-3.628150000	-1.402499000	1	-2.518508000	2.729948000	2.803595000
1	2.558232000	1.133649000	1.691900000	1	0.732093000	2.275496000	-2.764451000
1	2.377981000	2.129212000	-2.207653000	6	-1.525590000	-0.680318000	-2.180374000
1	-1.196530000	-4.007965000	0.731385000	7	-0.952333000	-1.550474000	0.050807000
1	1.513134000	-1.324991000	-0.577282000	7	-3.040683000	-1.863976000	-0.603981000
6	-1.522052000	1.408028000	1.217152000	6	-1.822642000	-1.328534000	-1.025716000
7	-2.628825000	0.330953000	-0.698671000	6	-1.573915000	-2.423788000	0.972068000
7	-3.688473000	2.033889000	0.168416000	6	-2.849147000	-2.609114000	0.574499000
6	-2.531672000	1.278506000	0.306027000	1	0.024279000	-1.687380000	-0.225313000
6	-3.880871000	0.398963000	-1.300413000	1	-3.744394000	-2.110322000	-1.282359000

1	-4.166480000	-0.266158000	-2.097268000	6	-3.976839000	-3.323393000	1.211203000
6	-4.536171000	1.451218000	-0.773505000	1	-3.649844000	-3.832877000	2.118379000
1	-5.489186000	1.882485000	-1.027224000	1	-4.790049000	-2.641586000	1.485291000
1	-2.047654000	-0.504414000	-0.605545000	1	-4.407183000	-4.081709000	0.546823000
1	-3.977941000	2.697165000	0.865922000	6	-0.845110000	-2.865352000	2.180140000
1	-1.575764000	-1.528717000	1.568907000	1	0.067821000	-3.415152000	1.922974000
1	-1.587324000	2.220470000	1.931954000	1	-0.533901000	-2.014942000	2.799167000
1	0.242991000	0.864188000	-1.281651000	1	-1.462697000	-3.520844000	2.795879000
				1	-2.337236000	-0.563679000	-2.893372000
				6	1.285611000	-1.201911000	-1.920013000
				7	2.049356000	0.172429000	-0.017826000
				7	3.177882000	-1.678966000	-0.382599000
				6	2.114532000	-0.919058000	-0.871569000
				6	3.178976000	0.190105000	0.816721000
				6	3.874652000	-0.945970000	0.597792000
				1	1.640944000	1.019274000	-0.416410000
				1	3.640583000	-2.343698000	-0.982772000
				6	5.067558000	-1.509701000	1.265262000
				1	5.467815000	-0.807267000	1.997502000
				1	4.841565000	-2.445240000	1.790282000
				1	5.870636000	-1.730505000	0.552277000
				6	3.364308000	1.280579000	1.798096000
				1	3.422998000	2.259316000	1.308225000
				1	2.529116000	1.332621000	2.506854000
				1	4.282580000	1.143228000	2.370697000
				1	1.527458000	-2.102619000	-2.480327000
P(Im ^c CH) ₃				P(Im ^d CH) ₃			
15	-0.039501000	0.405984000	-1.012684000	15	0.218887000	0.935586000	-1.023830000
6	-1.603400000	1.300255000	-0.844310000	6	1.816033000	1.748750000	-0.800470000
7	-2.800478000	0.479931000	1.200331000	7	3.129814000	0.436028000	0.870314000
7	-3.998118000	1.492864000	-0.334649000	7	4.259747000	1.667780000	-0.548779000
6	-0.572515000	-1.286505000	-0.637508000	6	-0.821760000	0.981974000	0.463889000
7	-0.293131000	-3.636645000	-0.014223000	7	-3.143657000	0.968280000	1.271452000
7	1.553562000	-2.623153000	-0.686152000	7	-2.710175000	2.416527000	-0.315762000
6	-2.699454000	1.090204000	-0.042325000	6	2.968660000	1.305684000	-0.195340000
6	-4.111787000	0.562620000	1.659451000	6	4.492908000	0.294022000	1.171902000
1	-4.396238000	0.152276000	2.613380000	6	5.190681000	1.050482000	0.292452000
6	-4.847845000	1.181936000	0.716302000	6	-2.119535000	1.433832000	0.460876000
1	-5.900725000	1.405087000	0.677959000	6	-4.338458000	1.639474000	0.986929000
6	0.186991000	-2.408708000	-0.473472000	6	-4.068235000	2.539608000	0.012210000
6	0.722441000	-4.582297000	-0.030539000	6	-2.985590000	-0.190525000	2.105177000
1	0.557230000	-5.591692000	0.307589000	1	-3.961018000	-0.526617000	2.457532000
6	1.844197000	-3.969808000	-0.450354000	1	-2.506586000	-0.998073000	1.536494000
1	2.844943000	-4.349889000	-0.568837000	1	-2.358290000	0.020978000	2.979472000
6	-1.670293000	-3.863116000	0.306136000	6	-1.962413000	3.386023000	-1.081584000
1	-1.782905000	-4.860460000	0.731410000	1	-1.829579000	3.084887000	-2.123715000
1	-2.021401000	-3.124703000	1.037562000	1	-2.473765000	4.351754000	-1.049120000
1	-2.313930000	-3.783658000	-0.579546000	1	-0.967718000	3.492725000	-0.638943000
6	2.334191000	-1.835868000	-1.616967000	6	2.061321000	0.172931000	1.809537000
1	2.358087000	-0.787889000	-1.315220000	1	1.434769000	-0.663047000	1.484335000
1	3.354665000	-2.223104000	-1.623169000	1	2.485280000	-0.053143000	2.788958000
1	1.926758000	-1.895203000	-2.633704000	1	1.421360000	1.057319000	1.885616000
6	-1.664613000	0.251250000	2.066442000	6	4.543551000	2.520232000	-1.667082000
1	-0.996099000	1.117566000	2.046292000	1	4.005005000	2.167841000	-2.553851000

1	-2.028608000	0.092697000	3.082596000	1	4.235887000	3.556241000	-1.479364000
1	-1.088933000	-0.620284000	1.743842000	1	5.613081000	2.511329000	-1.875401000
6	-4.360145000	2.151745000	-1.556450000	6	0.709492000	-0.811721000	-0.992864000
1	-3.998807000	1.579200000	-2.417206000	7	0.352889000	-3.193043000	-0.553813000
1	-5.445594000	2.231836000	-1.613417000	7	-1.492769000	-1.993758000	-0.802540000
1	-3.930720000	3.158764000	-1.617260000	6	-0.095392000	-1.900524000	-0.824146000
1	-1.816093000	1.910288000	-1.718148000	6	-0.733527000	-4.055357000	-0.367699000
1	-1.639235000	-1.422840000	-0.489735000	6	-1.860560000	-3.330876000	-0.540238000
6	1.080818000	0.699596000	0.392864000	6	1.740013000	-3.494288000	-0.368296000
7	3.337912000	1.329795000	1.146368000	1	2.189085000	-2.820671000	0.375923000
7	2.519315000	2.536931000	-0.495052000	1	1.853808000	-4.523159000	-0.027367000
6	2.215615000	1.467405000	0.337391000	1	2.308330000	-3.373691000	-1.299478000
6	4.283175000	2.294516000	0.825837000	6	-2.334156000	-1.169089000	-1.647283000
1	5.228259000	2.353377000	1.338573000	1	-1.862466000	-0.201463000	-1.814322000
6	3.779242000	3.035796000	-0.180579000	1	-2.504075000	-1.640771000	-2.625480000
1	4.197791000	3.875344000	-0.708812000	1	-3.303292000	-0.996964000	-1.168545000
6	3.491376000	0.250756000	2.078865000	6	-0.548669000	-5.477879000	-0.008166000
1	4.510111000	0.250382000	2.466402000	1	-0.029203000	-5.605047000	0.949725000
1	2.796183000	0.342770000	2.921719000	1	-1.515452000	-5.975261000	0.078111000
1	3.293231000	-0.709261000	1.586171000	1	0.034101000	-6.020742000	-0.761338000
6	1.547880000	3.240266000	-1.301791000	6	-3.284234000	-3.725448000	-0.461142000
1	0.558636000	3.133799000	-0.845737000	1	-3.376272000	-4.783326000	-0.210656000
1	1.813268000	4.300498000	-1.335495000	1	-3.825670000	-3.155718000	0.304904000
1	1.492699000	2.850401000	-2.320793000	1	-3.817595000	-3.565680000	-1.405800000
1	1.051284000	-0.013376000	1.213522000	6	-5.604915000	1.318778000	1.679773000
				1	-6.404203000	1.972688000	1.328874000
				1	-5.930962000	0.285673000	1.505641000
				1	-5.527054000	1.449547000	2.765351000
				6	-4.946494000	3.523400000	-0.658210000
				1	-4.923447000	3.414752000	-1.748373000
				1	-5.980054000	3.392058000	-0.334965000
				1	-4.668281000	4.560653000	-0.436831000
				6	6.648449000	1.226925000	0.115812000
				1	7.192326000	0.659638000	0.872008000
				1	6.997382000	0.881341000	-0.864987000
				1	6.953282000	2.275257000	0.212447000
				6	4.961245000	-0.593372000	2.259054000
				1	4.670719000	-0.238164000	3.254922000
				1	4.560084000	-1.608435000	2.154551000
				1	6.049765000	-0.665508000	2.249374000
				1	1.775055000	-1.014165000	-1.039805000
				1	-0.616010000	0.248635000	1.240225000
				1	1.976929000	2.541627000	-1.525341000

Table S4: Cartesian coordinates of optimized geometries of mono-phosphine-N₂ van der Waals complexes at M06L/6-311++G(d,p) level DFT. Atomic number followed by X, Y, Z coordinates in Å.

PH ₃ ⋯N ₂				PMe ₃ ⋯N ₂			
15	-1.739856000	-0.038980000	-0.122764000	15	-0.640425000	-0.000117000	-0.382661000
1	-1.264562000	-0.804368000	0.972208000	7	2.754966000	0.000753000	0.178327000
1	-1.158805000	1.155621000	0.372924000	7	3.497907000	-0.000722000	-0.635113000
7	2.259082000	-0.549291000	-0.022547000	6	-0.619145000	-1.398370000	0.821189000
7	2.241452000	0.551171000	0.020928000	1	-0.779036000	-2.345080000	0.300189000
1	-2.982526000	0.220292000	0.507669000	1	0.356694000	-1.451942000	1.308951000

		1	-1.388392000	-1.292949000	1.593535000		
		6	-2.442867000	-0.000105000	-0.780546000		
		1	-3.067370000	0.000333000	0.119158000		
		1	-2.694282000	0.879971000	-1.376764000		
		1	-2.694412000	-0.880660000	-1.376003000		
		6	-0.619052000	1.398630000	0.820639000		
		1	0.356774000	1.452399000	1.308392000		
		1	-0.779016000	2.345116000	0.299264000		
		1	-1.388318000	1.293427000	1.592997000		
P(Im ^a N) ₃ ···N ₂			P(Im ^b N) ₃ ···N ₂				
15	0.097030000	0.911366000	-0.329569000	15	0.149424000	0.012637000	-0.998924000
7	-0.308541000	-0.141046000	0.992876000	7	-1.066391000	-0.785636000	-0.066272000
7	-0.155576000	-2.190055000	-0.317814000	7	-2.485496000	1.154724000	0.230572000
7	-0.833560000	-2.343266000	1.735239000	7	-3.319047000	-0.788131000	0.717024000
7	-1.199538000	0.723121000	-1.422083000	7	1.594517000	-0.746749000	-0.451018000
7	-3.537074000	0.949742000	-1.780920000	7	2.826981000	-2.736911000	-0.013668000
7	-2.913431000	0.916911000	0.300739000	7	0.671798000	-2.956431000	-0.064893000
6	-0.413008000	-1.421675000	0.795410000	6	-2.161984000	-0.182798000	0.257509000
6	-0.363403000	-3.532149000	-0.053835000	6	-3.799523000	1.367559000	0.643655000
1	-0.209554000	-4.295419000	-0.796924000	6	-4.332327000	0.153725000	0.925357000
6	-0.789707000	-3.633716000	1.223889000	6	1.665087000	-2.014213000	-0.206704000
1	-1.080778000	-4.493376000	1.801358000	6	2.549662000	-4.074651000	0.286612000
6	-2.406263000	0.852904000	-0.989224000	6	1.200662000	-4.202830000	0.267579000
6	-4.686765000	1.027845000	-1.007364000	7	-3.950767000	-0.636938000	-2.373241000
1	-5.667573000	1.114159000	-1.441191000	7	-4.188161000	0.439843000	-2.360991000
6	-4.299257000	0.994924000	0.284842000	1	-1.732298000	1.824660000	0.078615000
1	-4.884739000	1.044346000	1.186618000	1	-3.448672000	-1.784701000	0.674477000
7	1.406224000	2.117097000	2.566981000	1	3.739850000	-2.323742000	-0.090810000
7	0.614631000	2.343875000	3.299247000	1	-0.287776000	-2.620320000	0.010936000
1	-3.479978000	0.956802000	-2.784075000	7	0.232210000	1.557684000	-0.237118000
1	-2.306952000	0.689447000	1.082196000	7	2.639571000	1.832920000	-0.348408000
1	0.291126000	-1.752218000	-1.123031000	7	1.450233000	3.548346000	0.237285000
1	-1.054259000	-2.077217000	2.679061000	6	1.335602000	2.222573000	-0.136221000
7	1.260214000	0.017350000	-1.251495000	6	3.530196000	2.858159000	-0.030443000
7	3.577471000	-0.324743000	-1.647409000	6	2.791248000	3.936298000	0.326996000
7	3.107169000	0.892489000	0.083690000	1	2.818184000	0.834102000	-0.448730000
6	2.505041000	0.194862000	-0.947150000	1	0.654072000	4.109881000	0.484184000
6	4.784291000	0.101400000	-1.106736000	6	3.627886000	-5.056146000	0.530834000
1	5.734369000	-0.192180000	-1.516950000	1	4.287706000	-5.169918000	-0.337344000
6	4.489727000	0.855037000	-0.027843000	1	4.260324000	-4.770406000	1.379352000
1	5.137063000	1.342373000	0.680342000	1	3.209393000	-6.038581000	0.752694000
1	3.447972000	-0.787487000	-2.530464000	6	0.332137000	-5.377327000	0.500736000
1	2.567991000	1.413352000	0.761298000	1	-0.359465000	-5.215574000	1.335172000
				1	-0.276557000	-5.613754000	-0.378950000
				1	0.928473000	-6.259703000	0.736729000
				6	-4.392788000	2.721628000	0.672400000
				1	-5.428905000	2.684745000	1.011321000
				1	-3.850070000	3.394969000	1.345134000
				1	-4.383697000	3.181733000	-0.322136000
				6	-5.692770000	-0.251922000	1.336160000
				1	-5.692293000	-0.798328000	2.286074000
				1	-6.334096000	0.621449000	1.460005000
				1	-6.167333000	-0.902937000	0.591089000
				6	4.993683000	2.678793000	-0.149502000

