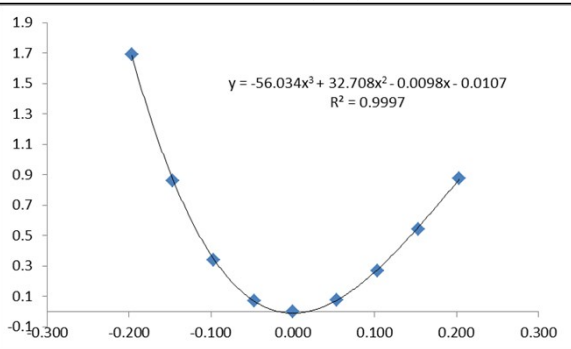
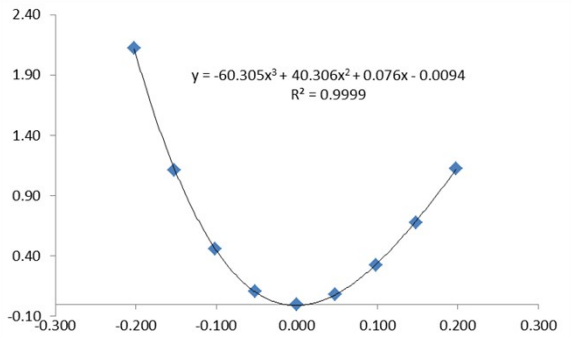
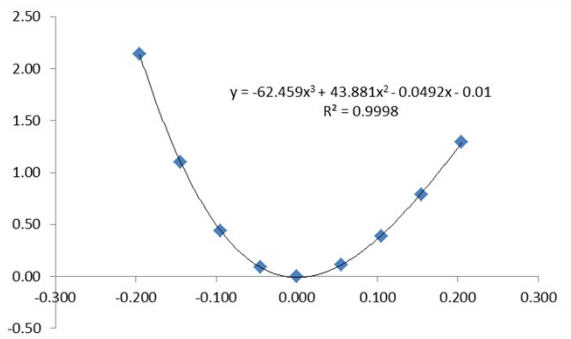
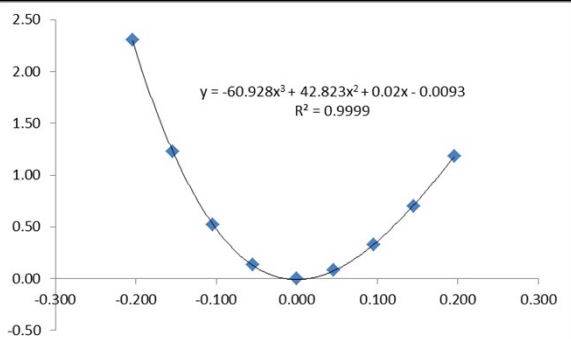
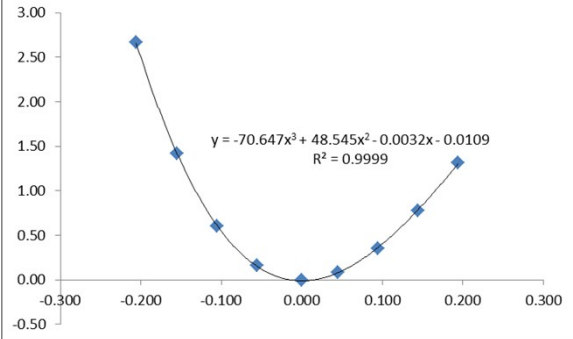
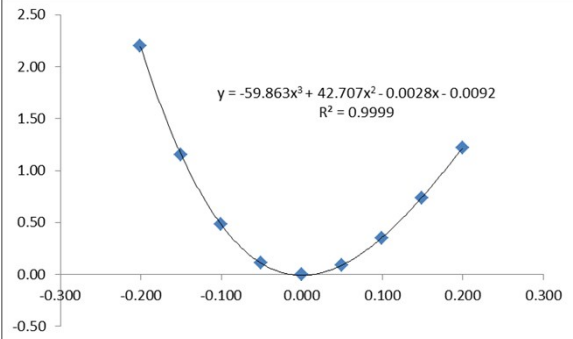
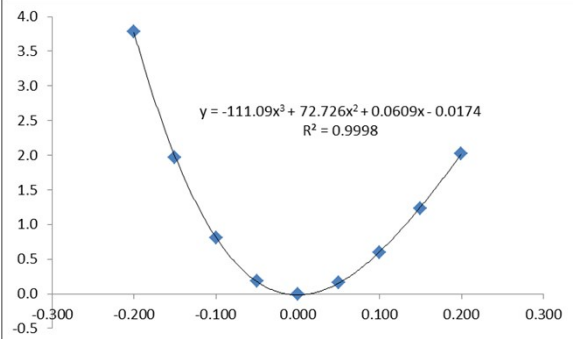
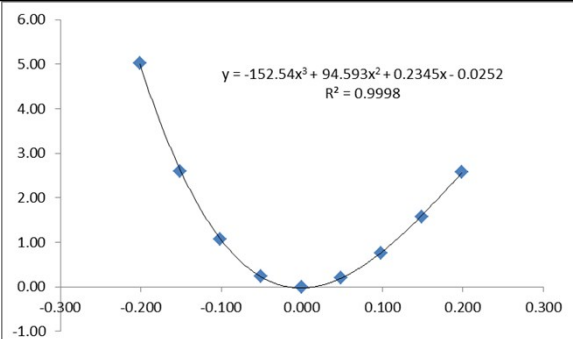
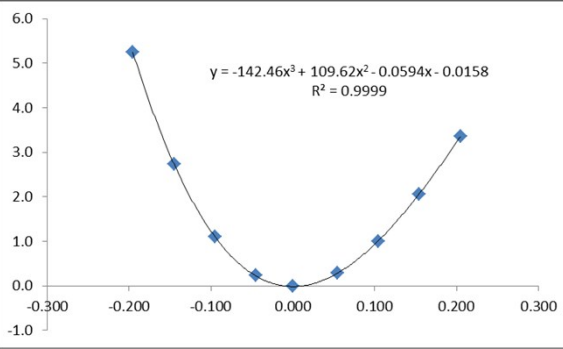
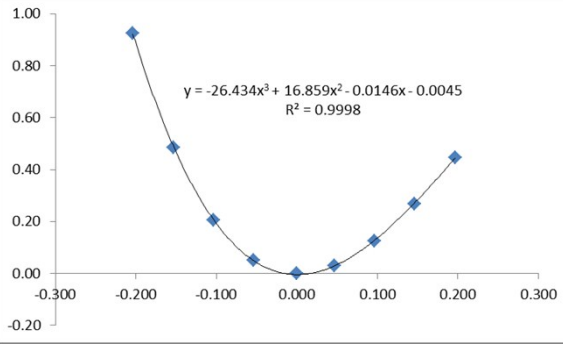
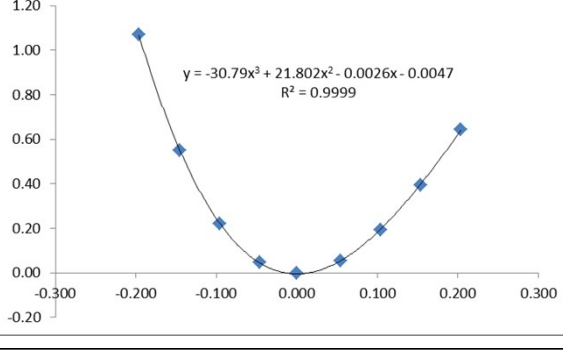
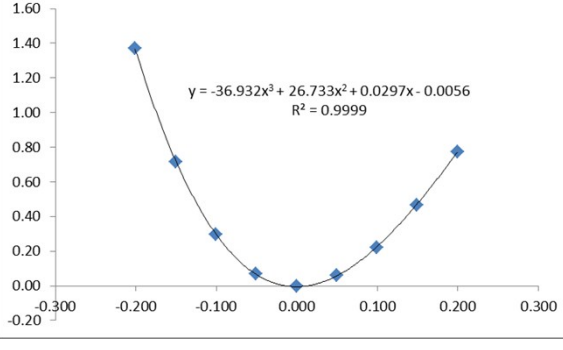


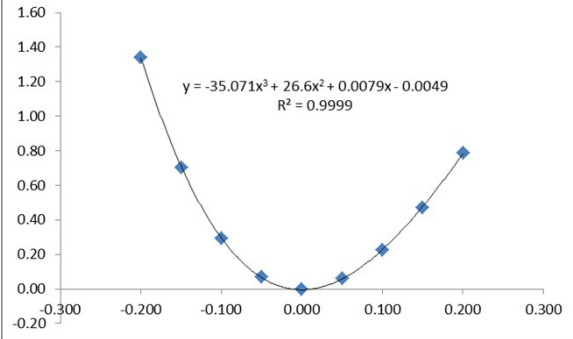
