

Synthesis and Characterization of Phosphorous(III) Diisocyanate and Triisocyanate

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Computed atomic coordinates (in Angstroms) and energies (in Hartrees) for all optimized structures.

syn-syn-CIP(NCO)₂

B3LYP/6-311+G(3df)

N	-0.03493400	-0.71114700	1.26093000
P	0.65608300	0.17483900	0.00000000
N	-0.03493400	-0.71114700	-1.26093000
C	0.02200400	-0.79184500	2.46368400
C	0.02200400	-0.79184500	-2.46368400
O	0.02200400	-0.93318700	-3.61609300
O	0.02200400	-0.93318700	3.61609300
Cl	-0.58637000	1.86862300	0.00000000
Zero-point correction=			0.029627
Thermal correction to Energy=			0.038098
Thermal correction to Enthalpy=			0.039042
Thermal correction to Gibbs Free Energy=			-0.006690
Sum of electronic and zero-point Energies=			-1137.938835
Sum of electronic and thermal Energies=			-1137.930364
Sum of electronic and thermal Enthalpies=			-1137.929420
Sum of electronic and thermal Free Energies=			-1137.975152

anti-syn-CIP(NCO)₂

B3LYP/6-311+G(3df)

P	0.04657900	0.46003800	0.89155900
N	-1.45294900	-0.28444100	0.70537000
N	1.00719300	-0.64310800	0.02002200
Cl	-0.11895900	1.99484300	-0.53543800
C	-2.09698500	-0.98138500	-0.04348100
O	-2.77871900	-1.65501500	-0.69450600
O	3.27513700	-1.22012800	-0.33818800
C	2.17574900	-0.90510100	-0.13770800
Zero-point correction=			0.029440
Thermal correction to Energy=			0.038028
Thermal correction to Enthalpy=			0.038972
Thermal correction to Gibbs Free Energy=			-0.008503
Sum of electronic and zero-point Energies=			-1137.936975
Sum of electronic and thermal Energies=			-1137.928387
Sum of electronic and thermal Enthalpies=			-1137.927443
Sum of electronic and thermal Free Energies=			-1137.974918

syn-syn-syn-P(NCO)₃

B3LYP/6-311+G(3df)

N	-0.00070700	1.48111200	-0.33271300
P	0.00000000	0.00000000	0.49825700

N	-1.28232700	-0.74116800	-0.33271300
N	1.28303400	-0.73994400	-0.33271300
C	2.30622700	-1.33113500	-0.09507800
C	-0.00031600	2.66281800	-0.09507800
C	-2.30591000	-1.33168300	-0.09507800
O	0.00000000	3.81598800	0.05102100
O	3.30474300	-1.90799400	0.05102100
O	-3.30474300	-1.90799400	0.05102100
Zero-point correction=			0.042050
Thermal correction to Energy=			0.052187
Thermal correction to Enthalpy=			0.053131
Thermal correction to Gibbs Free Energy=			0.002884
Sum of electronic and zero-point Energies=			-845.835939
Sum of electronic and thermal Energies=			-845.825802
Sum of electronic and thermal Enthalpies=			-845.824857
Sum of electronic and thermal Free Energies=			-845.875105

anti-syn-syn-P(NCO)₃

B3LYP/6-311+G(3df)

N	-0.00054600	1.45715700	0.76136100
P	0.00027500	-0.23819500	0.81647300
N	-1.28102900	-0.56151100	-0.26469100
N	1.28182700	-0.56027300	-0.26476600
C	2.35155500	-1.11832200	-0.25257400
C	-0.00101400	2.37927700	-0.02030600
C	-2.35021700	-1.12059300	-0.25243700
O	3.39010900	-1.63563900	-0.32247100
O	-3.38827400	-1.63891300	-0.32227300
O	-0.00281200	3.32244400	-0.69507100
Zero-point correction=			0.041908
Thermal correction to Energy=			0.052104
Thermal correction to Enthalpy=			0.053049
Thermal correction to Gibbs Free Energy=			0.000144
Sum of electronic and zero-point Energies=			-845.833995
Sum of electronic and thermal Energies=			-845.823799
Sum of electronic and thermal Enthalpies=			-845.822855
Sum of electronic and thermal Free Energies=			-845.875759

syn-syn-CIP(NCO)₂

BP86/6-311+G(3df)