				1	5.520703000	3.590791000	0.134043000
				1	5.360928000	1.873382000	0.496512000
				1	5.290905000	2.428602000	-1.173934000
				6	3.178175000	5.310218000	0.712142000
				1	2.788534000	6.060219000	0.013842000
				1	2.809071000	5.577612000	1.709122000
				1	4.263850000	5.412837000	0.728891000
$P(\text{Im}^c N)_3 \cdots N_2$				$P(\text{Im}^d N)_3 \cdots N_2$			
15	-0.348022000	0.123279000	-0.870342000	15	0.118187000	-0.238231000	-0.996409000
7	0.030754000	-1.526077000	-0.674040000	7	-0.623363000	-1.771130000	-0.935871000
7	1.135479000	-1.810195000	1.515080000	7	-2.255455000	-1.735092000	0.906020000
7	1.512278000	-3.256578000	-0.085034000	7	-2.618683000	-3.021916000	-0.818703000
7	0.925738000	0.842508000	0.013210000	7	1.183578000	-0.175117000	0.375743000
7	2.648287000	2.408949000	0.373034000	7	3.118024000	-1.538761000	-0.300809000
7	0.851598000	3.225754000	-0.578255000	7	3.344427000	-0.087399000	1.318003000
6	0.798464000	-2.093259000	0.197204000	6	-1.707810000	-2.103648000	-0.311390000
6	2.015329000	-2.768140000	1.999026000	6	-3.467089000	-2.399149000	1.122576000
1	2.394249000	-2.724101000	3.006379000	6	-3.689468000	-3.201543000	0.052243000
6	2.244022000	-3.661507000	1.013424000	6	2.405528000	-0.586646000	0.416716000
1	2.871900000	-4.536216000	0.989837000	6	4.454804000	-1.576511000	0.118805000
6	1.383882000	2.037409000	-0.086425000	6	4.590725000	-0.680854000	1.125782000
6	2.862508000	3.761602000	0.174181000	6	2.587822000	-2.350978000	-1.372256000
1	3.780614000	4.242189000	0.467108000	1	2.813290000	-1.923898000	-2.355289000
6	1.759943000	4.264002000	-0.419217000	1	3.023281000	-3.352260000	-1.319174000
1	1.533978000	5.264717000	-0.746865000	1	1.504771000	-2.439877000	-1.268114000
6	3.545851000	1.489127000	1.019908000	6	3.051145000	0.999111000	2.212671000
1	3.717390000	1.767851000	2.065046000	1	1.977697000	1.183127000	2.148671000
1	3.080878000	0.502784000	0.985749000	1	3.313754000	0.747619000	3.244515000
1	4.509710000	1.449173000	0.503994000	1	3.585021000	1.913758000	1.928557000
6	-0.484136000	3.375855000	-1.107430000	6	-1.572698000	-0.979130000	1.931338000
1	-1.162068000	2.702366000	-0.577895000	1	-2.050218000	-0.008944000	2.097476000
1	-0.812013000	4.406061000	-0.951174000	1	-1.575561000	-1.545660000	2.869194000
1	-0.531433000	3.145954000	-2.175518000	1	-0.543402000	-0.794590000	1.622382000
6	0.480487000	-0.843349000	2.370880000	6	-2.459047000	-3.636224000	-2.108439000
1	-0.391147000	-0.432343000	1.860030000	1	-1.613431000	-3.142530000	-2.588691000
1	0.168046000	-1.339589000	3.295627000	1	-2.244784000	-4.707463000	-2.025995000
1	1.147286000	-0.011634000	2.611562000	1	-3.356340000	-3.505867000	-2.720230000
6	1.487236000	-3.890881000	-1.375815000	7	3.957971000	1.641139000	-1.275495000
1	1.064517000	-3.173525000	-2.080676000	7	4.208520000	0.788568000	-1.927917000
1	2.499432000	-4.163739000	-1.684102000	7	-1.160783000	0.720703000	-0.416454000
1	0.861445000	-4.789557000	-1.375065000	7	-0.481029000	3.083582000	-0.452724000
7	-1.645614000	0.414175000	0.245284000	7	-2.577760000	2.566184000	-0.108378000
7	-3.878892000	0.548906000	0.939113000	6	-1.331952000	1.989921000	-0.353032000
7	-3.576997000	-0.680401000	-0.848382000	6	-1.194134000	4.281658000	-0.306521000
6	-2.884783000	0.099127000	0.075763000	6	-2.490564000	3.957175000	-0.084117000
6	-5.119853000	0.077327000	0.550986000	6	0.927348000	2.993732000	-0.749299000
1	-6.016312000	0.309942000	1.100438000	1	1.461607000	3.815718000	-0.266641000
6	-4.935376000	-0.674095000	-0.554545000	1	1.313235000	2.053174000	-0.355201000
1	-5.642035000	-1.218657000	-1.157709000	1	1.128945000	3.032099000	-1.826163000
6	-3.573566000	1.394433000	2.060836000	6	-3.767863000	1.781279000	0.076057000
1	-4.495998000	1.632135000	2.590687000	1	-3.485773000	0.735491000	-0.063585000
1	-2.879996000	0.896040000	2.744531000	1	-4.184849000	1.908215000	1.082012000
1	-3.096149000	2.320997000	1.728719000	1	-4.539510000	2.044216000	-0.654515000
6	-3.000944000	-1.356908000	-1.989805000	6	5.769754000	-0.288657000	1.928233000

1	-2.017310000	-1.756527000	-1.733192000	1	6.002839000	0.777757000	1.821118000
1	-3.655794000	-2.185905000	-2.267384000	1	5.625464000	-0.475308000	2.998638000
1	-2.896129000	-0.687779000	-2.848906000	1	6.650738000	-0.850162000	1.614908000
7	3.020731000	-0.503201000	-2.007524000	6	5.445685000	-2.468731000	-0.521441000
7	3.507051000	-1.197308000	-1.302474000	1	6.436318000	-2.304241000	-0.095249000
				1	5.206234000	-3.530236000	-0.389159000
				1	5.515133000	-2.289139000	-1.600639000
				6	-0.528245000	5.600481000	-0.383063000
				1	-0.004270000	5.745540000	-1.334784000
				1	-1.262652000	6.401568000	-0.288409000
				1	0.213061000	5.743467000	0.412350000
				6	-3.677614000	4.806722000	0.156948000
				1	-4.137056000	4.609050000	1.132468000
				1	-3.405088000	5.862539000	0.132319000
				1	-4.457584000	4.651029000	-0.597331000
				6	-4.813283000	-4.109340000	-0.267771000
				1	-5.541637000	-4.118595000	0.544138000
				1	-5.342589000	-3.810856000	-1.180326000
				1	-4.477816000	-5.141452000	-0.420066000
				6	-4.279336000	-2.153351000	2.334862000
				1	-3.759615000	-2.440731000	3.256080000
				1	-4.543037000	-1.094076000	2.439242000
				1	-5.209355000	-2.722246000	2.294296000
P(Im^aCH)₃…N₂				P(Im^bCH)₃…N₂			
15	-0.657467000	-0.474563000	0.099366000	15	0.177830000	-1.893868000	1.397466000
6	0.321577000	0.602331000	1.177936000	6	0.110463000	-0.112334000	1.786581000
7	1.278554000	2.064890000	-0.556464000	7	-0.497421000	0.955690000	-0.367023000
7	1.618728000	2.707167000	1.490041000	7	-0.427224000	2.278140000	1.386897000
6	0.440023000	-0.699196000	-1.343953000	6	-0.238925000	0.949636000	1.005622000
7	2.564214000	-1.680150000	-2.208228000	6	-1.119553000	2.169365000	-0.721118000
7	2.480689000	-1.240252000	-0.077143000	6	-1.068350000	2.985620000	0.352099000
6	1.006047000	1.713865000	0.746982000	1	-0.772230000	0.056373000	-0.769436000
6	2.099134000	3.181084000	-0.605471000	1	-0.557270000	2.511916000	2.358261000
1	2.439649000	3.600602000	-1.536037000	6	-1.451730000	4.403410000	0.523089000
6	2.302761000	3.593577000	0.662024000	1	-1.933739000	4.784360000	-0.378098000
1	2.841430000	4.440542000	1.049198000	1	-2.153194000	4.542205000	1.354074000
6	1.715817000	-1.186118000	-1.227678000	1	-0.582994000	5.038892000	0.729907000
6	3.839711000	-1.897032000	-1.689213000	6	-1.607463000	2.379943000	-2.100382000
1	4.645746000	-2.275216000	-2.293425000	1	-0.796925000	2.312512000	-2.835656000
6	3.783111000	-1.621045000	-0.371708000	1	-2.351977000	1.623519000	-2.377268000
1	4.538299000	-1.707497000	0.390072000	1	-2.074542000	3.359867000	-2.207055000
7	0.496797000	-2.556082000	3.228529000	1	0.306014000	0.121355000	2.831187000
7	1.415519000	-2.027333000	2.925870000	6	1.860101000	-2.255799000	0.893911000
1	2.324072000	-1.684265000	-3.183354000	7	2.279132000	-0.382676000	-0.657456000
1	2.153460000	-0.765176000	0.759997000	7	3.980877000	-1.663316000	-0.246342000
1	1.087706000	1.380650000	-1.291019000	6	2.636808000	-1.500774000	0.058532000
1	1.596597000	2.736821000	2.493631000	6	3.391547000	0.215742000	-1.251883000
6	-1.952348000	0.549427000	-0.605226000	6	4.457997000	-0.574317000	-0.993039000
7	-4.405300000	0.840430000	-0.873260000	1	1.391790000	0.086368000	-0.536965000
7	-3.745860000	-1.002835000	0.077540000	1	4.570873000	-2.259482000	0.309877000
6	-3.256820000	0.166749000	-0.478500000	6	5.875519000	-0.478323000	-1.400192000
6	-5.546154000	0.163715000	-0.435120000	1	6.049435000	0.434286000	-1.971707000
1	-6.538541000	0.527716000	-0.635970000	1	6.550578000	-0.457120000	-0.536252000
6	-5.132159000	-0.978115000	0.145551000	1	6.182767000	-1.324363000	-2.025812000

1	-5.698583000	-1.797460000	0.552948000	6	3.249621000	1.478664000	-2.006629000
1	-4.382535000	1.812991000	-1.125473000	1	2.588286000	1.366147000	-2.873871000
1	-3.119066000	-1.636720000	0.551728000	1	2.818545000	2.266320000	-1.376457000
1	-0.058046000	-0.830346000	-2.300179000	1	4.216625000	1.830979000	-2.367843000
1	0.136511000	0.526974000	2.245336000	1	2.341085000	-3.096395000	1.382633000
1	-1.752256000	1.512522000	-1.069883000	6	-0.769924000	-2.001884000	-0.158657000
				7	-2.817783000	-1.024988000	0.770099000
				7	-3.021124000	-1.869024000	-1.236209000
				6	-2.101728000	-1.698403000	-0.204096000
				6	-4.121233000	-0.755421000	0.338096000
				6	-4.268536000	-1.325393000	-0.877983000
				1	-2.332499000	-0.545348000	1.518472000
				1	-2.916560000	-2.611349000	-1.908116000
				6	-5.428458000	-1.405376000	-1.790439000
				1	-6.297310000	-0.912383000	-1.352690000
				1	-5.224743000	-0.926015000	-2.755126000
				1	-5.715872000	-2.442065000	-2.003682000
				6	-5.054573000	0.029004000	1.173449000
				1	-5.215629000	-0.440143000	2.150228000
				1	-4.676780000	1.041320000	1.362202000
				1	-6.025773000	0.125710000	0.686668000
				1	-0.335478000	-2.553887000	-0.985788000
				7	3.177112000	1.221625000	1.729348000
				7	3.636509000	0.406589000	2.314196000
P(Im^cCH)₃…N₂				P(Im^dCH)₃…N₂			
15	-0.169249000	-0.398751000	-0.807323000	15	-0.217980000	-0.679705000	-1.056416000
6	1.236460000	-1.516205000	-0.574259000	6	-1.657607000	-1.764376000	-0.900581000
7	2.346470000	-0.958002000	1.599859000	7	-3.165029000	-0.804431000	0.845522000
7	3.546469000	-2.022551000	0.098197000	7	-4.084298000	-2.091330000	-0.669761000
6	0.541479000	1.167517000	-0.238578000	6	0.797975000	-0.621248000	0.454726000
7	0.555986000	3.523894000	0.416129000	7	2.573406000	-2.303886000	-0.025964000
7	-1.307700000	2.840447000	-0.548285000	7	3.079780000	-0.696430000	1.374043000
6	2.281690000	-1.485000000	0.316240000	6	-2.867311000	-1.557017000	-0.276164000
6	3.591495000	-1.237276000	2.157577000	6	-4.534071000	-0.891607000	1.135338000
1	3.842382000	-0.913522000	3.153389000	6	-5.103477000	-1.684671000	0.197030000
6	4.326219000	-1.891929000	1.237949000	6	2.050973000	-1.168803000	0.573446000
1	5.344741000	-2.240765000	1.268716000	6	3.873867000	-2.538330000	0.434658000
6	-0.044533000	2.397991000	-0.148320000	6	4.190608000	-1.541833000	1.296474000
6	-0.274457000	4.627293000	0.280274000	6	1.769660000	-3.260688000	-0.751257000
1	0.003938000	5.593035000	0.667628000	1	1.765164000	-3.066636000	-1.827336000
6	-1.407012000	4.213868000	-0.317429000	1	2.150229000	-4.269477000	-0.572956000
1	-2.304025000	4.754947000	-0.567139000	1	0.736893000	-3.201962000	-0.393090000
6	1.900417000	3.519910000	0.912942000	6	2.975205000	0.531350000	2.109572000
1	2.126260000	4.493783000	1.347281000	1	2.544349000	1.311820000	1.470163000
1	2.024554000	2.751613000	1.686057000	1	2.326678000	0.429948000	2.989388000
1	2.625507000	3.309846000	0.116819000	1	3.963798000	0.846888000	2.443577000
6	-2.105094000	2.171383000	-1.552355000	6	-2.154929000	-0.396427000	1.797189000
1	-2.355649000	1.156994000	-1.237325000	1	-1.737800000	0.585645000	1.553025000
1	-3.028871000	2.736064000	-1.689425000	1	-2.588122000	-0.368175000	2.798442000
1	-1.579034000	2.114849000	-2.512680000	1	-1.330471000	-1.114270000	1.776690000
6	1.167946000	-0.674921000	2.392224000	6	-4.229959000	-2.889898000	-1.852973000
1	0.408586000	-1.443748000	2.218009000	1	-3.757927000	-2.389020000	-2.705515000
1	1.449628000	-0.669619000	3.446170000	1	-3.758884000	-3.873919000	-1.740822000
1	0.730274000	0.290575000	2.125773000	1	-5.287506000	-3.037597000	-2.069772000

