

Representatively chosen systems containing nearly all elements (H-Rn,
 # except Lanthanides) in (nearly) all common oxidation states.
 # Structure parameters were optimized for DFT(BP86)/def-SV(P) and are given
 # in atomic units.

#BaF			
0.0000000000000000	0.0000000000000000	-2.07069892703602	ba
0.0000000000000000	0.0000000000000000	2.07069892703602	f
#BaF2			
0.0000000000000000	0.0000000000000000	1.55847796152849	ba
3.50406263138391	0.0000000000000000	-0.77923898076424	f
-3.50406263138391	0.0000000000000000	-0.77923898076424	f
#BaH2			
0.0000000000000000	0.0000000000000000	1.68536306424487	ba
3.48553102731125	0.0000000000000000	-0.84268153212243	h
-3.48553102731125	0.0000000000000000	-0.84268153212243	h
#BaO			
0.0000000000000000	0.0000000000000000	-1.92962468481039	ba
0.0000000000000000	0.0000000000000000	1.92962468481039	o
#BaS			
0.0000000000000000	0.0000000000000000	-2.42999531404145	ba
0.0000000000000000	0.0000000000000000	2.42999531404145	s
#Be2F4			
-2.13361594547065	0.0000000000000000	0.0000000000000000	be
2.13361594547065	0.0000000000000000	0.0000000000000000	be
0.0000000000000000	2.13211302712278	0.0000000000000000	f
0.0000000000000000	-2.13211302712278	0.0000000000000000	f
-4.78939030299712	0.0000000000000000	0.0000000000000000	f
4.78939030299712	0.0000000000000000	0.0000000000000000	f
#Be2H4			
0.0000000000000000	0.0000000000000000	-1.92929449970282	be
0.0000000000000000	0.0000000000000000	1.92931071700141	be
2.05284948165387	0.0000000000000000	-0.00000554462538	h
-2.05284948165387	0.0000000000000000	-0.00000554462538	h
0.0000000000000000	0.0000000000000000	-4.46632923721534	h
0.0000000000000000	0.0000000000000000	4.46632410916751	h
#Be4			
1.98239336244068	-1.40175406475758	0.0000000000000000	be
-1.98240276048822	-1.40176820517744	0.0000000000000000	be
0.00000469902377	1.40176113496751	-1.98238088228083	be
0.00000469902377	1.40176113496751	1.98238088228083	be
#BeC2H6			
0.0000000000000000	0.0000000000000000	0.0000000000000000	be
-0.00020044556495	3.18689981828802	0.0000000000000000	c
0.00020044556495	-3.18689981828802	0.0000000000000000	c
1.94277443489397	3.99483630431448	0.0000000000000000	h
0.97131508976867	-3.99480784611534	-1.68303202724579	h
-0.97131508976866	3.99480784611534	-1.68303202724579	h
-1.94277443489397	-3.99483630431448	0.0000000000000000	h
-0.97131508976866	3.99480784611534	1.68303202724579	h
0.97131508976867	-3.99480784611534	1.68303202724579	h
#BeF2O2H4			
-0.00000032363640	-0.00000008566633	-0.88438717282531	be
0.00000013544101	-2.55923932656878	-2.01794116529110	f
-0.00000415512240	2.55924102532360	-2.01793952586888	f
2.70021194774609	-0.00000008523155	1.18317601953195	o
-2.70021065005859	0.00000715003053	1.18318161817594	o
3.67189018000387	1.47880857364976	0.63847717253928	h

-3.67189013209522	-1.47881214872542	0.63847438690258	h
3.67189002508221	-1.47880764617565	0.63847412415729	h
-3.67188702736059	1.47880254336382	0.63848454267826	h
#BeH2			
0.000000000000000	0.000000000000000	0.000000000000000	be
0.000000000000000	0.000000000000000	2.54057183216976	h
0.000000000000000	0.000000000000000	-2.54057183216976	h
#BeS			
0.000000000000000	0.000000000000000	-1.67244267945864	be
0.000000000000000	0.000000000000000	1.67244267945864	s
#CaCl2			
0.000000000000000	0.000000000000000	0.000000000000000	ca
0.000000000000000	0.000000000000000	-4.87191849109726	cl
0.000000000000000	0.000000000000000	4.87191849109726	cl
#CaF2			
0.000000000000000	0.000000000000000	0.000000000000000	ca
0.000000000000000	0.000000000000000	-3.97143043764854	f
0.000000000000000	0.000000000000000	3.97143043764854	f
#CaH2			
0.000000000000000	0.000000000000000	0.000000000000000	ca
0.000000000000000	0.000000000000000	4.04362377931292	h
0.000000000000000	0.000000000000000	-4.04362377931292	h
#CsF			
0.000000000000000	0.000000000000000	-2.43002010389848	f
0.000000000000000	0.000000000000000	2.43002010389848	cs
#CsH			
0.000000000000000	0.000000000000000	-2.51401278411792	cs
0.000000000000000	0.000000000000000	2.51401278411792	h
#CsO			
0.000000000000000	0.000000000000000	-2.61735090985010	o
0.000000000000000	0.000000000000000	2.61735090985010	cs
#K2S			
0.000000000000000	0.000000000000000	1.75493373992356	s
-4.68812462132366	0.000000000000000	-0.87746686996178	k
4.68812462132366	0.000000000000000	-0.87746686996178	k
#K3P			
0.000000000000000	0.000000000000000	1.89749417626207	p
2.58580346543032	-4.47874298051299	-0.63249805875402	k
2.58580346543032	4.47874298051299	-0.63249805875402	k
-5.17160693086064	0.000000000000000	-0.63249805875402	k
#KBr			
0.000000000000000	0.000000000000000	-2.75588742538509	k
0.000000000000000	0.000000000000000	2.75588742538509	br
#KCl			
0.000000000000000	0.000000000000000	-2.59307106746649	k
0.000000000000000	0.000000000000000	2.59307106746649	cl
#KF			
0.000000000000000	0.000000000000000	-2.13462007168556	k
0.000000000000000	0.000000000000000	2.13462007168556	f
#KH			
0.000000000000000	0.000000000000000	-2.20252950247800	k
0.000000000000000	0.000000000000000	2.20252950247800	h
#KI			
0.000000000000000	0.000000000000000	-3.00693295045154	k
0.000000000000000	0.000000000000000	3.00693295045154	i
#Li2			
0.000000000000000	0.000000000000000	2.64099487417752	li

0.0000000000000000	0.0000000000000000	-2.64099487417752	li
#Li2O			
0.0000000000000000	0.0000000000000000	0.0000000000000000	o
0.0000000000000000	0.0000000000000000	3.07886917104883	li
0.0000000000000000	0.0000000000000000	-3.07886917104883	li
#Li4C4H12			
1.64706365185023	-1.64706414193258	1.64706544369022	li
-1.64706403016091	1.64706609392631	1.64705887225055	li
-1.64706511498339	-1.64706283357271	-1.64706684500640	li
1.64706611886332	1.64706488898669	-1.64706698536379	li
-2.43039744530168	-2.43039421024393	2.43039371335858	c
-2.43039481981438	2.43039861558535	-2.43039404610143	c
2.43041016795889	-2.43037962486503	-2.43040830076453	c
2.43039584881608	2.43039712925517	2.43039442430495	c
-3.75314966263209	-3.75314808906104	1.42781762772074	h
-3.75315152314663	1.42782582005728	-3.75315082553213	h
3.75314761464945	-3.75315658904388	-1.42781372983920	h
3.75314887684819	1.42782119712603	3.75314726754457	h
3.75315353972696	-1.42784583286734	-3.75312947798914	h
-1.42781763382581	3.75315092168214	-3.75315637933721	h
-1.42782024327477	-3.75314815761710	3.75314688009472	h
3.75314899897099	3.75315138842044	1.42781694923781	h
1.42781612597795	-3.75315104845671	-3.75315272040008	h
-3.75315006597704	-1.42781843578250	3.75314714040825	h
1.42782002306320	3.75315047748770	3.75314651403628	h
-3.75316042760865	3.75314243091576	-1.42779552231280	h
#Li4Cl4			
2.74433107302748	-1.94051594179951	0.0000000000000000	li
0.00000067632057	1.94051446095008	2.74434044508148	li
-2.74434673087586	-1.94050438549579	0.0000000000000000	li
0.00000067632057	1.94051446095008	-2.74434044508148	li
3.45559531815124	2.44348827432849	0.0000000000000000	cl
-0.00000377172669	-2.44349841628354	3.45558889743391	cl
-3.45557361860438	2.44349993543522	0.0000000000000000	cl
-0.00000377172669	-2.44349841628354	-3.45558889743391	cl
#Li4H4			
1.70080534683096	1.70080537092335	1.70080629791783	li
-1.70080500921405	1.70080539807377	-1.70080575731674	li
-1.70080602667080	-1.70080602949547	1.70080562105870	li
1.70080538482293	-1.70080498514297	-1.70080576838347	li
-1.85949824812399	1.85949816528516	1.85949815526986	h
-1.85949848558192	-1.85949846568449	-1.85949840131317	h
1.85949821284325	-1.85949826186725	1.85949814331282	h
1.85949882509361	1.85949880790790	-1.85949829054584	h
#Li8			
2.74131108923626	2.74132478269676	2.74117649987501	li
-2.74132095967384	2.74139733087893	2.74123662814823	li
-2.74141505700265	-2.74140311587089	2.74132801066027	li
2.74142424897969	-2.74136699425814	2.7412852508306	li
2.74120592621730	-2.74115999255214	-2.74129238641303	li
2.74113282151043	2.74114762466293	-2.74121705828456	li
-2.74113063835797	2.74118015543297	-2.74125140645887	li
-2.74120743090921	-2.74111979099044	-2.74126581261013	li
#LiBH4			
-0.00024869116689	-0.69457330488353	0.0000000000000000	b
0.00086758333408	-2.99344227721830	0.0000000000000000	h
1.10203755028072	0.22558430838791	-1.90940541026977	h