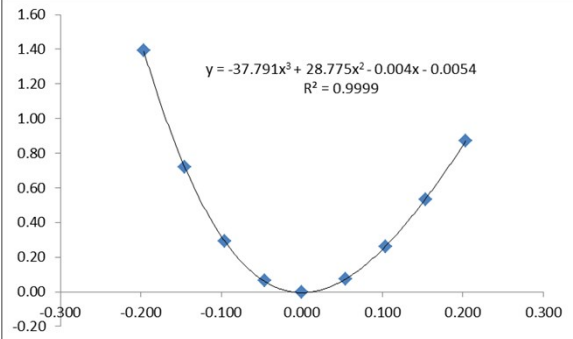
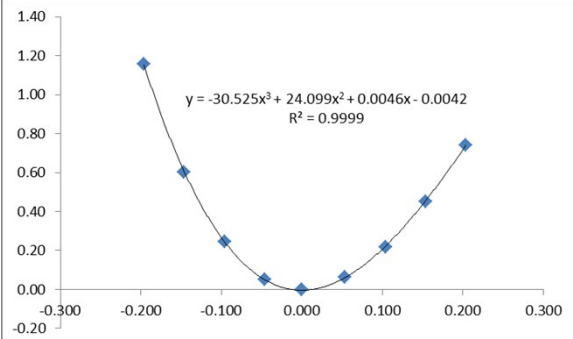
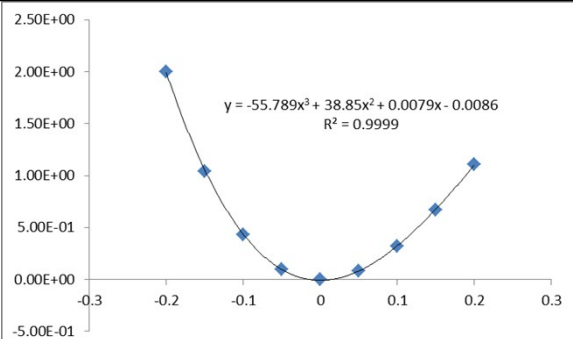
SUPPLEMENTARY MATERIAL FILE 2: E_r-E_{re} vs. $(r-r_e)$ data for forced constant calculations

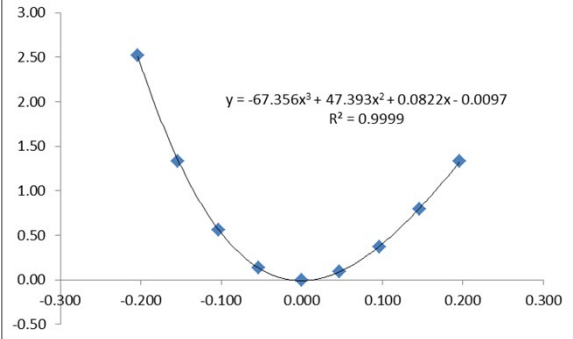
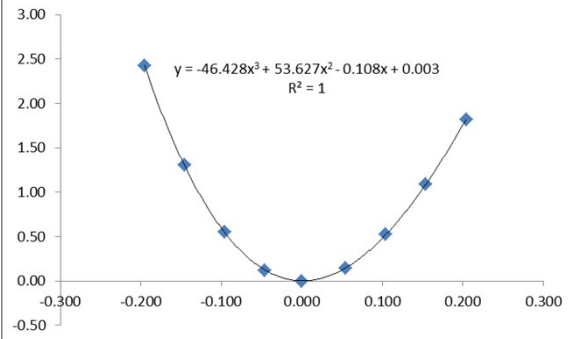
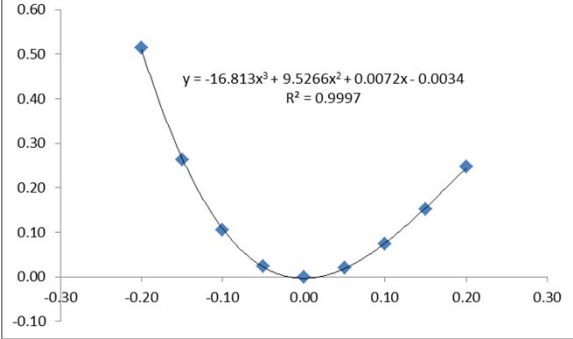
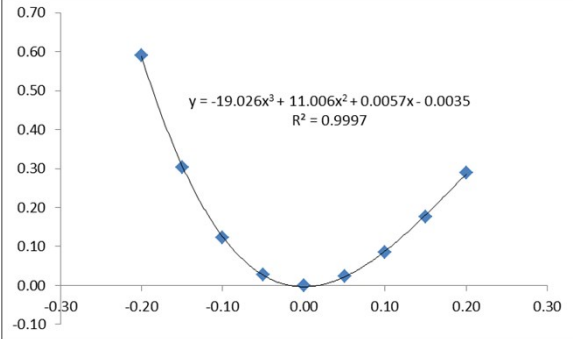
Geometry scan calculated at CCSD(T)/aug-cc-pVTZ computational level.

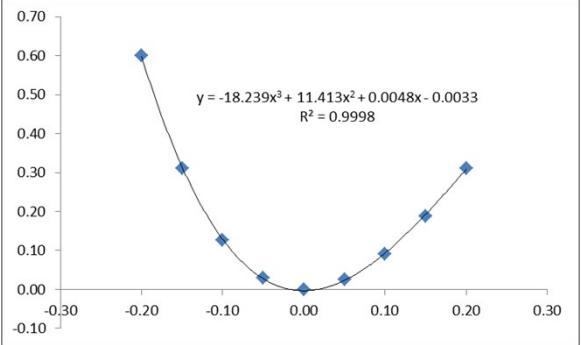
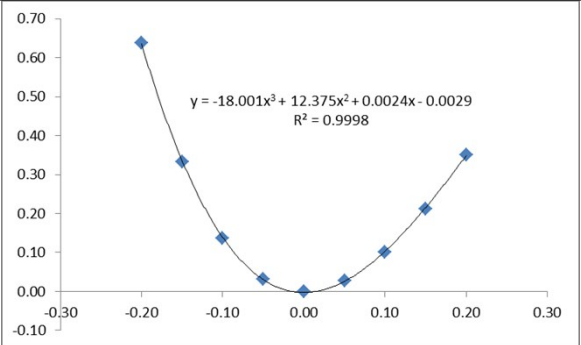