6	3.904974000	-2.732143000	-1.097328000	7	4.823877000	-0.413832000	-1.576859000
1	3.660882000	-2.133997000	-1.980186000	7	4.040337000	-0.760984000	-2.272944000
1	4.976845000	-2.929857000	-1.088955000	6	-1.002757000	0.950900000	-0.932859000
1	3.371573000	-3.687177000	-1.178307000	7	0.920992000	2.529215000	-0.609431000
1	1.445542000	-2.094404000	-1.470522000	7	-1.132068000	3.323713000	-0.358492000
1	1.572206000	1.128603000	0.098599000	6	-0.429785000	2.161902000	-0.675265000
6	-1.460587000	-0.650020000	0.452167000	6	1.006619000	3.906663000	-0.310070000
7	-3.841601000	-1.039974000	0.939569000	6	-0.245343000	4.383669000	-0.139779000
7	-3.022503000	-2.189509000	-0.742406000	6	1.910064000	1.920321000	-1.475884000
6	-2.671097000	-1.251217000	0.219611000	1	2.910002000	2.088439000	-1.067264000
6	-4.863853000	-1.835360000	0.440511000	1	1.745460000	0.845967000	-1.537736000
1	-5.854983000	-1.813145000	0.860853000	1	1.871690000	2.335846000	-2.493448000
6	-4.359810000	-2.541835000	-0.590510000	6	-2.559251000	3.351054000	-0.253157000
1	-4.825812000	-3.265312000	-1.237390000	1	-2.912266000	2.563435000	0.426974000
6	-3.949513000	-0.045145000	1.966800000	1	-2.883879000	4.317916000	0.130967000
1	-4.991304000	0.045054000	2.274126000	1	-3.043236000	3.183068000	-1.224451000
1	-3.346470000	-0.304530000	2.844927000	6	5.455918000	-1.242368000	1.999322000
1	-3.598986000	0.926296000	1.596288000	1	5.898779000	-0.295666000	1.664825000
6	-2.072103000	-2.942105000	-1.529843000	1	5.324643000	-1.171639000	3.085073000
1	-1.132058000	-3.024994000	-0.975360000	1	6.189201000	-2.027081000	1.809733000
1	-2.471231000	-3.944569000	-1.706451000	6	4.687037000	-3.664137000	-0.073459000
1	-1.856755000	-2.466125000	-2.489167000	1	5.700841000	-3.613006000	0.326076000
1	-1.422109000	-0.025046000	1.341204000	1	4.278814000	-4.643345000	0.202006000
7	3.110922000	0.354048000	-2.703540000	1	4.759315000	-3.647701000	-1.167989000
7	3.364441000	1.187015000	-2.026540000	6	2.318905000	4.576989000	-0.180175000
				1	2.887335000	4.576363000	-1.117854000
				1	2.189456000	5.617832000	0.120116000
				1	2.952515000	4.091689000	0.573074000
				6	-0.718641000	5.725553000	0.263401000
				1	-1.265535000	5.708348000	1.214275000
				1	0.126193000	6.404230000	0.385791000
				1	-1.389187000	6.167952000	-0.482293000
				6	-6.514310000	-2.079250000	-0.005815000
				1	-7.141515000	-1.655332000	0.779316000
				1	-6.914194000	-1.730963000	-0.965925000
				1	-6.648434000	-3.166769000	0.020803000
				6	-5.135753000	-0.173624000	2.280381000
				1	-4.788052000	-0.551117000	3.249298000
				1	-4.904205000	0.897621000	2.256076000
				1	-6.221635000	-0.277325000	2.266188000
				1	0.598435000	0.202405000	1.136278000
				1	-2.085808000	0.951770000	-1.002318000
				1	-1.692233000	-2.509600000	-1.690542000

Table S5: Cartesian coordinates of optimized geometries of mono-phosphine-N₂ hypervalent complexes at M06L/6-311++G(d,p) level DFT. Atomic number followed by X, Y, Z coordinates in Å.

(Im ^c N) ₃ P–N ₂				(Im ^d N) ₃ P–N ₂			
15	0.085593000	0.139665000	-0.715085000	15	-0.000377000	-0.277544000	-0.806758000
7	1.453550000	1.033044000	-0.892008000	7	-1.158071000	-1.452864000	-0.854879000
7	2.700639000	1.062861000	1.222555000	7	-2.509176000	-1.351166000	1.182182000
7	3.784402000	1.239817000	-0.665137000	7	-3.472162000	-1.875726000	-0.696545000
7	-1.102761000	0.703649000	0.316349000	7	1.268455000	-0.300397000	0.293254000
7	-2.546304000	2.570452000	0.560572000	7	2.570749000	-2.326898000	-0.201635000

7	-3.331322000	0.919162000	-0.630625000	7	3.596980000	-0.553571000	0.529886000
6	2.511066000	1.066389000	-0.146104000	6	-2.257198000	-1.501133000	-0.161671000
6	4.044611000	1.224382000	1.519069000	6	-3.851834000	-1.611508000	1.462965000
1	4.397811000	1.244013000	2.536154000	6	-4.450353000	-1.946028000	0.291654000
6	4.713919000	1.339630000	0.351889000	6	2.350658000	-1.024902000	0.176655000
1	5.762784000	1.482143000	0.154142000	6	3.924853000	-2.647059000	-0.087508000
6	-2.204822000	1.332418000	0.055504000	6	4.563844000	-1.543953000	0.378670000
6	-3.843446000	2.896542000	0.210967000	6	1.540381000	-3.274130000	-0.569022000
1	-4.302772000	3.821615000	0.515166000	1	1.500962000	-3.409660000	-1.652202000
6	-4.324948000	1.877867000	-0.536688000	1	1.737030000	-4.230996000	-0.078317000
1	-5.283006000	1.749978000	-1.011167000	1	0.569131000	-2.891408000	-0.257004000
6	-1.617218000	3.366418000	1.322168000	6	3.819209000	0.801217000	0.963797000
1	-1.947767000	4.404861000	1.322760000	1	2.954348000	1.389419000	0.654568000
1	-1.541125000	3.013787000	2.356058000	1	3.916772000	0.869244000	2.053390000
1	-0.628250000	3.298778000	0.864332000	1	4.724071000	1.204285000	0.504221000
6	-3.453032000	-0.354254000	-1.299168000	6	-1.517988000	-1.009787000	2.173058000
1	-2.764233000	-1.061739000	-0.831063000	1	-1.618728000	0.032036000	2.488017000
1	-4.475114000	-0.722115000	-1.192658000	1	-1.618854000	-1.670650000	3.039170000
1	-3.192212000	-0.278833000	-2.357482000	1	-0.523030000	-1.124133000	1.740938000
6	1.656418000	0.996529000	2.219356000	6	-3.662839000	-2.104626000	-2.105380000
1	1.611716000	0.003897000	2.673499000	1	-2.692744000	-1.968952000	-2.583644000
1	1.848195000	1.750107000	2.989274000	1	-4.020508000	-3.120455000	-2.297589000
1	0.692015000	1.185372000	1.747854000	1	-4.378558000	-1.393565000	-2.528741000
6	4.051764000	1.288613000	-2.080049000	7	0.502014000	0.208778000	-2.375659000
1	3.092046000	1.212907000	-2.590684000	7	0.935946000	-0.991113000	-2.232763000
1	4.533379000	2.231029000	-2.354309000	7	-0.913265000	0.971758000	-0.069580000
1	4.693688000	0.458214000	-2.386797000	7	-0.716244000	3.163190000	-1.047189000
7	-0.424313000	-0.547046000	-2.206555000	7	0.063259000	2.913567000	0.972023000
7	-0.669071000	0.715978000	-2.262018000	6	-0.541980000	2.207738000	-0.057754000
7	0.680533000	-1.116402000	0.289355000	6	-0.247659000	4.406972000	-0.632388000
7	0.157055000	-3.364897000	-0.408355000	6	0.226555000	4.255132000	0.632922000
7	-0.711774000	-2.682588000	1.476945000	6	-1.260431000	2.838256000	-2.341016000
6	0.094471000	-2.253876000	0.426028000	1	-1.902927000	3.646747000	-2.696905000
6	-0.562657000	-4.417557000	0.123461000	1	-0.473553000	2.634645000	-3.074838000
1	-0.629564000	-5.372503000	-0.370746000	1	-1.844221000	1.922561000	-2.226854000
6	-1.093153000	-3.998541000	1.296938000	6	0.398794000	2.294775000	2.228090000
1	-1.701342000	-4.523478000	2.014783000	1	0.543170000	1.228486000	2.039722000
6	0.869977000	-3.354083000	-1.661364000	1	1.326979000	2.717118000	2.620570000
1	1.349592000	-4.321230000	-1.825130000	1	-0.389902000	2.437538000	2.977605000
1	0.209064000	-3.113182000	-2.499109000	6	5.991633000	-1.297686000	0.676962000
1	1.625421000	-2.567944000	-1.601567000	1	6.421276000	-0.519317000	0.035849000
6	-1.040366000	-1.830365000	2.591366000	1	6.147061000	-0.979268000	1.713780000
1	-0.888756000	-0.798106000	2.269236000	1	6.575569000	-2.205527000	0.521876000
1	-2.086310000	-1.969154000	2.873996000	6	4.443976000	-3.983307000	-0.453378000
1	-0.409108000	-2.042257000	3.461926000	1	5.529384000	-4.011132000	-0.350164000
				1	4.034262000	-4.779553000	0.178279000
				1	4.202491000	-4.241777000	-1.489723000
				6	-0.316376000	5.601281000	-1.503778000
				1	-1.347991000	5.871643000	-1.757523000
				1	0.134296000	6.463346000	-1.010067000
				1	0.213600000	5.448328000	-2.450472000
				6	0.831396000	5.233622000	1.564088000
				1	1.864066000	4.973905000	1.826442000
				1	0.851202000	6.227593000	1.115148000
				1	0.274847000	5.309222000	2.505366000

	6	-5.847274000	-2.322487000	-0.017483000
	1	-6.457418000	-2.304501000	0.886268000
	1	-6.308628000	-1.639591000	-0.739688000
	1	-5.919225000	-3.330132000	-0.442131000
	6	-4.396217000	-1.505825000	2.834481000
	1	-3.930441000	-2.217984000	3.525321000
	1	-4.246042000	-0.506741000	3.258119000
	1	-5.468393000	-1.705898000	2.835139000

Table S6: Cartesian coordinates of optimized geometries of bis-phosphine-N₂ complexes at M06L/6-311++G(d,p) level DFT. Atomic number followed by X, Y, Z coordinates in Å.

H₃P–NN–PH₃				Me₃P–NN–PMe₃			
15	1.965802000	0.026825000	0.001648000	15	1.940465000	-0.048916000	-0.001563000
7	-0.487187000	0.544335000	-0.005079000	7	-0.449965000	0.597628000	-0.017328000
15	-1.965799000	-0.026840000	0.001647000	15	-1.940408000	0.048893000	-0.001551000
7	0.487174000	-0.544286000	-0.005077000	7	0.450048000	-0.597766000	-0.017793000
1	2.822521000	-1.075303000	-0.003390000	6	2.438828000	1.008570000	-1.405885000
1	2.460216000	0.840029000	-1.068492000	1	1.729466000	1.837370000	-1.456587000
1	2.457742000	0.827323000	1.082721000	1	3.451384000	1.406722000	-1.301904000
1	-2.822573000	1.075249000	-0.003466000	1	2.364066000	0.439652000	-2.334119000
1	-2.457740000	-0.827294000	1.082753000	6	3.049466000	-1.471158000	-0.008262000
1	-2.460117000	-0.840136000	-1.068461000	1	2.869757000	-2.072029000	-0.900130000
				1	4.092495000	-1.148104000	0.000809000
				1	2.859565000	-2.088426000	0.870224000
				6	2.422034000	0.980613000	1.429544000
				1	3.435714000	1.380694000	1.345617000
				1	1.712191000	1.808490000	1.488203000
				1	2.336516000	0.393348000	2.345365000
				6	-3.049341000	1.471199000	-0.008308000
				1	-2.870724000	2.071214000	-0.900971000
				1	-4.092363000	1.148163000	0.002337000
				1	-2.858367000	2.089300000	0.869358000
				6	-2.438390000	-1.008242000	-1.406236000
				1	-3.450792000	-1.406829000	-1.302433000
				1	-2.363846000	-0.438924000	-2.334244000
				1	-1.728676000	-1.836721000	-1.457248000
				6	-2.422711000	-0.980849000	1.429202000
				1	-1.713769000	-1.809514000	1.487538000
				1	-2.336571000	-0.394034000	2.345251000
				1	-3.436811000	-1.379854000	1.345158000
(Im^aN)₃P–NN–P(Im^aN)₃				(Im^bN)₃P–NN–P(Im^bN)₃			
15	2.017339000	-0.142235000	-0.332954000	7	-0.640852000	0.091184000	-0.519389000
7	2.302387000	-1.029840000	-1.691925000	7	0.549932000	0.349486000	0.315229000
7	0.313378000	-2.430599000	-1.813688000	15	-1.940868000	-0.451232000	0.306127000
7	2.036658000	-2.964155000	-3.023599000	7	-3.092950000	-0.483482000	-0.884561000
7	2.440218000	1.425387000	-0.798019000	7	-5.364360000	-0.810106000	-1.468677000
7	1.799384000	3.484918000	-1.790539000	7	-4.969454000	-0.678194000	0.653974000
7	0.231533000	1.993090000	-1.642818000	6	-4.338524000	-0.643503000	-0.566315000
6	1.591998000	-2.044435000	-2.102498000	6	-6.599143000	-0.913278000	-0.823255000
6	-0.037276000	-3.524644000	-2.579441000	6	-6.348620000	-0.817705000	0.506192000
1	-1.014145000	-3.972763000	-2.513004000	1	-5.198894000	-0.847400000	-2.459963000
6	1.031667000	-3.871887000	-3.331870000	1	-4.444488000	-0.409779000	1.483249000