1.10203755028072	0.22558430838791	1.90940541026977	h
-2.20471760670618	0.22450989127912	0.00000000000000	h
0.00002361397754	3.01233707404689	0.00000000000000	li
#LiCl			
0.00000000000000	0.00000000000000	-1.93849439881658	li
0.00000000000000	0.00000000000000	1.93849439881658	cl
#LiF			
0.00000000000000	0.00000000000000	-1.48697136026104	li
0.00000000000000	0.00000000000000	1.48697136026103	f
#LiH			
0.00000000000000	0.00000000000000	1.54697769798700	li
0.00000000000000	0.00000000000000	-1.54697769798700	h
#LiSLi			
0.00000000000000	0.00000000000000	0.00000000000000	s
0.00000000000000	0.00000000000000	3.94716240337943	li
0.00000000000000	0.00000000000000	-3.94716240337943	li
#Mg4			
2.14509045506480	-2.14509045506480	2.14509045506480	mg
-2.14509045506480	2.14509045506480	2.14509045506480	mg
-2.14509045506480	-2.14509045506480	-2.14509045506480	mg
2.14509045506480	2.14509045506480	-2.14509045506480	mg
#MgCl2			
0.00000000000000	0.00000000000000	0.00000000000000	mg
0.00000000000000	0.00000000000000	4.14223402210192	cl
0.00000000000000	0.00000000000000	-4.14223402210192	cl
#MgF			
0.00000000000000	0.00000000000000	-1.67915451808357	mg
0.00000000000000	0.00000000000000	1.67915451808357	f
#MgF2			
0.00000000000000	0.00000000000000	0.00000000000000	mg
0.00000000000000	0.00000000000000	3.32239429304949	f
0.00000000000000	0.00000000000000	-3.32239429304949	f
#MgH2			
0.00000000000000	0.00000000000000	0.00000000000000	mg
0.00000000000000	0.00000000000000	3.23157098894782	h
0.00000000000000	0.00000000000000	-3.23157098894782	h
#Na2O			
0.00000000000000	0.00000000000000	-0.00125987003817	o
3.76616708679694	0.00000000000000	0.00062993501909	na
-3.76616708679694	0.00000000000000	0.00062993501909	na
#Na2S			
0.00000000000000	0.00000000000000	0.00000000000000	s
0.00000000000000	0.00000000000000	-4.54664766104049	na
0.00000000000000	0.00000000000000	4.54664766104049	na
#Na3N			
0.00000000000000	0.00000000000000	0.98846813029527	n
-1.94602685234149	3.37061738114880	-0.32948937676509	na
-1.94602685234149	-3.37061738114880	-0.32948937676509	na
3.89205370468299	0.00000000000000	-0.32948937676509	na
#Na3P			
0.02166950952763	-0.00927750719924	1.85753834100637	p
1.53863108521887	-3.99579517958087	-0.62708109943298	na
2.65769485647032	3.35118326979984	-0.62224016723425	na
-4.21799545121683	0.65388941698028	-0.60821707433915	na
#NaCl			
0.00000000000000	0.00000000000000	-2.23125548600731	na
0.00000000000000	0.00000000000000	2.23125548600731	cl

#NaF	0.0000000000000000	0.0000000000000000	-1.81647944104883	na
	0.0000000000000000	0.0000000000000000	1.81647944104883	f
#NaH	0.0000000000000000	0.0000000000000000	-1.79420308214526	na
	0.0000000000000000	0.0000000000000000	1.79420308214526	h
#PLi3	-0.00040508715227	1.96231380420593	0.0000000000000000	p
	3.47020495828402	-0.65597305055359	0.0000000000000000	li
	-1.73489993556587	-0.65317037682617	3.00666083679482	li
	-1.73489993556587	-0.65317037682617	-3.00666083679482	li
#RbF	0.0000000000000000	0.0000000000000000	-2.29684487633273	f
	0.0000000000000000	0.0000000000000000	2.29684487633273	rb
#RbH	0.0000000000000000	0.0000000000000000	-2.33735012066011	rb
	0.0000000000000000	0.0000000000000000	2.33735012066011	h
#RbO	0.0000000000000000	0.0000000000000000	-2.46235472688576	o
	0.0000000000000000	0.0000000000000000	2.46235472688576	rb
#SrF	0.0000000000000000	0.0000000000000000	-1.95487637299250	sr
	0.0000000000000000	0.0000000000000000	1.95487637299250	f
#SrF2	0.0000000000000000	0.0000000000000000	1.21686253050211	sr
	3.54167198526231	0.0000000000000000	-0.60843126525105	f
	-3.54167198526231	0.0000000000000000	-0.60843126525105	f
#SrH2	0.0000000000000000	0.0000000000000000	1.36780798604125	sr
	-3.52443250853761	0.0000000000000000	-0.68390399302062	h
	3.52443250853761	0.0000000000000000	-0.68390399302062	h
#SrO	0.0000000000000000	0.0000000000000000	-1.83598401421036	sr
	0.0000000000000000	0.0000000000000000	1.83598401421036	o
#SrS	0.0000000000000000	0.0000000000000000	-2.31673677279564	sr
	0.0000000000000000	0.0000000000000000	2.31673677279564	s
#B2H6	0.0000000000000000	0.0000000000000000	1.68149280660034	b
	0.0000000000000000	0.0000000000000000	-1.68149280660034	b
	0.0000000000000000	-1.88412562931544	0.0000000000000000	h
	0.0000000000000000	1.88412562931544	0.0000000000000000	h
	1.99832414844106	0.0000000000000000	2.79335654905377	h
	-1.99832414844106	0.0000000000000000	2.79335654905377	h
	-1.99832414844106	0.0000000000000000	-2.79335654905377	h
	1.99832414844106	0.0000000000000000	-2.79335654905377	h
#B3N3H6	2.75503008971104	-0.00000323939483	0.0000000000000000	b
	1.33708167162979	2.31531468226869	0.0000000000000000	n
	-1.37762869492974	2.38537342180479	0.0000000000000000	b
	-2.67435276602476	0.00000211824938	0.0000000000000000	n
	-1.37764337777651	-2.38537456910514	0.0000000000000000	b
	1.33706851342589	-2.31531512981732	0.0000000000000000	n
	5.05300245977585	-0.00000804976266	0.0000000000000000	h
	2.30183999853162	3.98629277576524	0.0000000000000000	h
	-2.52609075956054	4.37610354836293	0.0000000000000000	h
	-4.60403920406282	0.00000416958359	0.0000000000000000	h

-2.52610296250991	-4.37610284086748	0.00000000000000	h
2.30183503179008	-3.98628688708722	0.00000000000000	h
#B4H4			
1.13513007545606	1.13512970003633	1.13512888659479	b
-1.13512170839976	1.13512235099020	-1.13512294487928	b
-1.13512831829025	-1.13512872380334	1.13512812346088	b
1.13513271243326	-1.13513209595804	-1.13513301541142	b
2.45171101991862	2.45170873428443	2.45170917853944	h
-2.45171753891449	2.45171830786967	-2.45171888582538	h
-2.45170898165818	-2.45171133452650	2.45171018828927	h
2.45170273945477	-2.45170693889277	-2.45170153076831	h
#BF3			
0.00057162011753	0.00000112131525	0.00000000000000	b
2.50269790165942	0.00000463627076	0.00000000000000	f
-1.25162960237501	2.16558024460409	0.00000000000000	f
-1.25163991940193	-2.16558600219009	0.00000000000000	f
#BH3			
0.00000000000000	0.00000000000000	-0.00001716605107	b
0.00000000000000	0.00000000000000	2.29252379962527	h
1.98536152775083	0.00000000000000	-1.14625331603055	h
-1.98536152775083	0.00000000000000	-1.14625331603055	h
#BH3CO			
-0.00003267004886	1.01111329216265	0.00000000000000	b
2.24066059731720	1.62213805210289	0.00000000000000	h
-1.12023754948246	1.62311914581523	1.94044267338909	h
-1.12023754948246	1.62311914581523	-1.94044267338909	h
-0.00018198607045	-1.85414688329676	0.00000000000000	c
0.00002915776702	-4.02534275259922	0.00000000000000	o
#BH3NH3			
-0.00005391609667	-0.00000006055366	1.59755328544083	b
0.00003677556503	-0.00000004984535	-1.51922811870669	n
-1.12198704238829	1.94345823821240	2.21019712023369	h
-1.81066670598354	-0.00000007552669	-2.23620407950898	h
-1.12200568324154	-1.94345788468772	2.21023739863948	h
0.90537147089552	-1.56819423165877	-2.23633381411281	h
2.24393364900982	-0.00000003812768	2.21011203996588	h
0.90537145223968	1.56819410218746	-2.23633383195137	h
#C2H2			
0.00000000000000	0.00000000000000	1.15246217269357	c
0.00000000000000	0.00000000000000	-1.15237758930046	c
0.00000000000000	0.00000000000000	3.19592252631204	h
0.00000000000000	0.00000000000000	-3.19600710970514	h
#C2H3N			
1.88736354706722	-0.38569072500046	0.00000000000000	n
-0.71824807664584	-0.19471094953120	-1.22023694426924	c
-0.71824807664584	-0.19471094953120	1.22023694426924	c
2.62906670020725	1.44277863614961	0.00000000000000	h
-1.53996704699139	-0.33383300604337	-3.10934257471802	h
-1.53996704699139	-0.33383300604337	3.10934257471802	h
#C2H4			
-0.00000595240645	-1.26733455985489	0.00000000000000	c
-0.00001103692376	1.26733990808114	0.00000000000000	c
1.77139591530185	-2.36353680346697	0.00000000000000	h
-1.77135302848125	-2.36354228611354	0.00000000000000	h
1.77143988920888	2.36354006871598	0.00000000000000	h
-1.77146578669927	2.36353367263826	0.00000000000000	h
#C2H6			

-0.00004769714133	0.00000349348608	1.44636083928208	c
0.00000804691144	0.00000483284596	-1.44638600827020	c
0.00000507341384	1.94903094277111	2.21977150357274	h
-1.68811904618790	0.97442869763498	-2.21944595476968	h
-1.68812247614916	-0.97443046693153	2.21943006405761	h
0.00000720306362	-1.94903334377391	-2.21978760781604	h
1.68813497191566	-0.97443316442446	2.21950311354087	h
1.68813392417380	0.97442900839179	-2.21944594959735	h
#C4H4			
0.99384594007199	0.99384464702096	0.99383622488147	c
-0.99383778119390	0.99384857359297	-0.99384786547507	c
-0.99383837692231	-0.99383758446481	0.99383909184982	c
0.99384393287549	-0.99383406319256	-0.99384192088452	c
2.18053060627208	2.18052818251503	2.18055255481919	h
-2.18053790501712	2.18055083059018	-2.18055040079725	h
-2.18053792505281	-2.18054059788475	2.18054096602118	h
2.18053150896658	-2.18055998817700	-2.18052865041484	h
#C6H6			
2.65617581771435	-0.00001755566762	0.00000000000000	c
1.32809320450038	2.30036580039517	0.00000000000000	c
-1.32814289699474	2.30032454944275	0.00000000000000	c
-2.65616474222357	-0.00002947176151	0.00000000000000	c
-1.32814664832257	-2.30031670879657	0.00000000000000	c
1.32804572900546	-2.30030596170580	0.00000000000000	c
4.73697603254869	-0.00001003497658	0.00000000000000	h
2.36858554692983	4.10225225927773	0.00000000000000	h
-2.36858598921966	4.10217914017551	0.00000000000000	h
-4.73684964271648	-0.00000987434447	0.00000000000000	h
-2.36856197133617	-4.10217066208403	0.00000000000000	h
2.36857556011450	-4.10226147995460	0.00000000000000	h
#CF4			
0.00000072798427	-0.00000084127378	0.00000134823270	c
1.45612263947210	1.45612426874410	1.45612670863342	f
-1.45612382956586	1.45612744820956	-1.45611634123477	f
-1.45611302972194	-1.45611774949082	1.45611910063923	f
1.45611349183143	-1.45613312618904	-1.45613081627060	f
#CH2O			
0.00001136906018	-0.00680178712325	0.00000000000000	c
0.00001124892632	-2.29137576741941	0.00000000000000	o
-1.79950764336418	1.14910699652609	0.00000000000000	h
1.79948502537768	1.14907055801657	0.00000000000000	h
#CH2O2			
-0.00257696271985	-0.00029911539700	0.43566389538811	c
0.91809787651456	1.10119962920547	-1.77030267443462	o
-0.89638419996679	-1.09806893130047	-1.78331456460493	o
1.35822195950510	-1.13175262110298	1.56631140453024	h
-1.37735867333304	1.12892103859498	1.55164193912118	h
#CH3N			
-0.51099882579378	-1.72615900810017	0.00000000000000	n
-0.28199635256966	0.67673092847568	0.00000000000000	c
1.26548359579527	-2.55925182755683	0.00000000000000	h
1.54014071938432	1.74203610207273	0.00000000000000	h
-2.01262913681617	1.86664380510858	0.00000000000000	h
#CH3OH			
-0.60943318920949	0.23208453617070	0.00000000000000	c
-1.40349374228799	-0.73023655246102	-1.70457168393205	h
-1.40349374228799	-0.73023655246102	1.70457168393205	h