N	-0.19034300	-0.70809100	1.26395600
P	0.66323000	0.04826000	0.00000000
N	-0.19034300	-0.70809100	-1.26395600
C	-0.10951000	-0.78052400	2.47849000

C	-0.10951000	-0.78052400	-2.47849000
O	-0.10951000	-0.91143600	-3.64412600
O	-0.10951000	-0.91143600	3.64412600
Cl	-0.24808000	1.94933200	0.00000000
Zero-point correction=			0.028567
Thermal correction to Energy=			0.037180
Thermal correction to Enthalpy=			0.038124
Thermal correction to Gibbs Free Energy=		-0.007803	
Sum of electronic and zero-point Energies=			-1138.003664
Sum of electronic and thermal Energies=			-1137.995052
Sum of electronic and thermal Enthalpies=			-1137.994107
Sum of electronic and thermal Free Energies=			-1138.040034

anti-syn-ClP(NCO)₂

BP86/6-311+G(3df)

P	0.03458100	0.48843400	0.87730200
N	-1.51077100	-0.18765500	0.67558400
N	0.95407100	-0.66481700	-0.00166700
Cl	-0.05587200	2.04332700	-0.54298300
C	-2.09226100	-0.98334600	-0.04591100
O	-2.72789700	-1.74370500	-0.66903400
O	3.23832000	-1.31204300	-0.28876100
C	2.13303100	-0.95828200	-0.11807100
Zero-point correction=			0.028354
Thermal correction to Energy=			0.037095
Thermal correction to Enthalpy=			0.038039
Thermal correction to Gibbs Free Energy=		-0.009470	
Sum of electronic and zero-point Energies=			-1138.001539
Sum of electronic and thermal Energies=			-1137.992798
Sum of electronic and thermal Enthalpies=			-1137.991854
Sum of electronic and thermal Free Energies=			-1138.039363

syn-syn-syn-P(NCO)₃

BP86/6-311+G(3df)

N	-0.00019300	1.48814200	-0.36542900
P	0.00000000	0.00000000	0.47951900
N	-1.28867300	-0.74423800	-0.36542900
N	1.28886500	-0.74390400	-0.36542900
C	2.31565100	-1.33684600	-0.08682600
C	-0.00008300	2.67383500	-0.08682600
C	-2.31556800	-1.33699000	-0.08682600
O	0.00000000	3.83550600	0.08517000
O	3.32164600	-1.91775300	0.08517000
O	-3.32164600	-1.91775300	0.08517000

Zero-point correction=	0.040521
Thermal correction to Energy=	0.050840
Thermal correction to Enthalpy=	0.051784
Thermal correction to Gibbs Free Energy=	0.001252
Sum of electronic and zero-point Energies=	-845.876977
Sum of electronic and thermal Energies=	-845.866658
Sum of electronic and thermal Enthalpies=	-845.865714
Sum of electronic and thermal Free Energies=	-845.916245

anti-syn-syn-P(NCO)₃

BP86/6-311+G(3df)

N	0.00002100	1.43390300	0.80596000
P	-0.00002400	-0.27788300	0.80585500
N	-1.28384700	-0.57041400	-0.30035600
N	1.28379200	-0.57048500	-0.30034600
C	2.38346800	-1.09483400	-0.25538400
C	0.00011200	2.35125300	-0.00141000
C	-2.38356400	-1.09467400	-0.25539600
O	3.45262900	-1.57756500	-0.30773000
O	-3.45276400	-1.57732200	-0.30774500
O	0.00019700	3.29823200	-0.69096000
Zero-point correction=			0.040377
Thermal correction to Energy=			0.050749
Thermal correction to Enthalpy=			0.051694
Thermal correction to Gibbs Free Energy=			-0.000589
Sum of electronic and zero-point Energies=			-845.874899
Sum of electronic and thermal Energies=			-845.864527
Sum of electronic and thermal Enthalpies=			-845.863582
Sum of electronic and thermal Free Energies=			-845.915865

syn-syn-ClP(NCO)₂

mPW1PW9/6-311+G(3df)