1	1.174766000	-4.673119000	-4.035767000	6	-7.254688000	-0.870312000	1.674275000
6	1.553373000	2.200631000	-1.362931000	1	-8.290777000	-0.990892000	1.355159000
6	0.636742000	4.070929000	-2.278945000	1	-7.012094000	-1.705923000	2.339585000
1	0.615277000	5.078474000	-2.655775000	1	-7.200961000	0.043736000	2.276296000
6	-0.331755000	3.133874000	-2.180122000	6	-7.857021000	-1.112959000	-1.574291000
1	-1.373633000	3.175078000	-2.449323000	1	-8.050160000	-0.295687000	-2.278506000
7	-0.590843000	-0.324188000	-0.442040000	1	-7.847354000	-2.042093000	-2.155790000
15	-2.017454000	-0.143400000	0.332586000	1	-8.706808000	-1.163957000	-0.892588000
7	-2.301926000	-1.030401000	1.692062000	7	-1.910800000	-2.008110000	0.893331000
7	-0.311772000	-2.429429000	1.815278000	7	0.446343000	-2.126271000	1.486590000
7	-2.034911000	-2.963632000	3.025052000	7	-0.726681000	-3.944629000	1.562229000
7	-2.440938000	1.424435000	0.796834000	6	-0.818430000	-2.599573000	1.286369000
7	-1.801368000	3.483649000	1.790899000	6	1.326802000	-3.167075000	1.761799000
7	-0.233271000	1.991939000	1.644450000	6	0.600733000	-4.313102000	1.809794000
6	-1.590754000	-2.044124000	2.103468000	1	0.692508000	-1.142055000	1.214835000
6	0.039576000	-3.522745000	2.581764000	1	-1.496531000	-4.570547000	1.394745000
1	1.016843000	-3.970065000	2.515862000	6	0.982911000	-5.716602000	2.072977000
6	-1.029279000	-3.870335000	3.334164000	1	2.064438000	-5.801031000	2.191691000
1	-1.171864000	-4.671201000	4.038583000	1	0.521951000	-6.113083000	2.985678000
6	-1.554820000	2.199517000	1.363136000	1	0.690069000	-6.382496000	1.251485000
6	-0.639284000	4.069599000	2.280705000	6	2.771121000	-2.907453000	1.963604000
1	-0.618282000	5.077034000	2.657856000	1	3.182968000	-2.321579000	1.133238000
6	0.329404000	3.132677000	2.182500000	1	2.957491000	-2.330012000	2.876287000
1	1.370999000	3.173930000	2.452786000	1	3.329034000	-3.843114000	2.041885000
7	0.590784000	-0.323334000	0.441685000	7	-2.511025000	0.464785000	1.588427000
1	-2.696380000	3.926799000	1.680976000	7	-2.694444000	2.594810000	2.630695000
1	0.267647000	1.110925000	1.345656000	7	-0.883712000	2.264294000	1.492352000
1	0.314243000	-1.752606000	1.294799000	6	-2.048087000	1.660819000	1.856076000
1	-2.956500000	-2.917234000	3.424007000	6	-1.923241000	3.756749000	2.760836000
1	-0.313134000	-1.753623000	-1.293888000	6	-0.790651000	3.533056000	2.045741000
1	2.958161000	-2.917414000	-3.422709000	1	-3.591246000	2.424492000	3.052598000
1	2.694254000	3.928348000	-1.680568000	1	-0.098870000	1.693376000	1.066569000
1	-0.268805000	1.111437000	-1.345031000	6	0.389320000	4.384046000	1.769211000
7	3.091827000	-0.559657000	0.849886000	1	0.341312000	5.321318000	2.326172000
7	4.997630000	0.681266000	-0.023441000	1	1.318638000	3.871433000	2.037596000
7	5.306528000	-0.625676000	1.678592000	1	0.463660000	4.624937000	0.702208000
6	4.331977000	-0.187762000	0.808037000	6	-2.389446000	4.923766000	3.540012000
6	6.322295000	0.809537000	0.358163000	1	-3.322464000	5.344632000	3.146131000
1	7.012771000	1.449125000	-0.164053000	1	-2.569241000	4.674812000	4.592645000
6	6.522004000	-0.010925000	1.412386000	1	-1.640830000	5.716889000	3.517346000
1	7.412288000	-0.226537000	1.976389000	15	1.949924000	0.502190000	-0.515279000
1	4.436576000	1.261154000	-0.648104000	7	1.996150000	1.516603000	-1.816961000
1	5.105680000	-1.281868000	2.413142000	7	-0.216708000	2.496402000	-1.620994000
7	-3.091778000	-0.561919000	-0.849996000	7	1.260025000	3.546282000	-2.805310000
7	-4.997690000	0.681008000	0.020156000	6	1.080151000	2.424313000	-2.033471000
7	-5.305994000	-0.628669000	-1.679853000	6	-0.841170000	3.616411000	-2.150374000
6	-4.331828000	-0.189617000	-0.809454000	6	0.077690000	4.289967000	-2.890542000
6	-6.322167000	0.808809000	-0.362207000	1	-0.676496000	1.638557000	-1.212161000
1	-7.012817000	1.449272000	0.158705000	1	2.140805000	3.763345000	-3.240202000
6	-6.521503000	-0.013314000	-1.415212000	6	-0.002794000	5.551244000	-3.658387000
1	-7.411568000	-0.229709000	-1.979260000	1	-1.009794000	5.966738000	-3.600072000
1	-4.436793000	1.261145000	0.644746000	1	0.687893000	6.315052000	-3.281384000
1	-5.104909000	-1.286124000	-2.413207000	1	0.229581000	5.405245000	-4.719859000
				6	-2.258609000	3.904521000	-1.832699000
				1	-2.903990000	3.059647000	-2.095987000

	1	-2.397902000	4.083755000	-0.759945000
	1	-2.614766000	4.784279000	-2.371453000
	7	2.956205000	1.071914000	0.670214000
	7	5.046552000	0.264772000	-0.285855000
	7	5.133446000	1.493132000	1.493002000
	6	4.243632000	0.939264000	0.600561000
	6	6.387830000	0.349805000	0.084029000
	6	6.448144000	1.128212000	1.193115000
	1	4.598074000	-0.378284000	-0.938429000
	1	4.826362000	2.043385000	2.276876000
	6	7.592622000	1.604265000	1.999293000
	1	8.529329000	1.204990000	1.608645000
	1	7.674805000	2.697289000	1.994460000
	1	7.515614000	1.292784000	3.047251000
	6	7.454281000	-0.306971000	-0.703273000
	1	7.316584000	-1.392941000	-0.752711000
	1	7.482164000	0.058791000	-1.735349000
	1	8.433306000	-0.121297000	-0.259477000
	7	2.662462000	-0.923668000	-1.064207000
	7	2.433123000	-3.203663000	-1.675545000
	7	0.600608000	-2.050070000	-1.688975000
	6	1.937690000	-1.940448000	-1.453498000
	6	1.389437000	-4.109773000	-1.906500000
	6	0.247731000	-3.377317000	-1.915886000
	1	3.378616000	-3.450213000	-1.435194000
	1	-0.059199000	-1.270666000	-1.437673000
	6	-1.165748000	-3.762277000	-2.130632000
	1	-1.268554000	-4.848192000	-2.182751000
	1	-1.800367000	-3.386933000	-1.319746000
	1	-1.562687000	-3.342398000	-3.061482000
	6	1.642468000	-5.553805000	-2.093161000
	1	2.248602000	-5.763925000	-2.982583000
	1	2.168965000	-5.990393000	-1.234894000
	1	0.700480000	-6.092971000	-2.205728000
(Im^cN)₃P–NN–P(Im^cN)₃				
15		-1.830907000	-0.024297000	-0.414979000
7		-2.766726000	0.738161000	-1.588306000
7		-2.912762000	3.146541000	-1.129122000
7		-4.676675000	2.088872000	-1.862452000
7		-1.210347000	-1.335038000	-1.207102000
7		0.567825000	-2.726217000	-1.870966000
7		0.518767000	-0.778597000	-2.863281000
6		-3.357874000	1.888549000	-1.490910000
6		-3.933851000	4.070371000	-1.271394000
1		-3.783945000	5.112364000	-1.044074000
6		-5.026252000	3.419952000	-1.730461000
1		-6.010225000	3.780916000	-1.977731000
6		-0.134250000	-1.524229000	-1.896576000
6		1.625336000	-2.691072000	-2.761736000
1		2.300339000	-3.522314000	-2.877981000
6		1.602980000	-1.479138000	-3.358167000
1		2.261223000	-1.047278000	-4.093493000
7		0.376880000	1.131424000	-0.345449000
15		1.736459000	0.712083000	0.399755000
(Im^dN)₃P–NN–P(Im^dN)₃				
15		1.421068000	1.070767000	-0.721992000
7		2.201624000	0.673392000	-2.159110000
7		3.401289000	-1.422892000	-1.854943000
7		4.543988000	0.332069000	-2.455902000
7		0.383986000	2.271342000	-1.141541000
7		-1.718909000	3.319049000	-1.062982000
7		-1.639169000	1.532437000	-2.312428000
6		3.258073000	-0.080822000	-2.144108000
6		4.739176000	-1.804477000	-1.929689000
6		5.452544000	-0.709169000	-2.305293000
6		-0.861704000	2.303508000	-1.473312000
6		-2.989194000	3.147937000	-1.608612000
6		-2.944676000	2.019828000	-2.360446000
7		-0.230104000	-0.819133000	-0.568800000
15		-1.576058000	-1.032472000	0.273133000
7		-1.270876000	-1.577919000	1.837383000
7		0.447766000	-3.272360000	1.457931000
7		0.605935000	-2.013856000	3.228835000
7		-2.728495000	0.152476000	0.509311000

7	1.684346000	1.161533000	2.013634000	7	-4.160693000	1.808747000	1.334529000
7	1.002497000	3.500013000	1.960544000	7	-2.108244000	1.944134000	2.080846000
7	-0.026047000	2.167816000	3.344528000	6	-0.171101000	-2.224603000	2.106638000
7	2.349216000	-0.837799000	0.442189000	6	1.608945000	-3.652608000	2.134648000
7	3.100742000	-3.024382000	0.796746000	6	1.706614000	-2.865755000	3.236271000
7	1.204426000	-2.552892000	1.790725000	6	-2.915421000	1.183738000	1.250123000
6	0.950900000	2.182526000	2.371559000	6	-4.104518000	2.926358000	2.165705000
6	0.049429000	4.249747000	2.626233000	6	-2.832165000	3.011275000	2.625145000
1	-0.063772000	5.306822000	2.452328000	7	0.829842000	-0.136990000	0.173796000
6	-0.592581000	3.419295000	3.478268000	7	2.561521000	1.869523000	0.191604000
1	-1.387101000	3.610117000	4.179833000	7	4.833942000	2.453141000	0.401578000
6	2.178755000	-1.984645000	0.978124000	7	4.393486000	0.342805000	0.780383000
6	2.712719000	-4.150539000	1.499418000	6	3.783033000	1.541793000	0.430687000
1	3.302734000	-5.051837000	1.505143000	6	6.045658000	1.828791000	0.690789000
6	1.542728000	-3.860299000	2.107249000	6	5.772026000	0.521115000	0.926856000
1	0.910032000	-4.465201000	2.735086000	7	-2.420003000	-2.089936000	-0.693746000
7	-0.788372000	0.806174000	0.480859000	7	-4.728095000	-2.150358000	0.134356000
7	-2.904730000	-0.588430000	0.717397000	7	-4.342807000	-2.523786000	-1.981657000
7	-4.152355000	-2.498630000	-0.248291000	6	-3.700203000	-2.216561000	-0.790307000
7	-4.246833000	-2.080460000	1.901532000	6	-5.962495000	-2.379799000	-0.484131000
6	-3.675193000	-1.616684000	0.719074000	6	-5.720953000	-2.611390000	-1.798467000
6	-4.955657000	-3.464699000	0.346561000	6	3.684442000	-0.818921000	1.276277000
1	-5.420556000	-4.241760000	-0.236433000	1	2.619606000	-0.739014000	1.004937000
6	-5.013264000	-3.206747000	1.669919000	1	4.098306000	-1.733056000	0.837364000
1	-5.532635000	-3.717061000	2.463472000	1	3.787053000	-0.887672000	2.366996000
7	2.891482000	1.444261000	-0.549217000	6	4.642894000	3.832917000	0.043604000
7	5.074316000	0.630665000	0.232253000	1	5.309914000	4.128135000	-0.772394000
7	4.831545000	1.209125000	-1.863126000	1	3.605100000	3.931272000	-0.280378000
6	4.128101000	1.102097000	-0.668091000	1	4.816133000	4.500649000	0.894591000
6	6.298562000	0.469488000	-0.398395000	6	-1.280837000	4.437606000	-0.274856000
1	7.164500000	0.115044000	0.135459000	1	-0.246932000	4.238350000	0.013043000
6	6.150563000	0.833223000	-1.690670000	1	-1.311140000	5.371705000	-0.848461000
1	6.861658000	0.857044000	-2.499164000	1	-1.900069000	4.555448000	0.620444000
6	-3.962764000	-1.458275000	3.166993000	6	-0.115779000	-3.942320000	0.305978000
1	-4.148744000	-0.383388000	3.108167000	1	0.380006000	-4.905439000	0.174685000
1	-4.600846000	-1.899314000	3.933112000	1	-1.183888000	-4.104138000	0.467905000
1	-2.912741000	-1.593574000	3.447616000	1	-0.019440000	-3.326053000	-0.591815000
6	-3.970075000	-2.398582000	-1.681395000	6	0.419071000	-0.879553000	4.092149000
1	-4.922339000	-2.621475000	-2.173216000	1	-0.587687000	-0.501107000	3.913183000
1	-3.655100000	-1.388369000	-1.941631000	1	0.523030000	-1.168061000	5.141389000
1	-3.205615000	-3.094645000	-2.036907000	1	1.138599000	-0.084250000	3.862829000
6	0.145888000	-3.864243000	-1.100598000	6	-4.547260000	-2.042309000	1.563849000
1	-0.630455000	-3.523194000	-0.413233000	1	-5.117806000	-2.828384000	2.068771000
1	-0.275440000	-4.648051000	-1.741449000	1	-3.489819000	-2.153221000	1.807471000
1	0.979186000	-4.281949000	-0.529752000	1	-4.874118000	-1.068238000	1.940682000
6	1.877397000	3.986189000	0.919963000	6	-3.637152000	-2.668213000	-3.227683000
1	1.920922000	5.075093000	0.976646000	1	-2.573499000	-2.588281000	-3.000116000
1	2.877828000	3.572212000	1.061107000	1	-3.837808000	-3.641349000	-3.685994000
1	1.528641000	3.661938000	-0.065146000	1	-3.908981000	-1.881948000	-3.940664000
6	-0.622932000	0.933759000	3.792582000	6	2.297181000	-2.301270000	-1.543950000
1	0.169064000	0.227199000	4.042069000	1	2.339748000	-3.194889000	-2.176909000
1	-1.231311000	1.129252000	4.677557000	1	2.318128000	-2.598560000	-0.490962000
1	-1.232300000	0.518413000	2.979265000	1	1.351670000	-1.770306000	-1.694781000
6	4.866573000	0.445412000	1.650966000	6	4.855490000	1.694095000	-2.801488000
1	5.707902000	0.879573000	2.198814000	1	5.674811000	2.071786000	-2.183259000