-1.34535487704355	2.19364844386480	0.00000000000000	h
2.05720432204887	0.37903865616194	0.00000000000000	o
2.70457122878014	-1.34429853127539	0.00000000000000	h
#CH4			
0.00000365772543	-0.00000430204539	-0.00000303470922	c
1.20635474089927	1.20638206443483	1.20635809459961	h
-1.20637417661767	1.20636079380735	-1.20635435342573	h
-1.20635629114801	-1.20637256903187	1.20636439312342	h
1.20637206914099	-1.20636598716490	-1.20636509958807	h
#CO			
0.00000000000000	0.00000000000000	-1.07901367410215	c
0.00000000000000	0.00000000000000	1.07901367410215	o
#CO2			
0.00000000000000	0.00000000000000	0.00002806040915	c
0.00000000000000	0.00000000000000	2.21994735057408	o
0.00000000000000	0.00000000000000	-2.21997541098322	o
#F2			
0.00000000000000	0.00000000000000	-1.33472243762606	f
0.00000000000000	0.00000000000000	1.33472243762606	f
#H2			
0.00000000000000	0.00000000000000	0.72490772298399	h
0.00000000000000	0.00000000000000	-0.72490772298399	h
#H2CO3			
-0.00000072368405	0.22080394668051	0.00000000000000	c
-0.00000085983362	2.51789433031705	0.00000000000000	o
2.06907082035747	-1.26682714026337	0.00000000000000	o
-2.06907034454166	-1.26683026979785	0.00000000000000	o
3.50618225374280	-0.10251893084200	0.00000000000000	h
-3.50618114604093	-0.10252193609435	0.00000000000000	h
#H2O			
-0.00000092153086	0.77139067871094	0.00000000000000	o
1.43408493447591	-0.38569466553748	0.00000000000000	h
-1.43408401294505	-0.38569601317346	0.00000000000000	h
#H2O2			
1.37391573291828	-0.11754325013582	0.47481512973650	o
-1.37391573291828	0.11754325013582	0.47481512973650	o
1.81764940640807	1.41027485517298	-0.47481512973649	h
-1.81764940640807	-1.41027485517298	-0.47481512973649	h
#HCN			
0.00000000000000	0.00000000000000	-2.10459881646616	h
0.00000000000000	0.00000000000000	-0.05057148541107	c
0.00000000000000	0.00000000000000	2.15517030187723	n
#HF			
0.00000000000000	0.00000000000000	0.88143111896247	h
0.00000000000000	0.00000000000000	-0.88143111896247	f
#HNC			
0.00000000000000	0.00000000000000	-2.02196172790527	h
0.00000000000000	0.00000000000000	-0.10820520253614	n
0.00000000000000	0.00000000000000	2.13016693044140	c
#HNO			
-1.79661507816673	0.48943320881840	0.00000000000000	o
0.47454096973458	0.69971484027459	0.00000000000000	n
1.32207410843215	-1.18914804909299	0.00000000000000	h
#HNO2			
-0.00005991769124	0.00467141411420	0.00000000000000	n
0.00050822247803	-2.00908183598864	0.00000000000000	h
2.08688969332883	1.00263775985379	0.00000000000000	o

-2.08733799811562	1.00177266202064	0.00000000000000	o
#HNO3			
-0.84920495946036	-0.15764648097179	0.00000000000000	n
-1.28916831029594	2.10044345874920	0.00000000000000	o
1.78029964374549	-0.83073113266367	0.00000000000000	o
-2.25079424696181	-1.94859046351144	0.00000000000000	o
2.60886787297262	0.83652461839769	0.00000000000000	h
#N2			
0.00000000000000	0.00000000000000	-1.05078974035833	n
0.00000000000000	0.00000000000000	1.05078974035833	n
#N2H2			
-1.17672812398851	0.92386039472759	0.00000000000000	n
1.17661864072211	0.92396010505874	0.00000000000000	n
-1.95539025873620	-0.92400022187768	0.00000000000000	h
1.95549974200260	-0.92382027790864	0.00000000000000	h
#N2H4			
1.34301342554004	0.11487732805038	0.44262664845470	n
-1.34301342554004	-0.11487732805038	0.44262664845470	n
2.06079980354008	0.61078546738212	-1.30448136798935	h
-2.06079980354008	-0.61078546738212	-1.30448136798935	h
2.08747379308132	-1.63000779480150	0.86185471953465	h
-2.08747379308132	1.63000779480150	0.86185471953465	h
#N4			
0.97352637877574	0.97353427649995	0.97350854749399	n
-0.97347107666161	0.97345970934768	-0.97348952076396	n
-0.97352288698680	-0.97351512802877	0.97348592757745	n
0.97346758487266	-0.97347885781885	-0.97350495430747	n
#NF3			
-0.00023917863373	0.86723125260972	0.00000000000000	n
2.36152560364088	-0.29019299685791	0.00000000000000	f
-1.18064321250358	-0.28851912787590	2.04401593693485	f
-1.18064321250358	-0.28851912787590	-2.04401593693485	f
#NH3			
-0.00002996273382	0.60419573896846	0.00000000000000	n
1.77459787410351	-0.20146478753319	0.00000000000000	h
-0.88728395568485	-0.20136547571764	1.53702086353764	h
-0.88728395568485	-0.20136547571764	-1.53702086353764	h
#NH4F			
0.00035295142012	0.99586270905472	0.00000000000000	n
1.79756586681634	1.73917600761303	0.00000000000000	h
-0.89974980156668	1.73568143900128	1.55739131188531	h
-0.89974980156668	1.73568143900128	-1.55739131188531	h
0.00153471995548	-2.18853841134706	0.00000000000000	h
0.00004606494142	-4.01786318332326	0.00000000000000	f
#OF2			
0.00000000000000	0.00000000000000	1.08966458588793	o
-2.12636045821744	0.00000000000000	-0.54483229294396	f
2.12636045821744	0.00000000000000	-0.54483229294396	f
#Al2O3			
0.00000000000000	0.00000000000000	0.00000000000000	o
0.00000000000000	0.00000000000000	-3.20592451951933	al
0.00000000000000	0.00000000000000	3.20592451951933	al
0.00000000000000	0.00000000000000	-6.26442328261665	o
0.00000000000000	0.00000000000000	6.26442328261665	o
#Al2S3			
0.00000000000000	0.00000000000000	3.16034259123655	s
-6.05680384209421	0.00000000000000	-2.01213979070925	s

6.05680384209421	0.0000000000000000	-2.01213979070925	s
-3.12156733278024	0.0000000000000000	0.43196849509098	al
3.12156733278024	0.0000000000000000	0.43196849509098	al
#AlCl3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	al
1.98010837147193	-3.42964830388186	0.0000000000000000	cl
1.98010837147193	3.42964830388186	0.0000000000000000	cl
-3.96021674294387	0.0000000000000000	0.0000000000000000	cl
#AlF3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	al
1.56643211516439	-2.71314001007231	0.0000000000000000	f
1.56643211516439	2.71314001007231	0.0000000000000000	f
-3.13286423032878	0.0000000000000000	0.0000000000000000	f
#AlH3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	al
1.51111027824900	-2.61731977776682	0.0000000000000000	h
1.51111027824900	2.61731977776682	0.0000000000000000	h
-3.02222055649801	0.0000000000000000	0.0000000000000000	h
#AlN			
0.0000000000000000	0.0000000000000000	1.70183203298110	n
0.0000000000000000	0.0000000000000000	-1.70183203298110	al
#CS2			
0.0000000000000000	0.0000000000000000	-0.00042370317242	c
0.0000000000000000	0.0000000000000000	2.96976471283164	s
0.0000000000000000	0.0000000000000000	-2.96934100965921	s
#Cl2			
0.0000000000000000	0.0000000000000000	1.94562946845339	cl
0.0000000000000000	0.0000000000000000	-1.94562946845339	cl
#ClF			
0.0000000000000000	0.0000000000000000	-1.58509614282258	cl
0.0000000000000000	0.0000000000000000	1.58509614282258	f
#ClF3			
-0.00003067860727	-0.83736782989924	0.0000000000000000	cl
-3.32968626746479	-0.75728391745932	0.0000000000000000	f
3.32967523209023	-0.75719934611368	0.0000000000000000	f
0.00004171398183	2.35185109347225	0.0000000000000000	f
#H2SO4			
-0.00001618652064	0.00000532998352	0.57726346501965	s
2.40449042802622	0.00000119792204	1.95483853136064	o
-2.40446876756433	0.00000117641825	1.95482480979171	o
-0.00000130197438	2.22843215334819	-1.58826869332215	o
-0.00000131291374	-2.22844560147121	-1.58825020322016	o
-0.00000143369034	3.83405981964557	-0.65522713489551	h
-0.00000142536279	-3.83405407584636	-0.65518077473415	h
#H3PO4			
0.00025271029759	0.00000002775195	0.18378624273833	p
2.75771513369481	0.00000046305733	-1.18697263987526	o
-1.38058842041890	2.38580178738371	-1.18704930153066	o
-1.38058701560059	-2.38580233754762	-1.18704935129008	o
0.00141162249612	0.00000008197607	3.01262148875343	o
4.05947580693281	-0.00000015128153	0.12202776723928	h
-2.02883988453177	3.51548597828379	0.12131791511576	h
-2.02883995287005	-3.51548584962367	0.12131787884917	h
#HCP			
0.0000000000000000	0.0000000000000000	-2.64853987727355	p
0.0000000000000000	0.0000000000000000	2.35551089579161	h
0.0000000000000000	0.0000000000000000	0.29302898148195	c