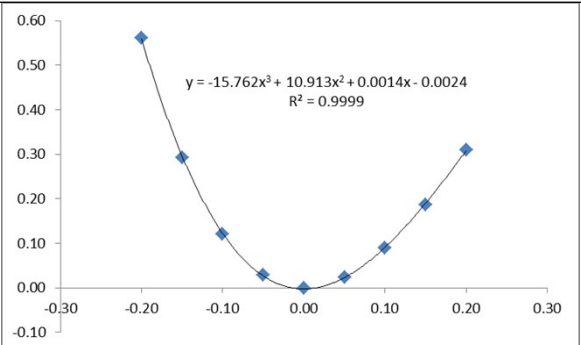
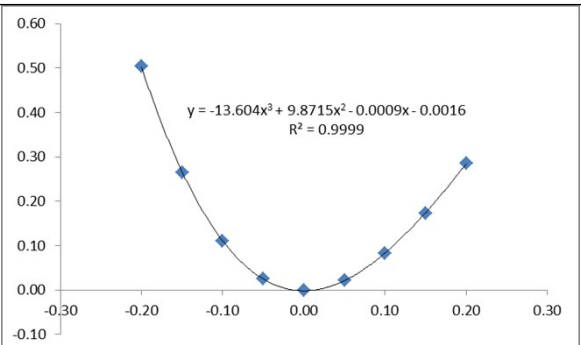
Complex	$(r-r_e)/\text{\AA}$	$E_r-E_{re}/\text{kJ mol}^{-1}$	E_r-E_{re} vs. $(r-r_e)$
N2...HF	-0.197	1.69	
	-0.147	0.86	
	-0.097	0.34	
	-0.047	0.07	
	0.000	0.00	
	0.053	0.08	
	0.103	0.27	
	0.153	0.54	
	0.203	0.88	
OC...HF	-0.202	2.12	
	-0.152	1.11	
	-0.102	0.46	
	-0.052	0.11	
	0.000	0.00	
	0.048	0.08	
	0.098	0.32	
	0.148	0.68	
	0.198	1.12	
C2H2...HF	-0.195	2.14	
	-0.145	1.10	
	-0.095	0.44	
	-0.045	0.09	
	0.000	0.00	
	0.055	0.11	