1	3.941319000	0.936825000	1.955956000	1	5.136437000	1.787803000	-3.856061000
1	4.778070000	-0.614211000	1.907082000	1	3.953036000	2.281357000	-2.617975000
6	4.216097000	1.651910000	-3.086243000	6	-0.669928000	1.834362000	2.184197000
1	3.136002000	1.599610000	-2.943079000	1	-0.369006000	1.819901000	3.235304000
1	4.487761000	2.685188000	-3.326804000	1	-0.307302000	0.927479000	1.691758000
1	4.513515000	1.006356000	-3.916187000	1	-0.175714000	2.677075000	1.688464000
6	-1.555582000	3.478449000	-0.742119000	6	-1.154243000	0.428672000	-3.108665000
1	-1.310594000	4.463833000	-1.149956000	1	-1.464455000	0.571836000	-4.150458000
1	-1.443035000	3.481385000	0.344820000	1	-0.065345000	0.408653000	-3.053017000
1	-0.854883000	2.730154000	-1.121256000	1	-1.518264000	-0.525559000	-2.720108000
6	-5.530759000	0.995421000	-2.247695000	6	-5.305482000	1.368003000	0.585442000
1	-5.613881000	0.267314000	-1.435280000	1	-4.998598000	0.487205000	0.017529000
1	-6.520776000	1.383951000	-2.486137000	1	-6.140148000	1.103104000	1.245006000
1	-5.124569000	0.478471000	-3.121090000	1	-5.650062000	2.137613000	-0.113998000
6	-0.058980000	-1.947998000	2.138001000	6	2.482268000	-4.749903000	1.660470000
1	-0.157250000	-1.873628000	3.225223000	1	3.388576000	-4.799861000	2.267092000
1	-0.140276000	-0.949075000	1.695853000	1	1.998425000	-5.732669000	1.717582000
1	-0.886875000	-2.550842000	1.747284000	1	2.789689000	-4.608356000	0.617814000
6	0.146861000	0.553688000	-3.281907000	6	2.713115000	-2.832295000	4.320535000
1	0.306866000	0.640800000	-4.360798000	1	2.295710000	-3.144088000	5.285577000
1	-0.909786000	0.709291000	-3.056931000	1	3.543319000	-3.502932000	4.092478000
1	0.716745000	1.303380000	-2.727241000	1	3.130554000	-1.829266000	4.466489000
6	4.286857000	-2.881315000	-0.005026000	6	-7.230891000	-2.340203000	0.276780000
1	4.154991000	-1.999920000	-0.635335000	1	-8.081801000	-2.478871000	-0.391606000
1	5.185129000	-2.742946000	0.608339000	1	-7.286053000	-3.123345000	1.041801000
1	4.428599000	-3.763972000	-0.634364000	1	-7.368116000	-1.383771000	0.794241000
				6	-6.638916000	-2.883468000	-2.926358000
				1	-6.555838000	-2.126775000	-3.715608000
				1	-6.442534000	-3.853973000	-3.396039000
				1	-7.674847000	-2.889530000	-2.585148000
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				6	-2.200932000	3.976002000	3.552841000
				1	-1.843582000	3.494317000	4.470536000
				1	-1.334060000	4.473511000	3.102413000
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				1	-5.011871000	3.773509000	-1.799511000
				1	-4.276849000	4.183791000	-0.240326000
				1	-3.866788000	5.106469000	-1.681636000
				6	-4.024081000	1.268939000	-3.038368000
				1	-3.817570000	1.092265000	-4.100225000
				1	-4.167840000	0.287409000	-2.566647000
				1	-4.969462000	1.811239000	-2.971794000
				6	5.173872000	-3.185699000	-1.622102000
				1	4.708710000	-3.925369000	-2.283569000
				1	6.255430000	-3.282534000	-1.731869000
				1	4.917948000	-3.477043000	-0.595446000
				6	6.907114000	-0.506158000	-2.484052000
				1	7.302012000	0.219873000	-1.759988000
				1	7.448771000	-1.442329000	-2.338972000
				1	7.156713000	-0.131596000	-3.482874000
				6	7.330428000	2.561974000	0.645681000

	1	8.158610000	1.901119000	0.906078000
	1	7.539636000	2.972913000	-0.350481000
	1	7.350108000	3.406136000	1.343915000
	6	6.665620000	-0.619311000	1.226054000
	1	6.425097000	-1.101163000	2.180571000
	1	6.592035000	-1.393690000	0.450929000
	1	7.706089000	-0.293324000	1.274136000
$(\text{Im}^a\text{CH})_3\text{P}-\text{NN}-\text{P}(\text{Im}^a\text{CH})_3$				
15	1.960093000	-0.098729000	-0.303789000	
6	2.160302000	-0.889946000	-1.867397000	
7	0.473746000	-2.690052000	-1.682274000	
7	1.955292000	-2.917128000	-3.266706000	
6	2.180779000	1.636491000	-0.659843000	
7	1.069084000	3.649416000	-1.594132000	
7	0.078240000	1.750675000	-1.957892000	
6	1.577389000	-2.089227000	-2.230142000	
6	0.143215000	-3.816582000	-2.414099000	
1	-0.708080000	-4.425014000	-2.158371000	
6	1.061500000	-3.978047000	-3.391039000	
1	1.182049000	-4.744628000	-4.136621000	
6	1.182845000	2.298585000	-1.363811000	
6	-0.119180000	3.933262000	-2.264306000	
1	-0.393780000	4.934727000	-2.546702000	
6	-0.727081000	2.745352000	-2.475965000	
1	-1.663810000	2.517017000	-2.955537000	
7	-0.581958000	-0.573537000	-0.462059000	
15	-1.960119000	-0.099227000	0.303670000	
6	-2.160165000	-0.890477000	1.867324000	
7	-0.473052000	-2.690045000	1.682171000	
7	-1.954419000	-2.917533000	3.266724000	
6	-2.181202000	1.635964000	0.659797000	
7	-1.069970000	3.649013000	1.594309000	
7	-0.078774000	1.750430000	1.958049000	
6	-1.576873000	-2.089567000	2.230101000	
6	-0.142112000	-3.816444000	2.414013000	
1	0.709393000	-4.424581000	2.158275000	
6	-1.060280000	-3.978194000	3.391011000	
1	-1.180563000	-4.744766000	4.136643000	
6	-1.183452000	2.298167000	1.363920000	
6	0.118238000	3.933062000	2.264505000	
1	0.392570000	4.934559000	2.547052000	
6	0.726360000	2.745263000	2.476134000	
1	1.663055000	2.517107000	2.955857000	
7	0.581989000	-0.573396000	0.461930000	
1	-1.739079000	4.321808000	1.263849000	
1	0.251493000	0.801485000	1.660795000	
1	0.199418000	-2.059777000	1.161383000	
1	-2.762374000	-2.754415000	3.840810000	
1	-0.198896000	-2.060062000	-1.161426000	
1	2.763158000	-2.753667000	-3.840819000	
1	1.738224000	4.322306000	-1.263932000	
1	-0.251795000	0.801611000	-1.660811000	
6	3.197368000	-0.446271000	0.914607000	
7	5.051693000	0.726574000	-0.219815000	
$(\text{Im}^b\text{CH})_3\text{P}-\text{NN}-\text{P}(\text{Im}^b\text{CH})_3$				
7	-0.085733000	-0.886423000	-1.111498000	
7	0.817535000	-0.091424000	-1.930324000	
15	-1.498637000	-0.166858000	-0.813235000	
6	-2.125183000	-1.218654000	0.480238000	
7	-4.004876000	0.132007000	1.370136000	
7	-3.360062000	-1.565140000	2.588458000	
6	-3.083838000	-0.894961000	1.398040000	
6	-4.697940000	0.206057000	2.581433000	
6	-4.292833000	-0.831076000	3.347282000	
1	-3.944498000	0.909744000	0.720423000	
1	-2.617396000	-2.091913000	3.026504000	
6	-4.722327000	-1.292876000	4.683884000	
1	-5.439466000	-0.596790000	5.121144000	
1	-5.197501000	-2.280167000	4.646256000	
1	-3.878675000	-1.372495000	5.380710000	
6	-5.716083000	1.256394000	2.799941000	
1	-5.292058000	2.258019000	2.661713000	
1	-6.552844000	1.165966000	2.097305000	
1	-6.123110000	1.203983000	3.810548000	
1	-1.416933000	-1.998779000	0.743245000	
6	-1.310170000	1.551736000	-0.335925000	
7	-3.617436000	2.388418000	-0.635285000	
7	-2.108118000	3.872318000	-0.009859000	
6	-2.257055000	2.524740000	-0.335524000	
6	-4.199505000	3.670104000	-0.739473000	
6	-3.277714000	4.576731000	-0.356009000	
1	-3.817055000	1.625180000	-1.296699000	
1	-1.195262000	4.296555000	-0.078901000	
6	-3.364112000	6.040874000	-0.166953000	
1	-4.341872000	6.414355000	-0.473574000	
1	-3.209199000	6.328435000	0.879269000	
1	-2.610574000	6.573395000	-0.758791000	
6	-5.627216000	3.818817000	-1.095045000	
1	-5.846710000	3.394315000	-2.081161000	
1	-6.280459000	3.306634000	-0.378387000	
1	-5.916958000	4.870274000	-1.118306000	
1	-0.278212000	1.842182000	-0.158521000	
6	-2.773441000	-0.041813000	-2.082543000	
7	-3.913714000	-2.206876000	-1.720858000	
7	-4.202886000	-1.309619000	-3.668780000	
6	-3.559304000	-1.112515000	-2.464206000	
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6	-4.855698000	-2.550763000	-3.690924000	
1	-3.492401000	-2.344213000	-0.803918000	
1	-3.959469000	-0.781921000	-4.490385000	
6	-5.602495000	-3.012269000	-4.880096000	

7	5.588770000	-0.396922000	1.563994000	1	-6.039081000	-3.995536000	-4.700404000
6	4.503611000	-0.072326000	0.766796000	1	-6.419920000	-2.331482000	-5.144800000
6	6.394165000	0.972302000	0.037007000	1	-4.958140000	-3.098521000	-5.762875000
1	6.996808000	1.583240000	-0.612136000	6	-5.172502000	-4.368350000	-1.885424000
6	6.732057000	0.276667000	1.139987000	1	-4.348431000	-5.008082000	-1.551517000
1	7.680905000	0.159858000	1.633487000	1	-5.816907000	-4.195627000	-1.016392000
1	4.443272000	1.238062000	-0.853342000	1	-5.750002000	-4.931551000	-2.619579000
1	5.492742000	-0.892207000	2.432450000	1	-2.510942000	0.644874000	-2.888100000
6	-3.197466000	-0.447037000	-0.914571000	15	2.187711000	-0.078403000	-1.063945000
7	-5.051746000	0.726068000	0.219724000	6	2.703659000	-1.765697000	-0.723871000
7	-5.588913000	-0.397920000	-1.563783000	7	4.975810000	-1.378737000	0.167376000
6	-4.503704000	-0.073032000	-0.766731000	7	4.469779000	-3.447992000	-0.281463000
6	-6.394167000	0.971882000	-0.037204000	6	3.946560000	-2.158387000	-0.317566000
1	-6.996791000	1.582984000	0.611806000	6	6.142694000	-2.129436000	0.324760000
6	-6.732107000	0.276034000	-1.140035000	6	5.839733000	-3.414281000	0.035444000
1	-7.680948000	0.159238000	-1.633550000	1	4.969107000	-0.367115000	0.116168000
1	-4.443267000	1.237563000	0.853201000	1	4.057648000	-4.175962000	-0.842309000
1	-5.492654000	-0.892353000	-2.432708000	6	6.647428000	-4.650780000	0.093435000
1	-2.698564000	2.232680000	-0.088955000	1	7.681735000	-4.422166000	0.354403000
1	-2.936861000	-1.150344000	-1.696675000	1	6.266144000	-5.358068000	0.839559000
1	-2.962674000	-0.521292000	2.499805000	1	6.662543000	-5.178727000	-0.867659000
1	2.698137000	2.233209000	0.088906000	6	7.389954000	-1.488228000	0.793703000
1	2.936508000	-1.149227000	1.696940000	1	7.675204000	-0.650541000	0.145967000
1	2.962681000	-0.520554000	-2.499923000	1	7.285599000	-1.084712000	1.808020000
				1	8.217424000	-2.198969000	0.802181000
				1	2.033342000	-2.511816000	-1.139853000
				6	3.388621000	0.820422000	-2.004586000
				7	4.823412000	1.671654000	-0.169252000
				7	5.411561000	2.221990000	-2.214240000
				6	4.442979000	1.517704000	-1.504942000
				6	5.839082000	2.642578000	-0.075712000
				6	6.201602000	2.980076000	-1.330982000
				1	4.077594000	1.542221000	0.523751000
				1	5.232921000	2.508758000	-3.163610000
				6	7.277298000	3.859156000	-1.837178000
				1	7.791737000	4.354605000	-1.012867000
				1	8.026282000	3.300949000	-2.410786000
				1	6.888694000	4.642646000	-2.498380000
				6	6.394813000	3.027672000	1.239386000
				1	5.626461000	3.444998000	1.899809000
				1	6.829877000	2.168808000	1.764480000
				1	7.176420000	3.780388000	1.127092000
				1	3.256947000	0.784624000	-3.080197000
				6	2.110170000	0.753675000	0.532590000
				7	1.423720000	-1.168862000	1.943206000
				7	0.580092000	0.771563000	2.490951000
				6	1.407450000	0.152282000	1.566570000
				6	0.478785000	-1.397566000	2.944628000
				6	-0.047799000	-0.200852000	3.289248000
				1	1.749499000	-1.847423000	1.255020000
				1	0.075659000	1.597489000	2.198560000
				6	-1.035710000	0.187250000	4.317765000
				1	-1.355099000	-0.682381000	4.896450000
				1	-0.625517000	0.918663000	5.023933000
				1	-1.936352000	0.633419000	3.874058000