#HC1	0.0000000000000000	0.0000000000000000	-1.22530682104886	cl
	0.0000000000000000	0.0000000000000000	1.22530682104886	h
#HSH	-0.00000891346937	1.19653856768716	0.0000000000000000	s
	1.84307080535555	-0.59826448731836	0.0000000000000000	h
	-1.84306189188618	-0.59827408036881	0.0000000000000000	h
#HSSH	1.98198459838609	-0.07543787142517	0.90366573347496	s
	-1.98198459838609	0.07543787142517	0.90366573347496	s
	2.42926401991953	1.72380811808687	-0.90366607995143	h
	-2.42926401991953	-1.72380811808687	-0.90366607995143	h
#P2	0.0000000000000000	0.0000000000000000	1.81038834147637	p
	0.0000000000000000	0.0000000000000000	-1.81038834147637	p
#PF3	0.00190593228732	0.00000637856307	-1.13522248396255	p
	2.65740159746508	0.00000628935462	0.38170793256163	f
	-1.32964926884328	2.29968766474854	0.37675740109626	f
	-1.32965826090911	-2.29970033266624	0.37675715030465	f
#PF5	0.00093568540199	0.00000556340549	0.0000000000000000	p
	0.00115403835462	-3.04805754510344	0.0000000000000000	f
	0.00115453827044	3.04805857150255	0.0000000000000000	f
	3.00853565827311	-0.00000245516935	0.0000000000000000	f
	-1.50588996015008	-0.00000206731762	2.60331280562780	f
	-1.50588996015008	-0.00000206731762	-2.60331280562780	f
#PH3	0.00021868262881	0.00000408524970	-1.13254033248507	p
	2.26639108333582	0.00000455950564	0.37803102689817	h
	-1.13330963847505	1.96296552283309	0.37726390137846	h
	-1.13330012748958	-1.96297416758843	0.37724540420844	h
#S2	0.0000000000000000	0.0000000000000000	-1.82795217547776	s
	0.0000000000000000	0.0000000000000000	1.82795217547776	s
#S5	-1.01219286085597	0.91031071217532	2.78939529359939	s
	2.56254320877922	-0.26701145071347	2.27262712733185	s
	2.56256180032893	-0.26700825963793	-2.27262274065567	s
	-1.01216802810249	0.91029852260584	-2.78940508703009	s
	-3.10074412014967	-1.28658952442978	0.00000540675450	s
#SF2	0.0000000000000000	0.0000000000000000	1.32266337773884	s
	2.37880811467657	0.0000000000000000	-0.66133188418768	f
	-2.37880811467657	0.0000000000000000	-0.66133188418768	f
#SF4	-0.00000226380055	-0.00002431422764	0.84926009844488	s
	-3.18886562268367	-0.00001733471558	0.66640784370306	f
	3.18886006659826	-0.00001733422028	0.66642737569287	f
	0.00000390405808	2.35445661105741	-1.09097973125881	f
	0.00000391582787	-2.35439762789392	-1.09111558658199	f
#SF6	0.0000000000000000	0.0000000000000000	0.00000118515990	s
	-2.15172851914079	-2.15172851914079	-0.00000033099473	f
	0.0000000000000000	0.0000000000000000	3.04300291311907	f
	-2.15172851914079	2.15172851914079	-0.00000033099473	f
	0.0000000000000000	0.0000000000000000	-3.04300276329175	f

2.15172851914079	-2.15172851914079	-0.00000033099473	f
2.15172851914079	2.15172851914079	-0.00000033099473	f
#SiCl4			
0.000000000000000	0.000000000000000	0.000000000000000	si
2.24180189786400	-2.24180189786400	2.24180189786400	cl
-2.24180189786400	2.24180189786400	2.24180189786400	cl
-2.24180189786400	-2.24180189786400	-2.24180189786400	cl
2.24180189786400	2.24180189786400	-2.24180189786400	cl
#SiF4			
0.000000000000000	0.000000000000000	0.000000000000000	si
1.74748733068482	-1.74748733068482	1.74748733068482	f
-1.74748733068482	1.74748733068482	1.74748733068482	f
-1.74748733068482	-1.74748733068482	-1.74748733068482	f
1.74748733068482	1.74748733068482	-1.74748733068482	f
#SiH4			
0.000000000000000	0.000000000000000	0.000000000000000	si
1.63806238513397	-1.63806238513397	1.63806238513397	h
-1.63806238513397	1.63806238513397	1.63806238513397	h
-1.63806238513397	-1.63806238513397	-1.63806238513397	h
1.63806238513397	1.63806238513397	-1.63806238513397	h
#SiO2			
0.000000000000000	0.000000000000000	0.000000000000000	si
0.000000000000000	0.000000000000000	-2.90863957585795	o
0.000000000000000	0.000000000000000	2.90863957585795	o
#SiS2			
0.000000000000000	0.000000000000000	0.000000000000000	si
0.000000000000000	0.000000000000000	-3.68153174204543	s
0.000000000000000	0.000000000000000	3.68153174204543	s
#As4			
1.64900717955662	-1.64900717955662	1.64900717955662	as
-1.64900717955662	1.64900717955662	1.64900717955662	as
-1.64900717955662	-1.64900717955662	-1.64900717955662	as
1.64900717955662	1.64900717955662	-1.64900717955662	as
#As4S4			
-1.41083883866857	-1.41083883866857	4.46081971940384	s
1.41083883866857	1.41083883866857	4.46081971940384	s
-1.41083883866857	1.41083883866857	-4.46081971940384	s
1.41083883866857	-1.41083883866857	-4.46081971940384	s
0.000000000000000	3.30253054743472	0.000000000000000	as
3.30253054743472	0.000000000000000	0.000000000000000	as
0.000000000000000	-3.30253054743472	0.000000000000000	as
-3.30253054743472	0.000000000000000	0.000000000000000	as
#AsCl3			
0.000000000000000	0.000000000000000	1.45363897308538	as
-1.85326772975506	3.20995386796359	-0.48454632436179	cl
-1.85326772975506	-3.20995386796359	-0.48454632436179	cl
3.70653545951011	0.000000000000000	-0.48454632436179	cl
#AsCl6-			
0.000000000000000	0.000000000000000	0.000000000000000	as
0.000000000000000	4.35128874572739	0.000000000000000	cl
0.000000000000000	0.000000000000000	4.35128874572739	cl
4.35128874572739	0.000000000000000	0.000000000000000	cl
0.000000000000000	0.000000000000000	-4.35128874572739	cl
-4.35128874572739	0.000000000000000	0.000000000000000	cl
0.000000000000000	-4.35128874572739	0.000000000000000	cl
#AsH3			
0.000000000000000	0.000000000000000	1.23244998693740	as

-1.20159017904000	2.08121523997307	-0.41081666231247	h
-1.20159017904000	-2.08121523997307	-0.41081666231247	h
2.40318035808001	0.00000000000000	-0.41081666231247	h
#Br2			
0.00000000000000	0.00000000000000	-2.20336345967580	br
0.00000000000000	0.00000000000000	2.20336345967580	br
#BrCl			
0.00000000000000	0.00000000000000	-2.07645102410186	br
0.00000000000000	0.00000000000000	2.07645102410186	cl
#BrO4-			
0.00000000000000	0.00000000000000	0.00000000000000	br
1.80474294078758	-1.80474294078758	1.80474294078758	o
-1.80474294078758	1.80474294078758	1.80474294078758	o
-1.80474294078758	-1.80474294078758	-1.80474294078758	o
1.80474294078758	1.80474294078758	-1.80474294078758	o
#GaCl			
0.00000000000000	0.00000000000000	-2.11198999351902	ga
0.00000000000000	0.00000000000000	2.11198999351902	cl
#GaCl3			
0.00000000000000	0.00000000000000	0.00000000000000	ga
2.02363708334148	-3.50504224442794	0.00000000000000	cl
2.02363708334148	3.50504224442794	0.00000000000000	cl
-4.04727416668296	0.00000000000000	0.00000000000000	cl
#GaF			
0.00000000000000	0.00000000000000	-1.69732010119943	ga
0.00000000000000	0.00000000000000	1.69732010119943	f
#GaF2			
0.00000000000000	0.00000000000000	1.16213096204235	ga
-2.87257490857190	0.00000000000000	-0.58106548102118	f
2.87257490857190	0.00000000000000	-0.58106548102118	f
#GaH3			
0.00000000000000	0.00000000000000	0.00000000000000	ga
1.49230772481659	-2.58475279990984	0.00000000000000	h
1.49230772481659	2.58475279990984	0.00000000000000	h
-2.98461544963317	0.00000000000000	0.00000000000000	h
#GaO			
0.00000000000000	0.00000000000000	-1.61698641616867	ga
0.00000000000000	0.00000000000000	1.61698641616867	o
#GeCl4			
0.00000000000000	0.00000000000000	0.00000000000000	ge
2.34720419578646	-2.34720419578646	2.34720419578646	cl
-2.34720419578646	2.34720419578646	2.34720419578646	cl
-2.34720419578646	-2.34720419578646	-2.34720419578646	cl
2.34720419578646	2.34720419578646	-2.34720419578646	cl
#GeF3			
0.00000000000000	0.00000000000000	0.93844457989423	ge
1.53348366776395	-2.65607162514423	-0.31281485996474	f
1.53348366776395	2.65607162514423	-0.31281485996474	f
-3.06696733552790	0.00000000000000	-0.31281485996474	f
#GeF4			
0.00000000000000	0.00000000000000	0.00000000000000	ge
1.87482477759343	-1.87482477759343	1.87482477759343	f
-1.87482477759343	1.87482477759343	1.87482477759343	f
-1.87482477759343	-1.87482477759343	-1.87482477759343	f
1.87482477759343	1.87482477759343	-1.87482477759343	f
#GeH4			
0.00000000000000	0.00000000000000	0.00000000000000	ge

1.69283500661777	-1.69283500661777	1.69283500661777	h
-1.69283500661777	1.69283500661777	1.69283500661777	h
-1.69283500661777	-1.69283500661777	-1.69283500661777	h
1.69283500661777	1.69283500661777	-1.69283500661777	h
#GeO			
0.000000000000000	0.000000000000000	-1.55696412775958	ge
0.000000000000000	0.000000000000000	1.55696412775958	o
#GeO2			
0.000000000000000	0.000000000000000	0.000000000000000	ge
0.000000000000000	0.000000000000000	3.09562411619127	o
0.000000000000000	0.000000000000000	-3.09562411619127	o
#HBr			
0.000000000000000	0.000000000000000	-1.35667371651595	h
0.000000000000000	0.000000000000000	1.35667371651595	br
#HBr3			
0.000000000000000	0.000000000000000	0.22579559169999	c
0.000000000000000	0.000000000000000	2.30613641574210	h
1.76507167530612	-3.05719382063092	-0.84397733581403	br
1.76507167530612	3.05719382063092	-0.84397733581403	br
-3.53014335061225	0.000000000000000	-0.84397733581403	br
#Se8			
4.73473332107232	-1.96119075580796	1.08203483157154	se
1.96119075580796	4.73473332107232	1.08203483157154	se
-4.73473332107232	1.96119075580796	1.08203483157154	se
-1.96119075580796	-4.73473332107232	1.08203483157154	se
4.73473332107232	1.96119075580796	-1.08203483157154	se
-1.96119075580796	4.73473332107232	-1.08203483157154	se
-4.73473332107232	-1.96119075580796	-1.08203483157154	se
1.96119075580796	-4.73473332107232	-1.08203483157154	se
#SeH2			
0.000000000000000	0.000000000000000	1.31443756714499	se
-1.99442696033084	0.000000000000000	-0.65721878357249	h
1.99442696033084	0.000000000000000	-0.65721878357249	h
#SeO			
0.000000000000000	0.000000000000000	-1.58117857273827	se
0.000000000000000	0.000000000000000	1.58117857273827	o
#SeO2			
0.000000000000000	0.000000000000000	1.10091950638887	se
-2.61260008861725	0.000000000000000	-0.55045975319444	o
2.61260008861725	0.000000000000000	-0.55045975319444	o
#I2			
0.000000000000000	0.000000000000000	-2.58717910006003	i
0.000000000000000	0.000000000000000	2.58717910006003	i
#ICl			
0.000000000000000	0.000000000000000	-2.27749291163188	i
0.000000000000000	0.000000000000000	2.27749291163189	cl
#IH			
0.000000000000000	0.000000000000000	-1.54901575226915	i
0.000000000000000	0.000000000000000	1.54901575226915	h
#IO4-			
0.000000000000000	0.000000000000000	0.000000000000000	i
2.03119023188409	-2.03119023188409	2.03119023188409	o
-2.03119023188409	2.03119023188409	2.03119023188409	o
-2.03119023188409	-2.03119023188409	-2.03119023188409	o
2.03119023188409	2.03119023188409	-2.03119023188409	o
#InCl			
0.000000000000000	0.000000000000000	-2.28501380453881	in

