Table S1 Absolute energies (Hartree) of various structures of Isocyanate (io), Isothiocyanate (it) and Isoselenocyanate (is) obtained using different theoretical methods. Number of imaginary frequencies are given in parenthesis.

Structure	Symmetry	HF/6-31+G*	MP2/6-31+G*	MP2(full)/6-31+G*	B3LYP/6-31+G*	B3PW91/6-31+G*	G2
Isocyanate							
io-1	C_s	-167.76651070(0)	-168.2317783(0)	-168.24376380(0)	-168.6871039(0)	-168.6182035(0)	-168.4567720(0)
io-2	$C_{\infty v}$	-167.76066550(0)	-168.2243437(1)	-168.23673060(1)	-168.6802656(1)	-168.6113828(1)	-168.4488790(1)
Thioisocyanate							
it-1	C_s	-490.3940464(0)	-490.8086303(0)	-490.82925730(0)	-491.6394015(0)	-491.5484610(0)	-491.0451410(0)
it-2	$C_{\infty v}$	-490.3940454(0)	-490.8040621(1)	-490.82497010(1)	-491.6353285(1)	-491.5444139(1)	-491.0413756(1)
Selenoisothiocyanate							
is-1	C_s	-2490.4824224(0)	-2490.8828861(0)	-2490.9269743(0)	-2492.8470274(0)	-2492.7865138(0)	-2493.28069439(0)
is-2	$C_{\infty v}$	-2490.4824225(0)	-2490.8811793(1)	-2490.9254983(1)	-2492.8451196(1)	-2492.7845971(1)	-2493.27743780(1)

Table S2 Absolute energies (Hartree) of various structures of Formamide, Thioformamide and Selenoformamide obtained using different theoretical methods. Numbers of imaginary frequencies are given in parenthesis.

Structure	Symmetry	HF/6-31+G*	MP2/6-31+G*	MP2(full)/6-31+G*	B3LYP/6-31+G*	B3PW91/6-31+G*	G2
Formamide							
f-1	C_1	-168.9385918(0)	-169.4104257(0)	-169.4218682(0)	-169.9025473(0)	-169.8350819(0)	-169.6457330(0)
f-2	*Cs*	-168.9128898(1)	-169.3830074(1)	-169.3942493(1)	-169.8730756(1)	-169.8051221(1)	-169.6202810(1)
f-3	*Cs*	-168.9086348(1)	-169.3791665(1)	-169.3904304(1)	-169.8700019(1)	-169.8019861(1)	-169.6182990(1)
Thioformamide							
tf-1	C_1	-491.5706373(0)	-491.9858174(0)	-492.0058646(0)	-492.8546091(0)	-492.7664215(0)	-492.2337005(0)
tf-2	*Cs*	-491.5371432(1)	-491.9548028(1)	-491.9746198(1)	-492.8195634(1)	-492.7308171(1)	-492.2049870(1)
tf-3	*Cs*	-491.5338452(1)	-491.9522506(1)	-491.9720873(1)	-492.8166459(1)	-492.7277680(1)	-492.2031810(1)
Selenoformamide							
sf-1	C_1	-2491.6513748(0)	-2492.0560636(0)	-2492.0992715(0)	-2494.0575872(0)	-2494.0000178(0)	-2494.4722675(0)
sf-2	*Cs*	-2491.6150938(1)	-2492.0230814(1)	-2492.0659766(1)	-2492.0213688(1)	-2493.9633111(1)	-2494.4426325(1)
sf-3	*Cs*	-2491.6116775(1)	-2492.0204022(1)	-2492.0632755(1)	-2494.0183535(1)	-2493.9601545(1)	-2494.4408394(1)

Table S3 Absolute energies (Hartree) of various structures of urea, thiourea, and selenourea obtained using different theoretical methods. Number of imaginary frequencies are given in parenthesis.

Structure	Symmetry	HF/6-31+G*	MP2/6-31+G*	MP2(full)/6-31+G*	B3LYP/6-31+G*	B3PW91/6-31+G*	G2
Urea							
u-1	C_2	-223.994377(0)	-224.628824(0)	-224.644074(0)	-225.278185(0)	-225.191236(0)	-224.938914(0)
u-2	C_{2v}	-223.992488(2)	-224.624954(2)	-224.640392(2)	-225.276156(2)	-225.189221(2)	-224.938530(2)
u-3	C_s	-223.992704(1)	-224.626672(0)	-224.641952(0)	-225.276642(0)	-225.189654(0)	-224.938791(1)
u-4	C_1	-223.992934(1)	-224.626298(1)	-224.641644(1)	-225.276793(1)	-225.189755(1)	-224.938913(0)
u-5	C_s	-223.980142(1)	-224.615446(1)	-224.630684(1)	-225.264984(1)	-225.177968(1)	-224.926926(1)
u-6	C_s	-223.969611(1)	-224.604740(2)	-224.619973(2)	-225.254919(1)	-225.167768(1)	-224.919725(2)
Thiourea							
tu-1	C_2	-546.622885(0)	-547.201210(0)	-547.225125(0)	-548.226723(0)	-548.119139(0)	-547.525014(0)
tu-2	C_{2v}	-546.622860(1)	-547.199040(2)	-547.223173(2)	-548.226009(1)	-548.118419(1)	-547.524768(1)
tu-3	C_s	---	-547.199512(0)	-547.223511(1)	---	---	-547.524769(1)
tu-4	C_1	---	-547.199584(1)	-547.223622(1)	-548.226068(1)	-548.118474(1)	-547.525036(0)
tu-5	C_s	-546.606053(1)	-547.187548(1)	-547.211457(1)	-548.212272(1)	-548.104603(1)	-547.510979(1)
tu-6	C_s	-546.592843(1)	-547.175647(2)	-547.199567(1)	-548.200315(1)	-548.092353(1)	-547.501898(1)
Selenourea							
su-1	C_2	---	-2547.276276(0)	-2547.323860(0)	-2549.435230(0)	-2549.358154(0)	-2549.764176(0)
su-2	C_{2v}	-2546.710186(0)	-2547.275115(2)	-2547.322912(1)	-2549.435055(1)	-2549.357979(1)	-2549.763913(0)
su-3	C_s	---	-2547.275115(1)	-2547.322903(1)	---	---	-2549.763917(0)
su-4	C_1	---	-2547.275260(1)	-2547.322982(1)	---	---	-2549.764172(0)
su-5	C_s	-2546.691844(1)	-2547.262438(1)	-2547.310011(1)	-2549.420495(1)	-2549.343374(1)	-2549.749129(1)
su-6	C_s	-2546.677625(1)	-2547.249548(1)	-2547.297095(1)	-2549.407966(1)	-2549.330552(1)	-2549.739629(1)