				6	0.249194000	-2.754426000	3.487969000
				1	-0.138339000	-3.437479000	2.721578000
				1	1.170432000	-3.204769000	3.874168000
				1	-0.470469000	-2.728337000	4.309877000
				1	1.866139000	1.812417000	0.408555000
$(\text{Im}^c\text{CH})_3\text{P}-\text{NN}-\text{P}(\text{Im}^c\text{CH})_3$				$(\text{Im}^d\text{CH})_3\text{P}-\text{NN}-\text{P}(\text{Im}^d\text{CH})_3$			
15	-1.859535000	0.198186000	-0.586928000	15	-1.497237000	-0.838333000	-0.170360000
6	-1.852823000	0.879888000	-2.230188000	6	-2.369278000	-0.933409000	-1.747654000
7	-1.237199000	3.271808000	-1.813679000	7	-3.776037000	1.102468000	-1.570961000
7	-0.770699000	2.448169000	-3.785234000	7	-4.660785000	-0.607278000	-2.616971000
6	-1.978422000	-1.584641000	-0.828913000	6	-0.619816000	-2.408518000	-0.050145000
7	-1.286150000	-3.914420000	-1.022109000	7	1.490409000	-3.644552000	0.144987000
7	0.075979000	-2.502338000	-1.995820000	7	1.335700000	-2.376185000	-1.628209000
6	-1.320425000	2.111691000	-2.557704000	6	-3.505670000	-0.188340000	-1.981847000
6	-0.623154000	4.267453000	-2.556685000	6	-5.094565000	1.441605000	-1.897145000
1	-0.448180000	5.245786000	-2.142107000	6	-5.647265000	0.381391000	-2.535260000
6	-0.340190000	3.766305000	-3.776082000	6	0.643844000	-2.750843000	-0.497214000
1	0.131385000	4.213917000	-4.634176000	6	2.680605000	-3.793742000	-0.572447000
6	-1.096560000	-2.553542000	-1.260160000	6	2.586004000	-2.991403000	-1.661343000
6	-0.295634000	-4.658700000	-1.641137000	7	0.297450000	0.908930000	-0.739175000
1	-0.269252000	-5.733133000	-1.572141000	15	1.780624000	1.164441000	-0.103428000
6	0.537966000	-3.788334000	-2.243377000	6	1.719319000	2.202858000	1.351873000
1	1.435170000	-3.954519000	-2.815122000	7	-0.212125000	3.696884000	0.864824000
7	0.570735000	0.968032000	-0.288478000	7	0.204978000	3.283479000	2.971852000
15	1.812060000	0.388391000	0.605997000	6	2.901927000	-0.133607000	0.418324000
6	1.736373000	0.973111000	2.286879000	7	4.083250000	-1.779603000	1.760859000
7	0.818294000	3.286762000	2.011618000	7	2.193870000	-1.094841000	2.646678000
7	0.489434000	2.303923000	3.937371000	6	0.636503000	2.993598000	1.688703000
6	2.176967000	-1.366873000	0.757539000	6	-1.161944000	4.384923000	1.624260000
7	1.873241000	-3.775007000	0.957787000	6	-0.895015000	4.145246000	2.931151000
7	0.298402000	-2.601110000	1.929258000	6	3.002992000	-0.929210000	1.533296000
6	1.056177000	2.107215000	2.687880000	6	3.950323000	-2.426524000	2.994191000
6	0.101087000	4.157030000	2.816846000	6	2.781369000	-2.009454000	3.532949000
1	-0.200680000	5.127168000	2.459861000	7	-0.689570000	0.518343000	0.231131000
6	-0.097041000	3.558296000	4.008889000	6	-2.755964000	-0.771273000	1.095736000
1	-0.605505000	3.895984000	4.895726000	7	-4.620299000	-2.210752000	0.280372000
6	1.466543000	-2.462477000	1.196396000	7	-5.167842000	-0.352246000	1.314633000
6	1.007532000	-4.670138000	1.564050000	6	-4.076724000	-1.103798000	0.912933000
1	1.152822000	-5.734837000	1.492044000	6	-6.021426000	-2.135433000	0.312167000
6	0.044795000	-3.946021000	2.167306000	6	-6.357458000	-0.975045000	0.924483000
1	-0.815855000	-4.255843000	2.735500000	6	2.592682000	1.767253000	-1.566946000
7	-0.705221000	0.877195000	0.354436000	7	5.040630000	1.811398000	-1.056918000
6	-3.263203000	0.530543000	0.453509000	7	4.445607000	1.723201000	-3.168804000
7	-5.307568000	-0.493145000	-0.583739000	6	3.926285000	1.774727000	-1.882152000
7	-5.437572000	0.175829000	1.507699000	6	6.210463000	1.759389000	-1.830074000
6	-4.556538000	0.088246000	0.432734000	6	5.844287000	1.697787000	-3.131703000
6	-6.619882000	-0.666752000	-0.151490000	1	3.611072000	-0.393588000	-0.361281000
1	-7.366706000	-1.094526000	-0.798567000	1	1.892954000	1.846401000	-2.392711000
6	-6.699626000	-0.262569000	1.130834000	1	2.321558000	1.859088000	2.189287000
1	-7.522121000	-0.281312000	1.825690000	1	-0.876805000	-2.878229000	0.896219000
6	3.150527000	0.945117000	-0.423850000	1	-2.580189000	0.116252000	1.699477000
7	5.280679000	-0.053005000	0.446675000	1	-2.327428000	-1.897378000	-2.244882000
7	5.280623000	0.731142000	-1.605837000	6	-5.020757000	0.989016000	1.807314000
6	4.460850000	0.558057000	-0.493956000	1	-4.624235000	1.005176000	2.828994000

6	6.557297000	-0.221254000	-0.081154000	1	-4.320277000	1.543422000	1.169217000
1	7.346044000	-0.672312000	0.496378000	1	-5.988311000	1.491315000	1.805638000
6	6.558283000	0.261364000	-1.339346000	6	-3.879764000	-3.444502000	0.141557000
1	7.341658000	0.302889000	-2.077068000	1	-4.473694000	-4.160544000	-0.429146000
6	-5.064269000	0.728039000	2.776494000	1	-2.936471000	-3.274377000	-0.381957000
1	-4.835469000	1.798544000	2.701885000	1	-3.648133000	-3.876348000	1.125553000
1	-5.883094000	0.592638000	3.483165000	6	1.150224000	-4.291105000	1.377607000
1	-4.171113000	0.224540000	3.164189000	1	0.859643000	-3.551222000	2.131878000
6	-4.929654000	-0.438786000	-1.979118000	1	0.312157000	-4.989811000	1.251364000
1	-5.752504000	-0.835384000	-2.575656000	1	2.013442000	-4.838972000	1.756164000
1	-4.718861000	0.592216000	-2.283842000	6	0.063248000	3.947396000	-0.533755000
1	-4.029653000	-1.031615000	-2.160211000	1	-0.415895000	4.882852000	-0.831377000
6	-2.412395000	-4.437759000	-0.308133000	1	1.146886000	4.038878000	-0.666607000
1	-2.451603000	-4.034409000	0.710218000	1	-0.261531000	3.114144000	-1.161762000
1	-3.35526000	-4.182139000	-0.808633000	6	0.933654000	2.910273000	4.150501000
1	-2.322913000	-5.522663000	-0.247163000	1	1.847964000	3.506136000	4.273950000
6	1.436749000	3.672212000	0.759827000	1	0.305873000	3.049666000	5.030707000
1	1.380796000	4.760257000	0.671899000	1	1.225850000	1.858973000	4.096452000
1	2.487388000	3.363769000	0.768444000	6	5.008891000	2.299410000	0.304016000
1	0.961297000	3.172285000	-0.089414000	1	5.750852000	3.094510000	0.433423000
6	0.524246000	1.328181000	4.987923000	1	4.016587000	2.703581000	0.515727000
1	1.551700000	1.122189000	5.309455000	1	5.199441000	1.505583000	1.033545000
1	-0.038605000	1.703407000	5.842561000	6	3.609864000	1.541418000	-4.320594000
1	0.077331000	0.385391000	4.656836000	1	2.924747000	0.698620000	-4.165379000
6	4.976129000	-0.136784000	1.858307000	1	2.998545000	2.429345000	-4.520409000
1	5.894814000	0.015299000	2.430278000	1	4.226601000	1.344366000	-5.197126000
1	4.256029000	0.644049000	2.118389000	6	-2.730752000	2.073194000	-1.300738000
1	4.527621000	-1.097720000	2.126588000	1	-2.990885000	3.024474000	-1.778181000
6	4.810313000	1.292759000	-2.838368000	1	-2.556390000	2.213346000	-0.230444000
1	3.905753000	0.771716000	-3.174194000	1	-1.787014000	1.698358000	-1.709539000
1	4.559932000	2.354838000	-2.730042000	6	-4.818063000	-1.940105000	-3.121627000
1	5.584313000	1.191786000	-3.599212000	1	-4.513004000	-2.667043000	-2.359599000
6	-1.910556000	3.508436000	-0.553810000	1	-5.860791000	-2.115137000	-3.386909000
1	-2.013687000	4.588304000	-0.418573000	1	-4.201870000	-2.110246000	-4.012171000
1	-2.904712000	3.051097000	-0.586753000	6	0.808313000	-0.688761000	2.758488000
1	-1.372372000	3.046365000	0.278700000	1	0.665051000	0.018933000	3.581627000
6	-0.656631000	1.531239000	-4.881942000	1	0.440231000	-0.218986000	1.837634000
1	-1.641377000	1.212336000	-5.242565000	1	0.173201000	-1.562097000	2.949095000
1	-0.128170000	2.018316000	-5.701416000	6	0.784543000	-1.524484000	-2.655854000
1	-0.099701000	0.637640000	-4.582759000	1	1.514279000	-1.423077000	-3.459456000
6	-0.527950000	-1.536273000	2.443684000	1	-0.128592000	-1.969973000	-3.063224000
1	-0.194100000	-1.226107000	3.441245000	1	0.552566000	-0.530061000	-2.239528000
1	-0.531866000	-0.661538000	1.774203000	6	-7.676717000	-0.337595000	1.122475000
1	-1.557314000	-1.899816000	2.513791000	1	-7.871620000	-0.098251000	2.173861000
6	0.713536000	-1.317615000	-2.515589000	1	-7.769700000	0.599051000	0.556053000
1	1.783996000	-1.518223000	-2.617930000	1	-8.474307000	-1.000613000	0.784029000
1	0.306574000	-1.053555000	-3.499382000	6	-6.878171000	-3.198110000	-0.259089000
1	0.602485000	-0.463347000	-1.828591000	1	-6.774897000	-4.153032000	0.270125000
6	3.070603000	-4.107151000	0.245497000	1	-7.928983000	-2.909322000	-0.201254000
1	3.036836000	-3.723480000	-0.780855000	1	-6.647529000	-3.394705000	-1.312929000
1	3.955502000	-3.679416000	0.735383000	6	-7.026797000	0.155251000	-3.016669000
1	3.173823000	-5.191849000	0.206778000	1	-7.515615000	-0.675575000	-2.489751000
1	2.762047000	1.507640000	-1.267464000	1	-7.634744000	1.046317000	-2.852811000
1	1.887431000	0.221255000	3.056480000	1	-7.066816000	-0.074475000	-4.087668000
1	2.985120000	-1.641356000	0.085454000	6	-5.664169000	2.763331000	-1.552026000

1	-2.749123000	-1.990645000	-0.179158000	1	-5.550878000	2.989841000	-0.485112000
1	-1.907979000	0.162111000	-3.043561000	1	-5.185397000	3.584535000	-2.098633000
1	-2.934638000	1.033425000	1.358205000	1	-6.729150000	2.796282000	-1.789001000
				6	3.586076000	-2.679756000	-2.706372000
				1	3.233895000	-2.914047000	-3.717831000
				1	3.855954000	-1.614298000	-2.697068000
				1	4.500007000	-3.253249000	-2.539342000
				6	3.765068000	-4.690092000	-0.119293000
				1	4.605915000	-4.648293000	-0.814071000
				1	4.144558000	-4.415805000	0.873352000
				1	3.443966000	-5.737599000	-0.060393000
				6	2.117590000	-2.385720000	4.800133000
				1	2.748556000	-3.064888000	5.375553000
				1	1.907966000	-1.512772000	5.428754000
				1	1.157037000	-2.889072000	4.635441000
				6	4.980539000	-3.346945000	3.522652000
				1	5.948588000	-2.853155000	3.674564000
				1	4.667423000	-3.747867000	4.487719000
				1	5.163195000	-4.201528000	2.858791000
				6	-1.591819000	4.587805000	4.158331000
				1	-0.943607000	5.174646000	4.820070000
				1	-2.444788000	5.217359000	3.901473000
				1	-1.972866000	3.745470000	4.749072000
				6	-2.240751000	5.186807000	1.004253000
				1	-2.841017000	4.595101000	0.303471000
				1	-2.912419000	5.573249000	1.772633000
				1	-1.858724000	6.049852000	0.446512000
				6	7.549701000	1.762351000	-1.201400000
				1	8.327377000	1.638244000	-1.956400000
				1	7.763216000	2.693965000	-0.664468000
				1	7.658898000	0.948561000	-0.474526000
				6	6.660893000	1.588841000	-4.359664000
				1	6.484118000	2.422060000	-5.049738000
				1	7.722382000	1.592892000	-4.108807000
				1	6.461362000	0.665120000	-4.916974000
				6	5.235402000	-1.794725000	0.906150000
				1	4.976908000	-2.156332000	-0.096984000
				1	5.653836000	-0.785256000	0.793155000
				1	5.996104000	-2.453286000	1.326451000