	0.105	0.39	
	0.155	0.79	
	0.205	1.29	
C2H4...HF	-0.204	2.31	
	-0.154	1.22	
	-0.104	0.52	
	-0.054	0.13	
	0.000	0.00	
	0.046	0.08	
	0.096	0.32	
	0.146	0.70	
	0.196	1.18	

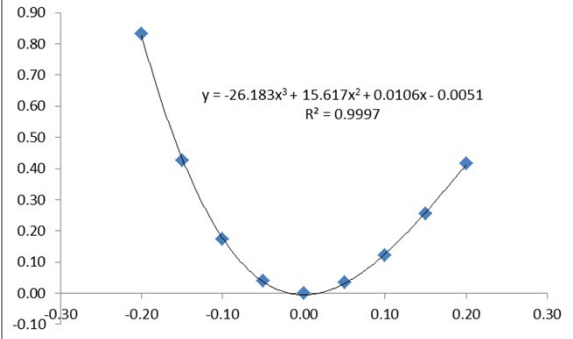
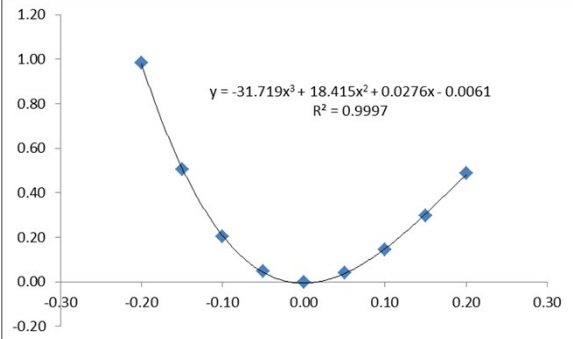
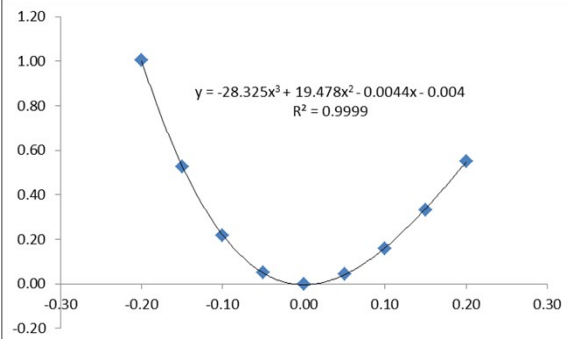
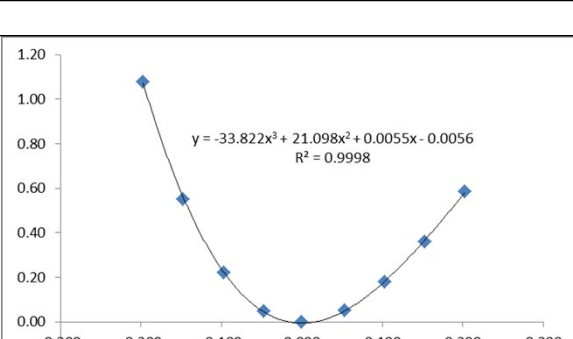
H2S...HF	-0.206	2.67	
	-0.156	1.42	
	-0.106	0.61	
	-0.056	0.16	
	0.000	0.00	
	0.044	0.08	
	0.094	0.35	
	0.144	0.78	
	0.194	1.31	
H3P...HF	-0.201	2.20	
	-0.151	1.15	
	-0.101	0.48	
	-0.051	0.11	