0.0000000000000000	0.0000000000000000	2.28501380453881	cl
#InCl3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	in
-2.18888514352907	3.79126028052504	0.0000000000000000	cl
-2.18888514352907	-3.79126028052504	0.0000000000000000	cl
4.37777028705814	0.0000000000000000	0.0000000000000000	cl
#InH			
0.0000000000000000	0.0000000000000000	-1.77323971157117	in
0.0000000000000000	0.0000000000000000	1.77323971157117	h
#InH3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	in
-1.65719731255026	2.87034994350365	0.0000000000000000	h
-1.65719731255026	-2.87034994350365	0.0000000000000000	h
3.31439462510052	0.0000000000000000	0.0000000000000000	h
#InO			
0.0000000000000000	0.0000000000000000	-1.77046376816122	in
0.0000000000000000	0.0000000000000000	1.77046376816122	o
#SbCl6-			
0.0000000000000000	0.0000000000000000	0.0000000000000000	sb
0.0000000000000000	4.64447503829980	0.0000000000000000	cl
0.0000000000000000	0.0000000000000000	4.64447503829980	cl
4.64447503829980	0.0000000000000000	0.0000000000000000	cl
0.0000000000000000	0.0000000000000000	-4.64447503829980	cl
-4.64447503829980	0.0000000000000000	0.0000000000000000	cl
0.0000000000000000	-4.64447503829980	0.0000000000000000	cl
#SbF			
0.0000000000000000	0.0000000000000000	-1.86318815100045	sb
0.0000000000000000	0.0000000000000000	1.86318815100045	f
#SbF3			
0.0000000000000000	0.0000000000000000	1.41635010067847	sb
-1.57661128992144	2.73077085793065	-0.47211670022616	f
-1.57661128992144	-2.73077085793065	-0.47211670022616	f
3.15322257984289	0.0000000000000000	-0.47211670022616	f
#SbH3			
0.0000000000000000	0.0000000000000000	1.40288124678412	sb
1.34916589534128	-2.33682387857025	-0.46762708226138	h
1.34916589534128	2.33682387857025	-0.46762708226138	h
-2.69833179068256	0.0000000000000000	-0.46762708226138	h
#SbO2			
0.0000000000000000	0.0000000000000000	1.18120858212824	sb
3.08998758817836	0.0000000000000000	-0.59060429106412	o
-3.08998758817836	0.0000000000000000	-0.59060429106412	o
#SnF3			
0.0000000000000000	0.0000000000000000	1.07456818814013	sn
1.71243475756358	-2.96602400474702	-0.35818939604671	f
1.71243475756358	2.96602400474702	-0.35818939604671	f
-3.42486951512717	0.0000000000000000	-0.35818939604671	f
#SnH4			
0.0000000000000000	0.0000000000000000	0.0000000000000000	sn
1.89044177023958	-1.89044177023958	1.89044177023958	h
-1.89044177023958	1.89044177023958	1.89044177023958	h
-1.89044177023958	-1.89044177023958	-1.89044177023958	h
1.89044177023958	1.89044177023958	-1.89044177023958	h
#SnO			
0.0000000000000000	0.0000000000000000	-1.76719363698803	sn
0.0000000000000000	0.0000000000000000	1.76719363698803	o
#SnO2			

0.0000000000000000	0.0000000000000000	0.00163548812459	sn
-3.51460840178293	0.0000000000000000	-0.00081774406230	o
3.51460840178293	0.0000000000000000	-0.00081774406230	o
#TeF3			
0.0000000000000000	0.0000000000000000	0.35475666747305	te
-1.87725312652868	3.25149779381520	-0.11825222249101	f
-1.87725312652868	-3.25149779381520	-0.11825222249101	f
3.75450625305736	0.0000000000000000	-0.11825222249101	f
#TeH2			
0.0000000000000000	0.0000000000000000	1.49820193039170	te
-2.24906865611118	0.0000000000000000	-0.74910096519585	h
2.24906865611118	0.0000000000000000	-0.74910096519585	h
#TeO			
0.0000000000000000	0.0000000000000000	-1.77896181226445	te
0.0000000000000000	0.0000000000000000	1.77896181226445	o
#TeO2			
0.0000000000000000	0.0000000000000000	1.29984292231352	te
-2.88498675314837	0.0000000000000000	-0.64992146115676	o
2.88498675314837	0.0000000000000000	-0.64992146115676	o
#XeF2			
0.0000000000000000	0.0000000000000000	0.0000000000000000	xe
0.0000000000000000	0.0000000000000000	3.90757878328295	f
0.0000000000000000	0.0000000000000000	-3.90757878328295	f
#XeF4			
0.0000000000000000	0.0000000000000000	0.0000000000000000	xe
2.72236103703447	-2.72236103703447	0.0000000000000000	f
2.72236103703447	2.72236103703447	0.0000000000000000	f
-2.72236103703447	2.72236103703447	0.0000000000000000	f
-2.72236103703447	-2.72236103703447	0.0000000000000000	f
#XeOF4			
0.0000000000000000	0.0000000000000000	-0.39099828949089	xe
0.0000000000000000	0.0000000000000000	3.04665434896357	o
2.70138310369918	-2.70138310369918	-0.66391401486817	f
2.70138310369918	2.70138310369918	-0.66391401486817	f
-2.70138310369918	2.70138310369918	-0.66391401486817	f
-2.70138310369918	-2.70138310369918	-0.66391401486817	f
#BiCl6-			
0.0000000000000000	0.0000000000000000	0.0000000000000000	bi
0.0000000000000000	4.82554937284918	0.0000000000000000	cl
0.0000000000000000	0.0000000000000000	4.82554937284918	cl
0.0000000000000000	-4.82554937284918	0.0000000000000000	cl
0.0000000000000000	0.0000000000000000	-4.82554937284918	cl
4.82554937284918	0.0000000000000000	0.0000000000000000	cl
-4.82554937284918	0.0000000000000000	0.0000000000000000	cl
#BiF			
0.0000000000000000	0.0000000000000000	-1.93137769997131	bi
0.0000000000000000	0.0000000000000000	1.93137769997131	f
#BiF3			
0.0000000000000000	0.0000000000000000	1.46232798160630	bi
1.63662897536318	-2.83472453846842	-0.48744266053543	f
1.63662897536318	2.83472453846842	-0.48744266053543	f
-3.27325795072636	0.0000000000000000	-0.48744266053543	f
#BiH3			
0.0000000000000000	0.0000000000000000	1.47386771700502	bi
1.40843659350503	-2.43948373918995	-0.49128923900167	h
1.40843659350503	2.43948373918995	-0.49128923900167	h
-2.81687318701006	0.0000000000000000	-0.49128923900167	h

#BiO2	0.0000000000000000	0.0000000000000000	1.37289088296138	bi
	-3.15041062335303	0.0000000000000000	-0.68644544148069	o
	3.15041062335303	0.0000000000000000	-0.68644544148069	o
#PbF3	0.0000000000000000	0.0000000000000000	1.10329818701537	pb
	-1.78036242435008	3.08367817486085	-0.36776606233846	f
	-1.78036242435008	-3.08367817486085	-0.36776606233846	f
	3.56072484870017	0.0000000000000000	-0.36776606233846	f
#PbH4	0.0000000000000000	0.0000000000000000	0.0000000000000000	pb
	1.91301550123300	-1.91301550123300	1.91301550123300	h
	-1.91301550123300	1.91301550123300	1.91301550123300	h
	-1.91301550123300	-1.91301550123300	-1.91301550123300	h
	1.91301550123300	1.91301550123300	-1.91301550123300	h
#PbO	0.0000000000000000	0.0000000000000000	-1.80754257937630	pb
	0.0000000000000000	0.0000000000000000	1.80754257937630	o
#PbO2	0.0000000000000000	0.0000000000000000	0.0000000000000000	pb
	0.0000000000000000	0.0000000000000000	3.61357863592328	o
	0.0000000000000000	0.0000000000000000	-3.61357863592328	o
#TlCl	0.0000000000000000	0.0000000000000000	-2.38342001986092	tl
	0.0000000000000000	0.0000000000000000	2.38342001986092	cl
#TlCl3	0.0000000000000000	0.0000000000000000	-0.01443837177572	tl
	-2.26117878730255	3.91647654460500	0.00481279059057	cl
	-2.26117878730255	-3.91647654460500	0.00481279059057	cl
	4.52235757460510	0.0000000000000000	0.00481279059057	cl
#TlH	0.0000000000000000	0.0000000000000000	-1.81347675018980	tl
	0.0000000000000000	0.0000000000000000	1.81347675018980	h
#TlH3	0.0000000000000000	0.0000000000000000	0.0000000000000000	tl
	-1.64536913789863	2.84986294404622	0.0000000000000000	h
	-1.64536913789863	-2.84986294404622	0.0000000000000000	h
	3.29073827579725	0.0000000000000000	0.0000000000000000	h
#TlO	0.0000000000000000	0.0000000000000000	-1.81795601245970	tl
	0.0000000000000000	0.0000000000000000	1.81795601245970	o
#CoCl3	0.0000000000000000	0.0000000000000000	0.0000000000000000	co
	2.00502719350387	-3.47280896970594	0.0000000000000000	cl
	2.00502719350387	3.47280896970594	0.0000000000000000	cl
	-4.01005438700775	0.0000000000000000	0.0000000000000000	cl
#CoF2	0.0000000000000000	0.0000000000000000	-0.01591379082412	co
	3.26355789294746	0.0000000000000000	0.00795689541206	f
	-3.26355789294746	0.0000000000000000	0.00795689541206	f
#CoF3	0.0000000000000000	0.0000000000000000	0.0000000000000000	co
	1.65123154872552	-2.86001693745324	0.0000000000000000	f
	1.65123154872552	2.86001693745324	0.0000000000000000	f
	-3.30246309745104	0.0000000000000000	0.0000000000000000	f
#CrCO6	0.0000000000000000	0.0000000000000000	0.0000000000000000	cr