N	-0.19034300	-0.70809100	1.26395600
P	0.66323000	0.04826000	0.00000000
N	-0.19034300	-0.70809100	-1.26395600
C	-0.10951000	-0.78052400	2.47849000
C	-0.10951000	-0.78052400	-2.47849000
O	-0.10951000	-0.91143600	-3.64412600
O	-0.10951000	-0.91143600	3.64412600
Cl	-0.24808000	1.94933200	0.00000000
Zero-point correction=			0.030214
Thermal correction to Energy=			0.038594
Thermal correction to Enthalpy=			0.039538
Thermal correction to Gibbs Free Energy=			-0.006054

Sum of electronic and zero-point Energies=	-1137.846647
Sum of electronic and thermal Energies=	-1137.838267
Sum of electronic and thermal Enthalpies=	-1137.837323
Sum of electronic and thermal Free Energies=	-1137.882914

anti-syn-ClP(NCO)₂

mPW1PW9/6-311+G(3df)

P	0.03835600	0.48426100	0.86966200
N	-1.46823300	-0.23379600	0.69119100
N	0.97494800	-0.62453300	-0.00494200
Cl	-0.11649400	1.99743800	-0.53880300
C	-2.05794700	-0.99581500	-0.03643200
O	-2.68916200	-1.72686500	-0.66871100
O	3.23451200	-1.24528700	-0.29546500
C	2.14048600	-0.90999200	-0.12617200
Zero-point correction=			0.030019
Thermal correction to Energy=			0.038516
Thermal correction to Enthalpy=			0.039460
Thermal correction to Gibbs Free Energy=			-0.007842
Sum of electronic and zero-point Energies=			-1137.844675
Sum of electronic and thermal Energies=			-1137.836178
Sum of electronic and thermal Enthalpies=			-1137.835234
Sum of electronic and thermal Free Energies=			-1137.882536

syn-syn-syn-P(NCO)₃

mPW1PW9/6-311+G(3df)

N	-0.00019300	1.48814200	-0.36542900
P	0.00000000	0.00000000	0.47951900
N	-1.28867300	-0.74423800	-0.36542900
N	1.28886500	-0.74390400	-0.36542900
C	2.31565100	-1.33684600	-0.08682600
C	-0.00008300	2.67383500	-0.08682600
C	-2.31556800	-1.33699000	-0.08682600
O	0.00000000	3.83550600	0.08517000
O	3.32164600	-1.91775300	0.08517000
O	-3.32164600	-1.91775300	0.08517000
Zero-point correction=			0.042825
Thermal correction to Energy=			0.052864
Thermal correction to Enthalpy=			0.053808
Thermal correction to Gibbs Free Energy=			0.003870
Sum of electronic and zero-point Energies=			-845.690343
Sum of electronic and thermal Energies=			-845.680304
Sum of electronic and thermal Enthalpies=			-845.679360

Sum of electronic and thermal Free Energies= -845.729298

anti-syn-syn-P(NCO)₃

mPW1PW9/6-311+G(3df)

N	0.00017800	1.43959100	0.78229600
P	-0.00013400	-0.24908500	0.80583000
N	-1.27387300	-0.54978100	-0.27541100
N	1.27353300	-0.55027300	-0.27536500
C	2.34423100	-1.10225600	-0.25320100
C	0.00068800	2.34954500	-0.01165600
C	-2.34483500	-1.10125100	-0.25326400
O	3.38280700	-1.61052600	-0.31424900
O	-3.38365000	-1.60903100	-0.31433100
O	0.00117300	3.27996700	-0.69634000
Zero-point correction=			0.042672
Thermal correction to Energy=			0.052781
Thermal correction to Enthalpy=			0.053725
Thermal correction to Gibbs Free Energy=			0.000846
Sum of electronic and zero-point Energies=			-845.688306
Sum of electronic and thermal Energies=			-845.678198
Sum of electronic and thermal Enthalpies=			-845.677253
Sum of electronic and thermal Free Energies=			-845.730132

syn-syn-CIP(NCO)₂

CCSD(T)-F12A/aug-cc-pVTZ energy= -1136.552634427431

anti-syn-CIP(NCO)₂

CCSD(T)-F12A/aug-cc-pVTZ energy= -1136.551532517824

syn-syn-syn-P(NCO)₃

CCSD(T)-F12A/aug-cc-pVTZ energy= -844.691387709193

anti-syn-syn-P(NCO)₃

CCSD(T)-F12A/aug-cc-pVTZ energy= -844.690187484567