	0.000	0.00	
	0.049	0.09	
	0.099	0.35	
	0.149	0.73	
	0.199	1.22	
HCN...HF	-0.200	3.79	
	-0.150	1.97	
	-0.100	0.81	
	-0.050	0.19	
	0.000	0.00	
	0.050	0.16	
	0.100	0.59	
	0.150	1.23	
	0.200	2.03	
H2O...HF	-0.201	5.02	
	-0.151	2.60	
	-0.101	1.06	
	-0.051	0.25	
	0.000	0.00	
	0.049	0.20	
	0.099	0.76	
	0.149	1.57	
	0.199	2.58	

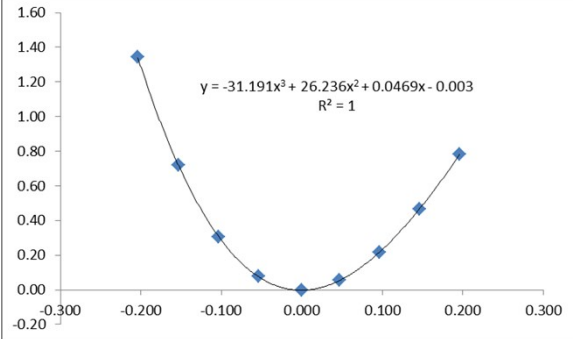
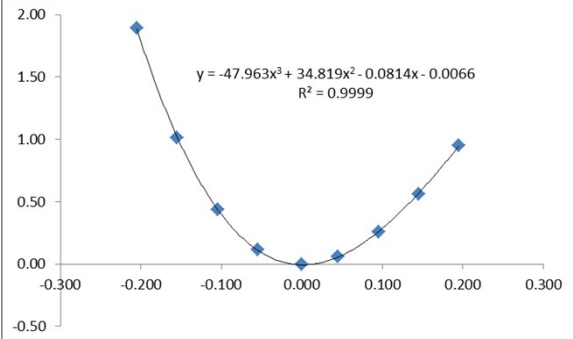
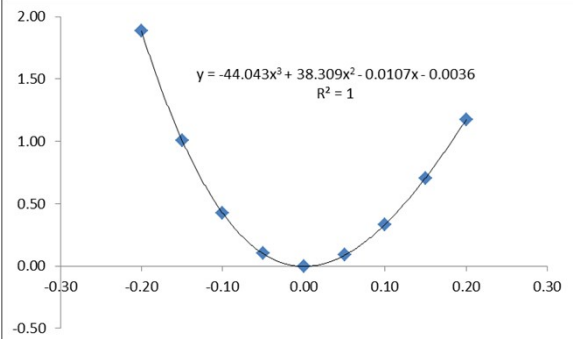
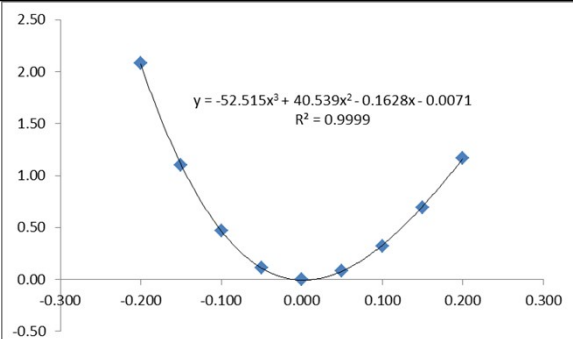
H3N...HF	-0.195	5.25	
	-0.145	2.73	