0.0000000000000000	3.59171681854581	0.0000000000000000	c
0.0000000000000000	0.0000000000000000	3.59171681854581	c
3.59171681854581	0.0000000000000000	0.0000000000000000	c
0.0000000000000000	0.0000000000000000	-3.59171681854581	c
-3.59171681854581	0.0000000000000000	0.0000000000000000	c
0.0000000000000000	-3.59171681854581	0.0000000000000000	c
0.0000000000000000	5.77973936611907	0.0000000000000000	o
0.0000000000000000	0.0000000000000000	5.77973936611907	o
5.77973936611907	0.0000000000000000	0.0000000000000000	o
0.0000000000000000	0.0000000000000000	-5.77973936611907	o
-5.77973936611907	0.0000000000000000	0.0000000000000000	o
0.0000000000000000	-5.77973936611907	0.0000000000000000	o
#CrCl3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	cr
2.02495084056461	-3.50731773868720	0.0000000000000000	cl
2.02495084056461	3.50731773868720	0.0000000000000000	cl
-4.04990168112921	0.0000000000000000	0.0000000000000000	cl
#CrF3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	cr
1.63137792162153	-2.82562944659461	0.0000000000000000	f
1.63137792162153	2.82562944659461	0.0000000000000000	f
-3.26275584324306	0.0000000000000000	0.0000000000000000	f
#CrO3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	cr
-1.50063115995876	2.59916941246959	0.0000000000000000	o
-1.50063115995876	-2.59916941246959	0.0000000000000000	o
3.00126231991752	0.0000000000000000	0.0000000000000000	o
#Cu2			
0.0000000000000000	0.0000000000000000	-2.07387116344728	cu
0.0000000000000000	0.0000000000000000	2.07387116344728	cu
#Cu2O			
0.0000000000000000	0.0000000000000000	1.63312192704579	o
2.28854347532692	0.0000000000000000	-0.81656096352289	cu
-2.28854347532692	0.0000000000000000	-0.81656096352289	cu
#Cu2S			
0.0000000000000000	0.0000000000000000	2.19080233145777	s
-2.28384138036123	0.0000000000000000	-1.09540116572889	cu
2.28384138036123	0.0000000000000000	-1.09540116572889	cu
#CuCN			
0.0000000000000000	0.0000000000000000	-3.01968451426437	cu
0.0000000000000000	0.0000000000000000	0.39611548720036	c
0.0000000000000000	0.0000000000000000	2.62356902706402	n
#CuCl			
0.0000000000000000	0.0000000000000000	-1.95954303758138	cu
0.0000000000000000	0.0000000000000000	1.95954303758138	cl
#CuF			
0.0000000000000000	0.0000000000000000	-1.64676654637877	cu
0.0000000000000000	0.0000000000000000	1.64676654637877	f
#CuH			
0.0000000000000000	0.0000000000000000	-1.37926640891550	cu
0.0000000000000000	0.0000000000000000	1.37926640891550	h
#FeCO5			
0.0000000000000000	0.0000000000000000	0.0000000000000000	fe
1.70357480283978	-2.95067811301262	0.0000000000000000	c
1.70357480283978	2.95067811301262	0.0000000000000000	c
-3.40714960567955	0.0000000000000000	0.0000000000000000	c
0.0000000000000000	0.0000000000000000	3.40816318478371	c

0.0000000000000000	0.0000000000000000	-3.40816318478371	c
2.79922085086665	-4.84839273530721	0.0000000000000000	o
2.79922085086665	4.84839273530721	0.0000000000000000	o
-5.59844170173329	0.0000000000000000	0.0000000000000000	o
0.0000000000000000	0.0000000000000000	5.59447063964439	o
0.0000000000000000	0.0000000000000000	-5.59447063964439	o
#FeF2			
0.0000000000000000	0.0000000000000000	0.0000000000000000	fe
3.29988416615965	0.0000000000000000	0.0000000000000000	f
-3.29988416615965	0.0000000000000000	0.0000000000000000	f
#FeF3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	fe
1.67360598116772	-2.89877059123365	0.0000000000000000	f
1.67360598116772	2.89877059123365	0.0000000000000000	f
-3.34721196233544	0.0000000000000000	0.0000000000000000	f
#FeO			
-0.66907143281002	0.0000000000000000	0.0000000000000000	fe
2.33556505384199	0.0000000000000000	0.0000000000000000	o
#Ferrocen			
0.0000000000000000	0.0000000000000000	0.0000000000000000	fe
2.31561104541701	0.0000000000000000	3.09927116392114	c
0.71556316539619	2.20227697394888	3.09927116392114	c
-1.87336868810470	1.36108202254167	3.09927116392114	c
-1.87336868810470	-1.36108202254167	3.09927116392114	c
0.71556316539619	-2.20227697394888	3.09927116392114	c
2.31561104541701	0.0000000000000000	-3.09927116392114	c
0.71556316539619	-2.20227697394888	-3.09927116392114	c
-1.87336868810470	-1.36108202254167	-3.09927116392114	c
-1.87336868810470	1.36108202254167	-3.09927116392114	c
0.71556316539619	2.20227697394888	-3.09927116392114	c
4.38900985665904	0.0000000000000000	3.08518706538327	h
1.35627863418680	4.17419642425924	3.08518706538327	h
-3.55078356251632	2.57979526591049	3.08518706538327	h
-3.55078356251632	-2.57979526591049	3.08518706538327	h
1.35627863418680	-4.17419642425924	3.08518706538327	h
4.38900985665904	0.0000000000000000	-3.08518706538327	h
1.35627863418680	-4.17419642425924	-3.08518706538327	h
-3.55078356251632	-2.57979526591049	-3.08518706538327	h
-3.55078356251632	2.57979526591049	-3.08518706538327	h
1.35627863418680	4.17419642425924	-3.08518706538327	h
#MnF2			
0.0000000000000000	0.0000000000000000	0.0000000000000000	mn
0.0000000000000000	0.0000000000000000	3.36165918231541	f
0.0000000000000000	0.0000000000000000	-3.36165918231541	f
#MnO			
0.0000000000000000	0.0000000000000000	-1.52065965443162	mn
0.0000000000000000	0.0000000000000000	1.52065965443162	o
#MnO2			
0.0000000000000000	0.0000000000000000	0.91350357143973	mn
2.66795187804954	0.0000000000000000	-0.45675178571986	o
-2.66795187804954	0.0000000000000000	-0.45675178571986	o
#MnO3F			
0.0000000000000000	0.0000000000000000	-0.07330413800993	mn
0.0000000000000000	0.0000000000000000	3.16649627047248	f
1.40721736620792	-2.43737197556538	-1.03106404415419	o
1.40721736620792	2.43737197556538	-1.03106404415419	o
-2.81443473241584	0.0000000000000000	-1.03106404415419	o

#MnO4-	0.0000000000000000	0.0000000000000000	0.0000000000000000	mn
	1.75938547049818	-1.75938547049818	1.75938547049818	o
	-1.75938547049818	1.75938547049818	1.75938547049818	o
	-1.75938547049818	-1.75938547049818	-1.75938547049818	o
	1.75938547049818	1.75938547049818	-1.75938547049818	o
#MnS	0.0000000000000000	0.0000000000000000	-1.92619713055598	mn
	0.0000000000000000	0.0000000000000000	1.92619713055598	s
#NiCO4	0.0000000000000000	0.0000000000000000	0.0000000000000000	ni
	1.98326378231725	-1.98326378231725	1.98326378231725	c
	-1.98326378231725	1.98326378231725	1.98326378231725	c
	-1.98326378231725	-1.98326378231725	-1.98326378231725	c
	1.98326378231725	1.98326378231725	-1.98326378231725	c
	3.24273654096679	-3.24273654096679	3.24273654096679	o
	-3.24273654096679	3.24273654096679	3.24273654096679	o
	-3.24273654096679	-3.24273654096679	-3.24273654096679	o
	3.24273654096679	3.24273654096679	-3.24273654096679	o
#NiCl2	0.0000000000000000	0.0000000000000000	0.00232084864856	ni
	-3.96670138124145	0.0000000000000000	-0.00116042432428	cl
	3.96670138124145	0.0000000000000000	-0.00116042432428	cl
#NiF2	0.0000000000000000	0.0000000000000000	0.0000000000000000	ni
	0.0000000000000000	0.0000000000000000	-3.26603962131760	f
	0.0000000000000000	0.0000000000000000	3.26603962131760	f
#NiF3	0.0000000000000000	0.0000000000000000	0.00152306552660	ni
	-1.66351766562508	2.88129711615101	-0.00050768850887	f
	-1.66351766562508	-2.88129711615101	-0.00050768850887	f
	3.32703533125016	0.0000000000000000	-0.00050768850887	f
#NiO	0.0000000000000000	0.0000000000000000	-1.51749092920855	ni
	0.0000000000000000	0.0000000000000000	1.51749092920855	o
#NiS	0.0000000000000000	0.0000000000000000	-1.85681514730456	ni
	0.0000000000000000	0.0000000000000000	1.85681514730456	s
#ScCl3	0.0000000000000000	0.0000000000000000	0.0000000000000000	sc
	2.15416668810895	-3.73112615177708	0.0000000000000000	cl
	2.15416668810895	3.73112615177708	0.0000000000000000	cl
	-4.30833337621790	0.0000000000000000	0.0000000000000000	cl
#ScF3	0.0000000000000000	0.0000000000000000	0.0000000000000000	sc
	1.73202055035891	-2.99994759297505	0.0000000000000000	f
	1.73202055035891	2.99994759297505	0.0000000000000000	f
	-3.46404110071783	0.0000000000000000	0.0000000000000000	f
#ScH3	0.0000000000000000	0.0000000000000000	0.0000000000000000	sc
	1.71347214324408	-2.96782080945268	0.0000000000000000	h
	1.71347214324408	2.96782080945268	0.0000000000000000	h
	-3.42694428648816	0.0000000000000000	0.0000000000000000	h
#ScO	0.0000000000000000	0.0000000000000000	-1.57175591846256	sc
	0.0000000000000000	0.0000000000000000	1.57175591846256	o
#TiCO4				

0.0000000000000000	0.0000000000000000	0.0000000000000000	ti
2.25209609785139	-2.25209609785139	2.25209609785139	c
-2.25209609785139	2.25209609785139	2.25209609785139	c
-2.25209609785139	-2.25209609785139	-2.25209609785139	c
2.25209609785139	2.25209609785139	-2.25209609785139	c
3.52294080235074	-3.52294080235074	3.52294080235074	o
-3.52294080235074	3.52294080235074	3.52294080235074	o
-3.52294080235074	-3.52294080235074	-3.52294080235074	o
3.52294080235074	3.52294080235074	-3.52294080235074	o
#TiCl4			
0.0000000000000000	0.0000000000000000	0.0000000000000000	ti
2.38225918250055	-2.38225918250055	2.38225918250055	cl
-2.38225918250055	2.38225918250055	2.38225918250055	cl
-2.38225918250055	-2.38225918250055	-2.38225918250055	cl
2.38225918250055	2.38225918250055	-2.38225918250055	cl
#TiF3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	ti
1.67141378359608	-2.89497359365934	0.0000000000000000	f
1.67141378359608	2.89497359365934	0.0000000000000000	f
-3.34282756719215	0.0000000000000000	0.0000000000000000	f
#TiF4			
0.0000000000000000	0.0000000000000000	0.0000000000000000	ti
1.91049002205680	-1.91049002205680	1.91049002205680	f
-1.91049002205680	1.91049002205680	1.91049002205680	f
-1.91049002205680	-1.91049002205680	-1.91049002205680	f
1.91049002205680	1.91049002205680	-1.91049002205680	f
#TiH4			
0.0000000000000000	0.0000000000000000	0.0000000000000000	ti
1.85401673992524	-1.85401673992524	1.85401673992524	h
-1.85401673992524	1.85401673992524	1.85401673992524	h
-1.85401673992524	-1.85401673992524	-1.85401673992524	h
1.85401673992524	1.85401673992524	-1.85401673992524	h
#TiO			
0.0000000000000000	0.0000000000000000	-1.52666508702031	ti
0.0000000000000000	0.0000000000000000	1.52666508702031	o
#TiO2			
0.0000000000000000	0.0000000000000000	1.20428895304113	ti
-2.52745691819368	0.0000000000000000	-0.60214447652056	o
2.52745691819368	0.0000000000000000	-0.60214447652056	o
#TiS2			
0.0000000000000000	0.0000000000000000	1.47408703528939	ti
-3.26474084717958	0.0000000000000000	-0.73704351764470	s
3.26474084717958	0.0000000000000000	-0.73704351764470	s
#VH5			
0.19112681055705	0.02226992514811	-0.53930273355572	v
1.21909073594429	0.14802719321707	-3.48934725444155	h
1.35539695757176	-1.88711320691551	1.52413775854092	h
1.36313902267154	1.74011620101324	1.68211209473418	h
-2.05809542406512	1.79208170165047	0.49003911695103	h
-2.07065810267952	-1.81538181411337	0.33236101777113	h
#VO			
0.0000000000000000	0.0000000000000000	-1.49605986356322	v
0.0000000000000000	0.0000000000000000	1.49605986356322	o
#VOF3			
0.0000000000000000	0.0000000000000000	0.02138488636646	v
0.0000000000000000	0.0000000000000000	2.99447623694060	o
-1.54851197430779	2.68210141562988	-1.00528704110235	f