Table S7: Cartesian coordinates of optimized geometries of transition states for the activation of N₂ at M06L/6-311++G(d,p) level DFT. Atomic number followed by X, Y, Z coordinates in Å.

ts1				ts2			
15	-2.012109000	0.138798000	-0.420113000	15	2.074900000	-0.270176000	-0.596846000
7	-2.234977000	1.089393000	-1.733485000	7	1.997285000	-1.146146000	-1.943931000
7	-0.251383000	2.498233000	-1.764579000	7	-0.019135000	-2.474853000	-1.726564000
7	-1.957896000	3.081487000	-2.973801000	7	1.480061000	-3.094170000	-3.184091000
7	-2.408601000	-1.407903000	-0.934924000	7	2.461072000	1.291571000	-0.997251000
7	-1.718110000	-3.501080000	-1.813212000	7	1.789480000	3.427009000	-1.783212000
7	-0.155110000	-2.010606000	-1.623768000	7	0.198756000	1.975399000	-1.572600000
6	-1.522528000	2.125439000	-2.088228000	6	1.200995000	-2.161369000	-2.220829000
6	0.106840000	3.627621000	-2.472690000	6	-0.512381000	-3.567996000	-2.405376000
1	1.081062000	4.074730000	-2.370859000	1	-1.482017000	-3.980426000	-2.179794000

6	-0.951961000	4.005452000	-3.225061000	6	0.410689000	-3.970515000	-3.312922000
1	-1.087796000	4.837021000	-3.894296000	1	0.417042000	-4.784673000	-4.017038000
6	-1.489356000	-2.205502000	-1.418472000	6	1.539499000	2.131054000	-1.421500000
6	-0.530051000	-4.110436000	-2.201616000	6	0.604102000	4.080496000	-2.099053000
1	-0.491120000	-5.132471000	-2.535314000	1	0.579906000	5.116163000	-2.388368000
6	0.435267000	-3.173178000	-2.077619000	6	-0.380709000	3.166451000	-1.959838000
1	1.492751000	-3.226951000	-2.273322000	1	-1.445387000	3.254613000	-2.091370000
7	0.612179000	0.337844000	-0.464022000	7	-0.583585000	-0.382887000	-0.399858000
15	2.028698000	0.142845000	0.345478000	15	-1.956478000	-0.068715000	0.496143000
7	2.300669000	1.085064000	1.673692000	7	-2.079594000	-0.872342000	1.929461000
7	0.277443000	2.438306000	1.806343000	7	-0.310463000	-2.553393000	1.852579000
7	1.994136000	3.009459000	3.007281000	7	-1.909071000	-2.783481000	3.300582000
7	2.395048000	-1.412786000	0.845235000	7	-2.274409000	1.514634000	0.769875000
7	1.638804000	-3.389391000	1.926356000	7	-1.556964000	3.593749000	1.656319000
7	0.144747000	-1.817426000	1.660455000	7	-0.078311000	1.950154000	1.720429000
6	1.568392000	2.076939000	2.087754000	6	-1.471893000	-1.962191000	2.285382000
6	-0.095233000	3.523686000	2.576259000	6	-0.016611000	-3.664462000	2.623363000
1	-1.081786000	3.950490000	2.514998000	1	0.865057000	-4.258057000	2.453210000
6	0.969854000	3.892470000	3.322587000	6	-1.013803000	-3.819835000	3.521613000
1	1.097879000	4.696375000	4.026251000	1	-1.174122000	-4.570147000	4.275856000
6	1.450155000	-2.120000000	1.436995000	6	-1.331288000	2.269767000	1.365887000
6	0.438062000	-3.891672000	2.416519000	6	-0.399705000	4.133217000	2.199863000
1	0.359077000	-4.876748000	2.843608000	1	-0.336431000	5.162205000	2.513398000
6	-0.473267000	-2.904806000	2.241094000	6	0.486313000	3.099406000	2.226467000
1	-1.522462000	-2.887168000	2.490029000	1	1.504958000	3.110960000	2.588161000
7	-0.586939000	0.289224000	0.399258000	7	0.673754000	-0.438162000	0.360117000
1	2.517599000	-3.874724000	1.874485000	1	-2.422925000	4.074240000	1.479805000
1	-0.350050000	-0.823712000	1.186016000	1	0.658026000	0.321474000	1.072618000
1	-0.337188000	1.766459000	1.287622000	1	0.335895000	-2.017487000	1.251433000
1	2.915543000	2.978249000	3.407952000	1	-2.748700000	-2.583258000	3.816065000
1	0.360592000	1.794019000	-1.256550000	1	-0.516767000	-1.627954000	-1.107887000
1	-2.873631000	3.050748000	-3.387852000	1	2.329700000	-3.084670000	-3.722832000
1	-2.616863000	-3.941891000	-1.725988000	1	2.704655000	3.839097000	-1.733685000
1	0.331798000	-1.116493000	-1.334612000	1	-0.298255000	1.096813000	-1.266149000
7	-3.098972000	0.519292000	0.760275000	7	3.211738000	-0.805540000	0.454448000
7	-4.974413000	-0.765540000	-0.114941000	7	4.987555000	0.787559000	-0.032743000
7	-5.310149000	0.516293000	1.599648000	7	5.391422000	-0.812068000	1.367671000
6	-4.330170000	0.112954000	0.721023000	6	4.405361000	-0.301727000	0.558807000
6	-6.294244000	-0.931085000	0.268991000	6	6.281401000	0.963210000	0.425612000
1	-6.969276000	-1.584091000	-0.256633000	1	6.908590000	1.768677000	0.085226000
6	-6.510613000	-0.126506000	1.332102000	6	6.540058000	-0.036798000	1.295869000
1	-7.403140000	0.059544000	1.902945000	1	7.429143000	-0.272469000	1.853321000
1	-4.401630000	-1.317870000	-0.754006000	1	4.392828000	1.390635000	-0.602604000
1	-5.122904000	1.169967000	2.340211000	1	5.241111000	-1.623473000	1.942341000
7	3.122473000	0.536140000	-0.826304000	7	-3.095410000	-0.649426000	-0.551614000
7	4.955945000	-0.826625000	0.015933000	7	-4.804101000	1.022164000	-0.100432000
7	5.337152000	0.496925000	-1.658801000	7	-5.294473000	-0.618704000	-1.429438000
6	4.341048000	0.095840000	-0.795378000	6	-4.272421000	-0.112195000	-0.657823000
6	6.271344000	-1.018904000	-0.368552000	6	-6.098900000	1.224730000	-0.541056000
1	6.925031000	-1.706858000	0.139379000	1	-6.691862000	2.064015000	-0.220626000
6	6.517052000	-0.189510000	-1.406201000	6	-6.413300000	0.201156000	-1.365543000
1	7.417762000	-0.012317000	-1.967015000	1	-7.323372000	-0.024708000	-1.892702000
1	4.358648000	-1.376807000	0.637838000	1	-4.158027000	1.621296000	0.427666000
1	5.173388000	1.178933000	-2.378848000	1	-5.189061000	-1.461356000	-1.967264000
ts3				ts4			
15	-1.984401000	0.151850000	-0.739249000	15	-1.783781000	0.138772000	-1.288887000

7	-1.622668000	0.985199000	-2.053111000	7	-1.230007000	1.004023000	-2.480109000
7	-0.110721000	2.755948000	-1.308481000	7	0.152851000	2.771057000	-1.561197000
7	-1.155093000	2.955749000	-3.244649000	7	-1.052081000	3.200771000	-3.359462000
7	-2.319834000	-1.408010000	-1.122927000	7	-1.834413000	-1.453585000	-1.531921000
7	-1.540617000	-3.465248000	-2.014019000	7	-0.759742000	-3.448537000	-2.216479000
7	0.007900000	-1.992274000	-1.516888000	7	0.577726000	-1.782259000	-1.668958000
6	-1.002064000	2.166107000	-2.131975000	6	-0.736036000	2.258649000	-2.419318000
6	0.287816000	3.922164000	-1.932901000	6	0.387362000	4.064152000	-1.969926000
1	1.008768000	4.583829000	-1.472937000	1	1.070611000	4.706698000	-1.434460000
6	-0.340381000	4.068139000	-3.130003000	6	-0.342595000	4.356522000	-3.082343000
1	-0.294615000	4.831612000	-3.888625000	1	-0.424648000	5.242395000	-3.689853000
6	-1.323615000	-2.202029000	-1.531112000	6	-0.702912000	-2.145535000	-1.802371000
6	-0.321713000	-4.066274000	-2.295619000	6	0.531747000	-3.929411000	-2.349487000
1	-0.250429000	-5.069622000	-2.679698000	1	0.740914000	-4.936538000	-2.669010000
6	0.616740000	-3.138183000	-1.978589000	6	1.332058000	-2.883411000	-2.006686000
1	1.691565000	-3.216137000	-2.042827000	1	2.411838000	-2.851824000	-1.989244000
7	0.619214000	0.154357000	-0.244386000	7	0.717840000	0.499819000	-0.147468000
15	2.013433000	0.079847000	0.917036000	15	1.867328000	0.256694000	1.330136000
7	1.597456000	0.885907000	2.236803000	7	1.239186000	1.029046000	2.551480000
7	0.486271000	2.920437000	1.441040000	7	-0.571537000	2.418793000	1.753219000
7	0.972942000	2.732660000	3.539571000	7	0.537234000	3.077277000	3.524585000
7	2.389799000	-1.458315000	1.148159000	7	2.069969000	-1.325434000	1.471616000
7	1.760875000	-3.594641000	1.978421000	7	1.239906000	-3.448078000	2.118700000
7	0.153054000	-2.081242000	1.865065000	7	-0.285243000	-1.921143000	1.660393000
6	1.058761000	2.078102000	2.340717000	6	0.450822000	2.109407000	2.565656000
6	0.024919000	4.055583000	2.077202000	6	-1.121693000	3.598137000	2.200243000
1	-0.483664000	4.833464000	1.533648000	1	-1.955282000	4.057167000	1.692588000
6	0.329184000	3.950240000	3.390267000	6	-0.451172000	4.023761000	3.303142000
1	0.156570000	4.616812000	4.216461000	1	-0.574240000	4.884989000	3.937460000
6	1.448261000	-2.302117000	1.657337000	6	1.025755000	-2.149175000	1.750437000
6	0.603815000	-4.225317000	2.405591000	6	0.012844000	-4.071569000	2.263716000
1	0.592966000	-5.258194000	2.711642000	1	-0.075947000	-5.106139000	2.550097000
6	-0.365047000	-3.270626000	2.322594000	6	-0.905824000	-3.108190000	1.976541000
1	-1.413197000	-3.368457000	2.565171000	1	-1.982703000	-3.194500000	1.980698000
7	-0.680921000	0.318525000	0.396937000	7	-0.697167000	0.424421000	0.179732000
1	2.683528000	-3.993193000	1.928323000	1	2.147949000	-3.850497000	2.281338000
1	-0.712135000	-0.425141000	1.111387000	1	-0.780843000	-0.415013000	0.810926000
1	0.256342000	2.697161000	0.446654000	1	-0.854967000	1.434534000	0.839770000
1	1.319654000	2.323668000	4.390854000	1	1.232807000	3.076427000	4.252162000
1	0.746135000	1.000551000	-0.820938000	1	0.820033000	1.445601000	-0.615675000
1	-1.759365000	2.711571000	-4.011795000	1	-1.706717000	3.045925000	-4.108482000
1	-2.454165000	-3.863238000	-2.149004000	1	-1.613380000	-3.938209000	-2.426454000
1	0.530786000	-0.829752000	-0.906426000	1	0.899172000	-0.290274000	-0.837959000
7	-3.210017000	0.751244000	0.168896000	7	-3.176383000	0.658881000	-0.604070000
7	-4.830787000	-1.038530000	-0.135645000	7	-4.130481000	-1.509283000	-0.048164000
7	-5.423004000	0.707389000	0.999508000	7	-5.185921000	0.269471000	0.585081000
6	-4.363827000	0.169391000	0.307948000	6	-4.060363000	-0.145233000	-0.079059000
6	-6.131118000	-1.247008000	0.285197000	6	-5.267898000	-1.926752000	0.617997000
1	-6.679031000	-2.140794000	0.041910000	1	-5.508973000	-2.967322000	0.748964000
6	-6.507480000	-0.158512000	0.992250000	6	-5.929424000	-0.818839000	1.019287000
1	-7.437369000	0.079066000	1.477817000	1	-6.848629000	-0.705851000	1.566124000
1	-4.169049000	-1.637152000	-0.640142000	1	-3.388734000	-2.027606000	-0.530195000
1	-5.364250000	1.605945000	1.446911000	1	-5.386056000	1.243007000	0.739719000
7	3.131332000	0.852684000	0.014762000	7	3.184979000	0.959842000	0.680548000
7	4.597615000	-1.034047000	-0.430969000	7	4.271061000	-1.055010000	-0.147111000
7	5.089952000	0.879364000	-1.312546000	7	5.132625000	0.859956000	-0.660514000
6	4.166286000	0.258309000	-0.514818000	6	4.094561000	0.287037000	0.022839000

6	5.755861000	-1.210537000	-1.166297000	6	5.387139000	-1.307087000	-0.923603000
1	6.258103000	-2.159968000	-1.229695000	1	5.699373000	-2.305713000	-1.174992000
6	6.066744000	-0.018158000	-1.720510000	6	5.927208000	-0.112186000	-1.250278000
1	6.884055000	0.272084000	-2.356361000	1	6.792682000	0.132954000	-1.839748000
1	4.035266000	-1.684474000	0.126320000	1	3.606579000	-1.682059000	0.316452000
1	5.009980000	1.849182000	-1.567932000	1	5.233667000	1.857994000	-0.738998000

Table S8: Cartesian coordinates of optimized geometries of products for the activation of N₂ at M06L/6-311++G(d,p) level DFT. Atomic number followed by X, Y, Z coordinates in Å.