	-0.095	1.10	
	-0.045	0.23	
	0.000	0.00	
	0.055	0.29	
	0.105	1.01	
	0.155	2.05	
	0.205	3.35	
N2...HCl	-0.204	0.92	
	-0.154	0.49	
	-0.104	0.20	
	-0.054	0.05	
	0.000	0.00	
	0.046	0.03	
	0.096	0.12	
	0.146	0.27	
	0.196	0.45	
OC...HCl	-0.196	1.07	
	-0.146	0.55	
	-0.096	0.22	
	-0.046	0.05	
	0.000	0.00	
	0.054	0.06	
	0.104	0.19	
	0.154	0.39	
	0.204	0.64	
C2H2...HCl	-0.201	1.37	
	-0.151	0.72	
	-0.101	0.30	
	-0.051	0.07	
	0.000	0.00	
	0.049	0.06	
	0.099	0.22	
	0.149	0.47	
	0.199	0.77	

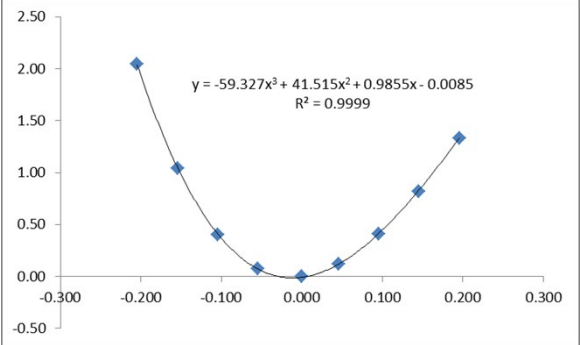