-1.54851197430779	-2.68210141562988	-1.00528704110235	f
3.09702394861558	0.00000000000000	-1.00528704110235	f
#ZnCl2			
0.00000000000000	0.00000000000000	0.00000000000000	zn
0.00000000000000	0.00000000000000	3.97259040076298	cl
0.00000000000000	0.00000000000000	-3.97259040076298	cl
#ZnF2			
0.00000000000000	0.00000000000000	0.00000000000000	zn
0.00000000000000	0.00000000000000	3.28287621534218	f
0.00000000000000	0.00000000000000	-3.28287621534218	f
#ZnH2			
0.00000000000000	0.00000000000000	0.00000000000000	zn
0.00000000000000	0.00000000000000	-2.92711569055511	h
0.00000000000000	0.00000000000000	2.92711569055511	h
#ZnMe2			
3.68342584557891	0.00005713689622	0.00026506182462	c
-3.68356713887322	0.00023772392501	0.00027909608166	c
4.44876667227890	1.40886676936816	-1.35377226518157	h
4.44905348065180	-1.87650086846691	-0.54356099559000	h
4.45013283461305	0.46800749693417	1.89658631099636	h
-4.44857871394426	1.21933922067696	-1.52675501888773	h
-4.45004569978716	0.71048953578705	1.82005490636899	h
-4.44913036491722	-1.93120927472341	-0.29420173043471	h
-0.00005691560083	0.00071225960275	0.00110463482239	zn
#Ag2			
0.00000000000000	0.00000000000000	-2.43284975341900	ag
0.00000000000000	0.00000000000000	2.43284975341900	ag
#AgCl			
0.00000000000000	0.00000000000000	-2.17427221124677	ag
0.00000000000000	0.00000000000000	2.17427221124677	cl
#CdF2			
0.00000000000000	0.00000000000000	0.00000000000000	cd
0.00000000000000	0.00000000000000	3.65399698977701	f
0.00000000000000	0.00000000000000	-3.65399698977701	f
#CdMe2			
-0.01552765207821	-0.00211074960291	-0.00256455209819	cd
-0.00518470223702	-0.00014740649893	4.03174197678488	c
-0.00362618205013	-0.00022460589332	-4.02970589844624	c
1.03909570930236	1.66912049287321	4.74981657043364	h
0.94231936085281	-1.72490849239420	4.75261331167082	h
-1.95136186467702	0.05616956014136	4.80782591209543	h
-1.54974432309212	-1.20222871244731	-4.77501608328692	h
1.81386811131603	-0.73818341030734	-4.76612177697937	h
-0.26983845733673	1.94251332412944	-4.76858946017406	h
#MoCO6			
0.00000000000000	0.00000000000000	0.00000000000000	mo
0.00000000000000	3.90295652556995	0.00000000000000	c
0.00000000000000	0.00000000000000	3.90295652556995	c
3.90295652556995	0.00000000000000	0.00000000000000	c
0.00000000000000	0.00000000000000	-3.90295652556995	c
-3.90295652556995	0.00000000000000	0.00000000000000	c
0.00000000000000	-3.90295652556995	0.00000000000000	c
0.00000000000000	6.09006160839460	0.00000000000000	o
0.00000000000000	0.00000000000000	6.09006160839460	o
6.09006160839460	0.00000000000000	0.00000000000000	o
0.00000000000000	0.00000000000000	-6.09006160839460	o
-6.09006160839460	0.00000000000000	0.00000000000000	o

0.0000000000000000	-6.09006160839460	0.0000000000000000	o
#MoF3			
0.0000000000000000	0.0000000000000000	-0.00159671171885	mo
1.77637872237622	-3.07677820063990	0.00053223723962	f
1.77637872237622	3.07677820063990	0.00053223723962	f
-3.55275744475244	0.0000000000000000	0.00053223723962	f
#MoH			
0.0000000000000000	0.0000000000000000	-1.62042478286011	mo
0.0000000000000000	0.0000000000000000	1.62042478286011	h
#MoO2			
0.0000000000000000	0.0000000000000000	1.20329050676615	mo
2.70432477568260	0.0000000000000000	-0.60164525338307	o
-2.70432477568260	0.0000000000000000	-0.60164525338307	o
#MoO3			
0.0000000000000000	0.0000000000000000	-0.87497023552764	mo
-1.52984968466562	2.64977738178409	0.29165674517588	o
-1.52984968466562	-2.64977738178409	0.29165674517588	o
3.05969936933125	0.0000000000000000	0.29165674517588	o
#NbF3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	nb
-1.76123486076723	3.05054826291034	0.0000000000000000	f
-1.76123486076723	-3.05054826291034	0.0000000000000000	f
3.52246972153446	0.0000000000000000	0.0000000000000000	f
#NbO			
0.0000000000000000	0.0000000000000000	1.61827909896555	nb
0.0000000000000000	0.0000000000000000	-1.61827909896555	o
#NbO2			
0.0000000000000000	0.0000000000000000	1.35090407793570	nb
2.58725120191969	0.0000000000000000	-0.67545203896785	o
-2.58725120191969	0.0000000000000000	-0.67545203896785	o
#NbO2F			
-0.02610891780556	0.86342528822632	0.06758988948919	nb
2.62395976524113	0.01237672503655	-1.69666564370223	o
-2.62102600254883	-0.14687228651066	-1.69136676770083	o
0.02317515511327	-0.72892972675222	3.32044252191387	f
#PdCO4			
0.00000919143467	0.00000531380106	-0.00001191622877	pd
2.18351277656177	2.18350949811326	2.18351805760958	c
-2.18350195361372	-2.18350090015659	2.18350128273601	c
2.18351494366302	-2.18352263605300	-2.18351671330313	c
-2.18351964856344	2.18351087841231	-2.18351593700892	c
3.44064404148229	3.44064088770018	3.44067413451479	o
-3.44064406985283	-3.44062025793711	3.44067735832652	o
3.44066163241694	-3.44068081079362	-3.44066336280415	o
-3.44067691352870	3.44065802691347	-3.44066290384197	o
#PdF			
0.0000000000000000	0.0000000000000000	-1.82090621303246	pd
0.0000000000000000	0.0000000000000000	1.82090621303246	f
#PdO2			
0.0000000000000000	0.0000000000000000	0.00368780697011	pd
-3.56296972714997	0.0000000000000000	-0.00184390348506	o
3.56296972714997	0.0000000000000000	-0.00184390348506	o
#RhF			
0.0000000000000000	0.0000000000000000	-1.80303434766506	rh
0.0000000000000000	0.0000000000000000	1.80303434766506	f
#RhF4			
0.0000000000000000	0.0000000000000000	0.0000000000000000	rh

2.11095283269456	-2.11095283269456	2.11095283269456	f
-2.11095283269456	2.11095283269456	2.11095283269456	f
-2.11095283269456	-2.11095283269456	-2.11095283269456	f
2.11095283269456	2.11095283269456	-2.11095283269456	f
#RhF6			
0.000000000000000	0.000000000000000	0.000000000000000	rh
2.51299833250292	-2.51299833250292	0.000000000000000	f
2.51299833250292	2.51299833250292	0.000000000000000	f
-2.51299833250292	2.51299833250292	0.000000000000000	f
-2.51299833250292	-2.51299833250292	0.000000000000000	f
0.000000000000000	0.000000000000000	3.55393480343994	f
0.000000000000000	0.000000000000000	-3.55393480343994	f
#RhO			
0.000000000000000	0.000000000000000	-1.63450098884323	rh
0.000000000000000	0.000000000000000	1.63450098884323	o
#RuCO5			
0.000000000000000	0.000000000000000	0.000000000000000	ru
1.84480011535838	-3.19528752960964	0.000000000000000	c
1.84480011535838	3.19528752960964	0.000000000000000	c
-3.68960023071676	0.000000000000000	0.000000000000000	c
0.000000000000000	0.000000000000000	3.69125554048716	c
0.000000000000000	0.000000000000000	-3.69125554048716	c
2.94039490193387	-5.09291336446596	0.000000000000000	o
2.94039490193387	5.09291336446596	0.000000000000000	o
-5.88078980386773	0.000000000000000	0.000000000000000	o
0.000000000000000	0.000000000000000	5.87379294085885	o
0.000000000000000	0.000000000000000	-5.87379294085885	o
#RuF			
0.000000000000000	0.000000000000000	-1.79559672059692	ru
0.000000000000000	0.000000000000000	1.79559672059692	f
#RuO			
0.000000000000000	0.000000000000000	-1.63370929862074	ru
0.000000000000000	0.000000000000000	1.63370929862074	o
#RuO2			
0.000000000000000	0.000000000000000	0.000000000000000	ru
0.000000000000000	0.000000000000000	3.22936844775946	o
0.000000000000000	0.000000000000000	-3.22936844775946	o
#RuO4			
-0.00003901512132	-0.00004974867915	0.00003175074579	ru
1.87142850130396	1.87147977103538	1.87148905199029	o
-1.87142232278019	-1.87137312944410	1.87142093412647	o
1.87151789303364	-1.87153124203117	-1.87151937514838	o
-1.87148505643610	1.87147434911906	-1.87142236171416	o
#Tc2O7			
0.000000000000000	0.000000000000000	0.000000000000000	o
0.000000000000000	0.000000000000000	3.55098914866315	tc
0.000000000000000	0.000000000000000	-3.55098914866315	tc
2.62571861860354	-1.51595935126696	4.65860875354015	o
2.62571861860354	1.51595935126696	-4.65860875354015	o
0.000000000000000	3.03191870253393	4.65860875354015	o
-2.62571861860354	1.51595935126696	-4.65860875354015	o
-2.62571861860354	-1.51595935126696	4.65860875354015	o
0.000000000000000	-3.03191870253393	-4.65860875354015	o
#TcO			
0.000000000000000	0.000000000000000	-1.65131440458535	tc
0.000000000000000	0.000000000000000	1.65131440458535	o
#TcO3F			