$(\text{Im}^{\text{a}}\text{N}')_3\text{P}-\text{NNH}-\text{P}(\text{Im}^{\text{a}}\text{N}')_3$				$(\text{Im}^{\text{a}}\text{N}')_3\text{P}-\text{HNNH}-\text{P}(\text{Im}^{\text{a}}\text{N}')_3$			
15	2.074366000	-0.271699000	-0.564902000	15	2.005062000	-0.076874000	-0.578150000
7	2.042518000	-1.203793000	-1.883234000	7	1.828230000	-0.876859000	-1.947004000
7	0.036615000	-2.566361000	-1.734352000	7	0.487895000	-2.800850000	-1.249793000
7	1.611905000	-3.187632000	-3.092408000	7	1.567087000	-2.866068000	-3.176260000
7	2.455579000	1.272607000	-1.023457000	7	2.410001000	1.497325000	-0.950565000
7	1.780156000	3.388031000	-1.859605000	7	1.772519000	3.650837000	-1.708159000
7	0.192768000	1.936835000	-1.616400000	7	0.162035000	2.216021000	-1.553585000
6	1.278421000	-2.229134000	-2.170710000	6	1.317226000	-2.114864000	-2.055753000
6	-0.410622000	-3.685361000	-2.405413000	6	0.224274000	-3.994840000	-1.889281000
1	-1.383136000	-4.106730000	-2.215661000	1	-0.429621000	-4.733223000	-1.446261000
6	0.566678000	-4.087651000	-3.250829000	6	0.876474000	-4.061265000	-3.081690000
1	0.622666000	-4.919951000	-3.930479000	1	0.918857000	-4.815301000	-3.849924000
6	1.531164000	2.101078000	-1.467870000	6	1.506868000	2.347820000	-1.372760000
6	0.593132000	4.031072000	-2.191067000	6	0.602486000	4.322534000	-2.039513000
1	0.566632000	5.059984000	-2.503558000	1	0.595296000	5.361382000	-2.317705000
6	-0.388908000	3.116973000	-2.031088000	6	-0.396463000	3.420626000	-1.933964000
1	-1.453936000	3.199082000	-2.164618000	1	-1.455732000	3.526807000	-2.091787000
7	-0.584067000	-0.378233000	-0.408303000	7	-0.639187000	-0.184158000	-0.374344000
15	-1.957316000	-0.054094000	0.463789000	15	-2.055802000	-0.115171000	0.633707000
7	-2.119179000	-0.857467000	1.899819000	7	-1.790209000	-0.847890000	2.055067000
7	-0.342104000	-2.532158000	1.857428000	7	-0.474943000	-2.827525000	1.431124000
7	-1.955543000	-2.753177000	3.292976000	7	-1.190058000	-2.624409000	3.462702000
7	-2.289149000	1.530123000	0.744297000	7	-2.549648000	1.409603000	0.832888000
7	-1.563472000	3.624037000	1.586543000	7	-2.125234000	3.570637000	1.723476000
7	-0.086857000	1.979278000	1.674814000	7	-0.402979000	2.184378000	1.667086000
6	-1.511348000	-1.939110000	2.273130000	6	-1.190310000	-1.997326000	2.242631000
6	-0.048407000	-3.629056000	2.649920000	6	-0.013025000	-3.915383000	2.145356000
1	0.838872000	-4.219548000	2.498531000	1	0.598393000	-4.669864000	1.680181000
6	-1.054439000	-3.778817000	3.538935000	6	-0.459351000	-3.800878000	3.416040000
1	-1.218344000	-4.520981000	4.300542000	1	-0.333808000	-4.437420000	4.273899000
6	-1.342256000	2.293548000	1.319458000	6	-1.703942000	2.306773000	1.396686000
6	-0.401144000	4.172914000	2.109943000	6	-1.041871000	4.276628000	2.224601000
1	-0.334454000	5.207496000	2.403876000	1	-1.125139000	5.299602000	2.552536000
6	0.482887000	3.138008000	2.152754000	6	-0.000976000	3.398914000	2.173682000
1	1.503534000	3.154974000	2.508992000	1	1.022880000	3.568320000	2.475365000
7	0.663450000	-0.426016000	0.367892000	7	0.609736000	-0.232305000	0.390440000
1	-2.426203000	4.104565000	1.395150000	1	-3.075585000	3.893642000	1.652614000
1	0.648028000	0.342634000	1.072816000	1	0.538587000	0.521881000	1.091183000
1	0.313342000	-1.991679000	1.270444000	1	-0.145539000	-2.619627000	0.466699000
1	-2.796805000	-2.546321000	3.803060000	1	-1.647771000	-2.218937000	4.261280000
1	-0.498017000	-1.823040000	-1.175240000	1	-0.676244000	-1.065811000	-0.896301000
1	2.489581000	-3.180225000	-3.583688000	1	2.157988000	-2.554964000	-3.929429000
1	2.693897000	3.804199000	-1.817302000	1	2.693620000	4.047436000	-1.646708000
1	-0.301783000	1.057786000	-1.284192000	1	-0.350267000	1.356077000	-1.279627000

7	3.203971000	-0.768272000	0.511232000	7	3.136456000	-0.629339000	0.472830000
7	4.968784000	0.830591000	0.002929000	7	4.959498000	0.886855000	-0.084588000
7	5.367411000	-0.719065000	1.459758000	7	5.345981000	-0.727919000	1.304275000
6	4.389792000	-0.246243000	0.619027000	6	4.351959000	-0.177775000	0.530223000
6	6.252150000	1.036986000	0.477735000	6	6.276316000	1.006027000	0.324368000
1	6.875412000	1.839170000	0.122711000	1	6.925457000	1.782727000	-0.040997000
6	6.507462000	0.068299000	1.383715000	6	6.523695000	-0.004428000	1.186129000
1	7.389287000	-0.138466000	1.963697000	1	7.422617000	-0.278000000	1.709597000
1	4.376184000	1.407182000	-0.596292000	1	4.373049000	1.515340000	-0.633853000
1	5.214760000	-1.510612000	2.060978000	1	5.184673000	-1.540323000	1.874606000
7	-3.097128000	-0.625189000	-0.593658000	7	-3.096453000	-0.942001000	-0.326013000
7	-4.825615000	1.004752000	-0.068421000	7	-4.876368000	0.709032000	-0.428169000
7	-5.310644000	-0.606378000	-1.436078000	7	-5.170723000	-1.183130000	-1.438812000
6	-4.283855000	-0.104729000	-0.666006000	6	-4.263608000	-0.487486000	-0.679151000
6	-6.129329000	1.199196000	-0.485287000	6	-6.121758000	0.756111000	-1.027948000
1	-6.730469000	2.019752000	-0.132962000	1	-6.766752000	1.613952000	-0.949514000
6	-6.440860000	0.193792000	-1.333061000	6	-6.311572000	-0.423698000	-1.658811000
1	-7.355781000	-0.032289000	-1.851766000	1	-7.145219000	-0.790787000	-2.230668000
1	-4.176739000	1.604601000	0.456958000	1	-4.340817000	1.407563000	0.097676000
1	-5.201147000	-1.432862000	-1.997434000	1	-4.981810000	-2.110398000	-1.779458000
(Im^aN'')₃P-H₂NNH-P(Im^aN'')₃				(Im^aN'')₃P-H₂NNH₂-P(Im^aN'')₃			
15	-1.629971000	-0.174503000	-1.420152000	15	-1.854572000	0.166197000	-1.328827000
7	-1.356559000	0.802552000	-2.638097000	7	-1.243772000	0.956766000	-2.535643000
7	-0.204314000	2.746380000	-1.722961000	7	0.227913000	2.683548000	-1.693013000
7	-1.417465000	2.975926000	-3.554456000	7	-1.034328000	3.146054000	-3.442209000
7	-1.279200000	-1.727338000	-1.748277000	7	-1.948905000	-1.429233000	-1.461956000
7	0.170983000	-3.190345000	-2.920962000	7	-0.971432000	-3.477793000	-2.138080000
7	1.141273000	-1.496306000	-1.895575000	7	0.442986000	-1.854891000	-1.657741000
6	-1.007188000	2.097604000	-2.584178000	6	-0.708893000	2.200152000	-2.511199000
6	-0.124101000	4.047601000	-2.169129000	6	0.483091000	3.968910000	-2.111355000
1	0.468325000	4.784592000	-1.645676000	1	1.203850000	4.591036000	-1.601891000
6	-0.862374000	4.218072000	-3.300584000	6	-0.281155000	4.280909000	-3.195323000
1	-1.037034000	5.069803000	-3.936832000	1	-0.360887000	5.167423000	-3.802148000
6	-0.042218000	-2.071003000	-2.159916000	6	-0.851082000	-2.172152000	-1.751405000
6	1.528573000	-3.313507000	-3.168093000	6	0.296047000	-4.010543000	-2.295555000
1	1.937240000	-4.120553000	-3.753251000	1	0.457428000	-5.030622000	-2.601375000
6	2.100370000	-2.258040000	-2.526356000	6	1.145234000	-2.989664000	-1.995276000
1	3.148541000	-1.999043000	-2.476424000	1	2.225305000	-2.999073000	-2.009049000
7	0.664435000	0.628268000	-0.233887000	7	0.704634000	0.462625000	-0.168313000
15	1.696351000	0.570564000	1.288572000	15	1.854339000	0.164734000	1.328554000
7	1.248827000	1.771628000	2.237770000	7	1.243218000	0.954019000	2.536041000
7	-0.760199000	2.853666000	1.382056000	7	-0.228513000	2.681629000	1.695295000
7	0.328610000	3.801070000	2.989365000	7	1.035372000	3.143163000	3.443535000
7	1.649412000	-0.908276000	1.883824000	7	1.948569000	-1.430829000	1.459950000
7	0.731758000	-2.410028000	3.476587000	7	0.971148000	-3.479318000	2.136453000
7	-0.720448000	-1.177435000	2.361568000	7	-0.443312000	-1.856593000	1.655626000
6	0.335055000	2.705169000	2.170581000	6	0.708817000	2.197655000	2.512524000
6	-1.422869000	4.024293000	1.689843000	6	-0.482900000	3.966943000	2.114218000
1	-2.308313000	4.327375000	1.158836000	1	-1.203865000	4.589461000	1.605528000
6	-0.749879000	4.622969000	2.697769000	6	0.282330000	4.278319000	3.197678000
1	-0.933067000	5.541448000	3.226387000	1	0.362836000	5.164602000	3.804736000
6	0.573647000	-1.430949000	2.534919000	6	0.850746000	-2.173779000	1.749478000
6	-0.522355000	-2.790424000	3.922771000	6	-0.296308000	-4.011995000	2.294277000
1	-0.658516000	-3.556814000	4.667739000	1	-0.457666000	-5.032024000	2.600277000
6	-1.395195000	-2.015794000	3.218830000	6	-1.145528000	-2.991262000	1.993588000
1	-2.474764000	-2.016836000	3.265149000	1	-2.225597000	-3.000730000	2.007327000

7	-0.762547000	0.443646000	-0.014814000	7	-0.705118000	0.462331000	0.168189000
1	1.622059000	-2.738053000	3.813256000	1	1.849097000	-3.940548000	2.307705000
1	-0.888927000	-0.188249000	0.799208000	1	-0.828346000	-0.346399000	0.845516000
1	-1.029868000	2.133606000	0.687438000	1	-0.846576000	1.388444000	0.664686000
1	1.049269000	3.959414000	3.673040000	1	1.729196000	3.010051000	4.160869000
1	0.706780000	1.557820000	-0.737161000	1	0.846040000	1.389321000	-0.663619000
1	-2.028931000	2.717752000	-4.311254000	1	-1.727563000	3.013369000	-4.160190000
1	-0.571206000	-3.743289000	-3.316333000	1	-1.849371000	-3.939375000	-2.308418000
1	1.029115000	-0.136581000	-0.892874000	1	0.827985000	-0.345201000	-0.846623000
7	-3.141931000	-0.096576000	-0.776735000	7	-3.200009000	0.782584000	-0.644573000
7	-3.371143000	-2.437899000	-0.147924000	7	-4.153802000	-1.301223000	0.173479000
7	-4.928822000	-1.057188000	0.442624000	7	-5.125636000	0.553093000	0.713436000
6	-3.727585000	-1.119226000	-0.222504000	6	-4.060584000	0.051159000	0.014921000
6	-4.323568000	-3.168168000	0.535914000	6	-5.245822000	-1.627982000	0.956283000
1	-4.225439000	-4.226651000	0.703883000	1	-5.495074000	-2.646073000	1.199945000
6	-5.298908000	-2.310828000	0.910810000	6	-5.854670000	-0.471324000	1.299386000
1	-6.208205000	-2.474400000	1.461715000	1	-6.728546000	-0.285235000	1.898024000
1	-2.515548000	-2.719514000	-0.637156000	1	-3.457338000	-1.883009000	-0.301882000
1	-5.428809000	-0.192632000	0.559041000	1	-5.288505000	1.542229000	0.799984000
7	3.130162000	0.888005000	0.597660000	7	3.199573000	0.781820000	0.644679000
7	3.913732000	-1.409299000	0.384097000	7	4.154342000	-1.301372000	-0.173753000
7	5.074050000	0.163068000	-0.536667000	7	5.125773000	0.553453000	-0.712691000
6	3.941032000	-0.059476000	0.196715000	6	4.060669000	0.050895000	-0.014725000
6	4.994547000	-2.011467000	-0.231312000	6	5.246486000	-1.627472000	-0.956672000
1	5.145513000	-3.076543000	-0.211984000	1	5.496134000	-2.645400000	-1.200602000
6	5.724968000	-1.031763000	-0.808470000	6	5.855063000	-0.470486000	-1.299160000
1	6.635153000	-1.073112000	-1.379806000	1	6.729069000	-0.283897000	-1.897453000
1	3.130562000	-1.808257000	0.905803000	1	3.457611000	-1.883531000	0.300785000
1	5.334371000	1.082772000	-0.851102000	1	5.288122000	1.542687000	-0.799106000