0.0000000000000000	0.0000000000000000	-0.03575380241616	tc
0.0000000000000000	0.0000000000000000	3.47832150786421	f
1.51189127548743	-2.61867250466434	-1.14752256848268	o
1.51189127548743	2.61867250466434	-1.14752256848268	o
-3.02378255097485	0.0000000000000000	-1.14752256848268	o
#YF			
0.0000000000000000	0.0000000000000000	-1.84234806551158	y
0.0000000000000000	0.0000000000000000	1.84234806551158	f
#YF3			
0.0000000000000000	0.0000000000000000	0.00977112603694	y
-1.89922978387516	3.28956248091983	-0.00325704201177	f
-1.89922978387516	-3.28956248091983	-0.00325704201177	f
3.79845956775031	0.0000000000000000	-0.00325704201177	f
#YO			
0.0000000000000000	0.0000000000000000	-1.72806290572366	y
0.0000000000000000	0.0000000000000000	1.72806290572366	o
#ZrF			
0.0000000000000000	0.0000000000000000	-1.78049044438309	zr
0.0000000000000000	0.0000000000000000	1.78049044438309	f
#ZrF3			
0.0000000000000000	0.0000000000000000	0.00444657710922	zr
-1.82070257365541	3.15354936304259	-0.00148219236669	f
-1.82070257365541	-3.15354936304259	-0.00148219236669	f
3.64140514731082	0.0000000000000000	-0.00148219236669	f
#ZrO			
0.0000000000000000	0.0000000000000000	-1.66498802952802	zr
0.0000000000000000	0.0000000000000000	1.66498802952802	o
#ZrO2			
0.0000000000000000	0.0000000000000000	1.36096020616404	zr
-2.71171774062042	0.0000000000000000	-0.68048010308202	o
2.71171774062042	0.0000000000000000	-0.68048010308202	o
#Au2			
0.0000000000000000	0.0000000000000000	-2.42327065240856	au
0.0000000000000000	0.0000000000000000	2.42327065240856	au
#Au3-			
0.0000000000000000	0.0000000000000000	0.0000000000000000	au
0.0000000000000000	0.0000000000000000	4.97146253204511	au
0.0000000000000000	0.0000000000000000	-4.97146253204511	au
#AuCl			
0.0000000000000000	0.0000000000000000	-2.15000661513040	au
0.0000000000000000	0.0000000000000000	2.15000661513040	cl
#AuCl3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	au
2.21054988848081	-3.82878471951448	0.0000000000000000	cl
2.21054988848081	3.82878471951448	0.0000000000000000	cl
-4.42109977696162	0.0000000000000000	0.0000000000000000	cl
#HfF			
0.0000000000000000	0.0000000000000000	1.78068737689156	hf
0.0000000000000000	0.0000000000000000	-1.78068737689156	f
#HfF3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	hf
1.81947112203196	-3.15141642626371	0.0000000000000000	f
1.81947112203196	3.15141642626371	0.0000000000000000	f
-3.63894224406392	0.0000000000000000	0.0000000000000000	f
#HfO			
0.0000000000000000	0.0000000000000000	-1.66226332616427	hf
0.0000000000000000	0.0000000000000000	1.66226332616427	o

#HfO2				
	0.0000000000000000	0.0000000000000000	1.37910110648005	hf
	2.72240351204331	0.0000000000000000	-0.68955055324002	o
	-2.72240351204331	0.0000000000000000	-0.68955055324002	o
#HgF2				
	0.0000000000000000	0.0000000000000000	0.0000000000000000	hg
	0.0000000000000000	0.0000000000000000	-3.69723523229824	f
	0.0000000000000000	0.0000000000000000	3.69723523229824	f
#HgMe2				
	0.0000000000000000	0.0000000000000000	0.0000000000000000	hg
	0.0000000000000000	0.0000000000000000	4.03656130521134	c
	0.0000000000000000	0.0000000000000000	-4.03656130521134	c
	1.70138176612670	-0.98229322066757	4.76366724761748	h
	1.70138176612670	0.98229322066757	-4.76366724761748	h
	0.0000000000000000	1.96458644133514	4.76366724761748	h
	-1.70138176612670	0.98229322066757	-4.76366724761748	h
	-1.70138176612670	-0.98229322066757	4.76366724761748	h
	0.0000000000000000	-1.96458644133514	-4.76366724761748	h
#Hg2Cl2				
	-0.00092289111444	-2.49971029372210	0.0000000000000000	hg
	0.00086843425201	2.49894980264274	0.0000000000000000	hg
	0.00005416705884	-6.97426742991672	0.0000000000000000	cl
	0.00000028980360	6.97502792099608	0.0000000000000000	cl
#IrF6				
	0.0000000000000000	0.0000000000000000	0.0000000000000000	ir
	0.0000000000000000	0.0000000000000000	3.59726293025323	f
	0.0000000000000000	0.0000000000000000	-3.59726293025323	f
	2.54361009647590	-2.54361009647590	0.0000000000000000	f
	2.54361009647590	2.54361009647590	0.0000000000000000	f
	-2.54361009647590	2.54361009647590	0.0000000000000000	f
	-2.54361009647590	-2.54361009647590	0.0000000000000000	f
#OsCO5				
	0.0000000000000000	0.0000000000000000	0.0000000000000000	os
	1.86245714222963	-3.22587039726125	0.0000000000000000	c
	1.86245714222963	3.22587039726125	0.0000000000000000	c
	-3.72491428445925	0.0000000000000000	0.0000000000000000	c
	0.0000000000000000	0.0000000000000000	3.74847701997556	c
	0.0000000000000000	0.0000000000000000	-3.74847701997556	c
	2.95959230898802	-5.12616424885734	0.0000000000000000	o
	2.95959230898802	5.12616424885734	0.0000000000000000	o
	-5.91918461797604	0.0000000000000000	0.0000000000000000	o
	0.0000000000000000	0.0000000000000000	5.93170395303675	o
	0.0000000000000000	0.0000000000000000	-5.93170395303675	o
#OsO2				
	0.0000000000000000	0.0000000000000000	-0.90139173199185	os
	2.96334365356516	0.0000000000000000	0.45069586599592	o
	-2.96334365356516	0.0000000000000000	0.45069586599592	o
#OsO3				
	0.0000000000000000	0.0000000000000000	0.0000000000000000	os
	1.63177166219432	-2.82631142527168	0.0000000000000000	o
	1.63177166219432	2.82631142527168	0.0000000000000000	o
	-3.26354332438864	0.0000000000000000	0.0000000000000000	o
#OsO4				
	0.0000000000000000	0.0000000000000000	0.0000000000000000	os
	1.90033009057400	-1.90033009057400	1.90033009057400	o
	-1.90033009057400	1.90033009057400	1.90033009057400	o
	-1.90033009057400	-1.90033009057400	-1.90033009057400	o

1.90033009057400	1.90033009057400	-1.90033009057400	o
#OsOF5			
0.0000000000000000	0.0000000000000000	0.22822360502953	os
0.0000000000000000	0.0000000000000000	3.47998909744502	o
0.0000000000000000	0.0000000000000000	-3.39562990080580	f
-2.53530418774888	2.53530418774888	-0.07814570041718	f
-2.53530418774888	-2.53530418774888	-0.07814570041718	f
2.53530418774888	-2.53530418774888	-0.07814570041718	f
2.53530418774888	2.53530418774888	-0.07814570041718	f
#PtCO4			
0.0000000000000000	0.0000000000000000	0.0000000000000000	pt
2.17219503977633	-2.17219503977633	2.17219503977633	c
-2.17219503977633	2.17219503977633	2.17219503977633	c
-2.17219503977633	-2.17219503977633	-2.17219503977633	c
2.17219503977633	2.17219503977633	-2.17219503977633	c
3.43196912076035	-3.43196912076035	3.43196912076035	o
-3.43196912076035	3.43196912076035	3.43196912076035	o
-3.43196912076035	-3.43196912076035	-3.43196912076035	o
3.43196912076035	3.43196912076035	-3.43196912076035	o
#PtO			
0.0000000000000000	0.0000000000000000	-1.67069134020836	pt
0.0000000000000000	0.0000000000000000	1.67069134020836	o
#PtO2			
0.0000000000000000	0.0000000000000000	0.0000000000000000	pt
0.0000000000000000	0.0000000000000000	-3.28869598692728	o
0.0000000000000000	0.0000000000000000	3.28869598692728	o
#ReH			
0.0000000000000000	0.0000000000000000	-1.56532428006416	re
0.0000000000000000	0.0000000000000000	1.56532428006416	h
#ReO			
0.0000000000000000	0.0000000000000000	-1.67864437842535	re
0.0000000000000000	0.0000000000000000	1.67864437842535	o
#ReO2			
0.0000000000000000	0.0000000000000000	0.0000000000000000	re
0.0000000000000000	0.0000000000000000	-3.36557123070835	o
0.0000000000000000	0.0000000000000000	3.36557123070835	o
#ReO3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	re
-1.64935415797960	2.85676520129566	0.0000000000000000	o
-1.64935415797960	-2.85676520129566	0.0000000000000000	o
3.29870831595921	0.0000000000000000	0.0000000000000000	o
#ReO3F			
0.0000000000000000	0.0000000000000000	-0.00862182543285	re
0.0000000000000000	0.0000000000000000	3.55207214412449	f
-1.52651151621215	2.64399550441844	-1.18115010623055	o
-1.52651151621215	-2.64399550441844	-1.18115010623055	o
3.05302303242429	0.0000000000000000	-1.18115010623055	o
#TaF			
0.0000000000000000	0.0000000000000000	-1.73663852825574	ta
0.0000000000000000	0.0000000000000000	1.73663852825574	f
#TaF3			
0.0000000000000000	0.0000000000000000	-0.00088004990885	ta
-1.76481713541870	3.05675294461335	0.00029334996962	f
-1.76481713541870	-3.05675294461335	0.00029334996962	f
3.52963427083740	0.0000000000000000	0.00029334996962	f
#TaO2F			
0.0000000000000000	0.0000000000000000	0.03006542312973	ta

0.0000000000000000	0.0000000000000000	3.72739793762169	f
2.74274130577697	0.0000000000000000	-1.87873168037571	o
-2.74274130577697	0.0000000000000000	-1.87873168037571	o
#WCO6			
0.0000000000000000	0.0000000000000000	0.0000000000000000	w
0.0000000000000000	3.93720141856123	0.0000000000000000	c
0.0000000000000000	0.0000000000000000	3.93720141856123	c
3.93720141856123	0.0000000000000000	0.0000000000000000	c
0.0000000000000000	0.0000000000000000	-3.93720141856123	c
-3.93720141856123	0.0000000000000000	0.0000000000000000	c
0.0000000000000000	-3.93720141856123	0.0000000000000000	c
0.0000000000000000	6.12568593744740	0.0000000000000000	o
0.0000000000000000	0.0000000000000000	6.12568593744740	o
6.12568593744740	0.0000000000000000	0.0000000000000000	o
0.0000000000000000	0.0000000000000000	-6.12568593744740	o
-6.12568593744740	0.0000000000000000	0.0000000000000000	o
0.0000000000000000	-6.12568593744740	0.0000000000000000	o
#WF3			
0.0000000000000000	0.0000000000000000	0.00187166361740	w
-1.79324602416154	3.10599322431868	-0.00062388787247	f
-1.79324602416154	-3.10599322431868	-0.00062388787247	f
3.58649204832309	0.0000000000000000	-0.00062388787247	f
#WH			
0.0000000000000000	0.0000000000000000	-1.62254316912897	w
0.0000000000000000	0.0000000000000000	1.62254316912897	h
#WO			
0.0000000000000000	0.0000000000000000	-1.58822148469933	w
0.0000000000000000	0.0000000000000000	1.58822148469933	o
#WO2			
0.0000000000000000	0.0000000000000000	1.21145734769756	w
-2.74201323107353	0.0000000000000000	-0.60572867384878	o
2.74201323107353	0.0000000000000000	-0.60572867384878	o
#WO3			
0.0000000000000000	0.0000000000000000	0.0000000000000000	w
1.67015014718729	-2.89278491119702	0.0000000000000000	o
1.67015014718729	2.89278491119702	0.0000000000000000	o
-3.34030029437458	0.0000000000000000	0.0000000000000000	o