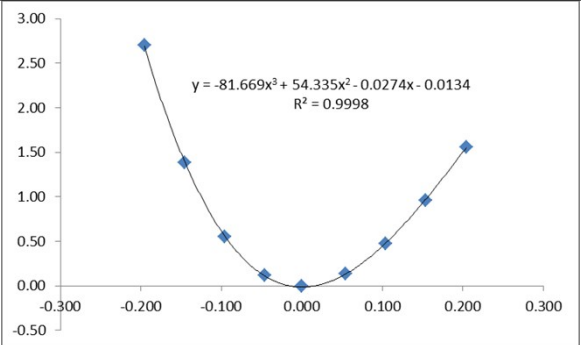
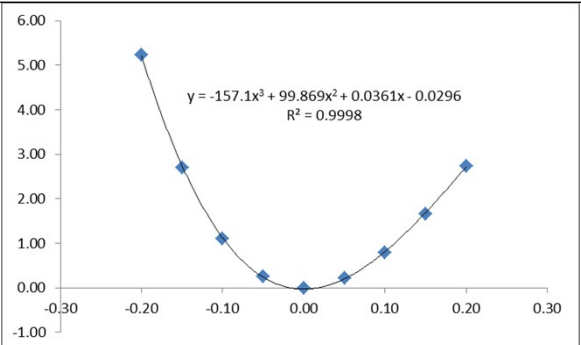
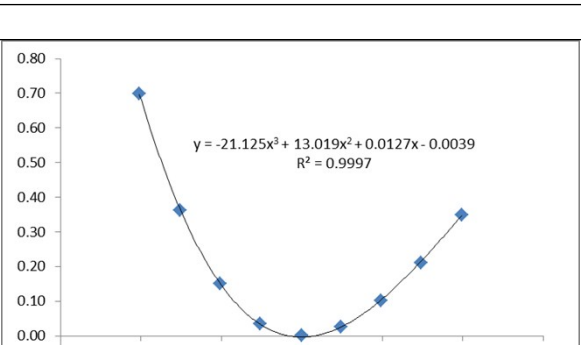
C2H4...HCl	-0.200	1.34	
	-0.150	0.70	
	-0.100	0.29	
	-0.050	0.07	
	0.000	0.00	
	0.050	0.06	
	0.100	0.22	
	0.150	0.47	
	0.200	0.79	
H2S...HCl	-0.196	1.39	
	-0.146	0.72	
	-0.096	0.29	
	-0.046	0.06	
	0.000	0.00	
	0.054	0.07	
	0.104	0.26	
	0.154	0.53	
	0.204	0.87	
H3P...HCl	-0.196	1.16	
	-0.146	0.60	
	-0.096	0.24	
	-0.046	0.05	
	0.000	0.00	
	0.054	0.06	
	0.104	0.22	
	0.154	0.45	
	0.204	0.74	
HCN...HCl	-0.200	2.00	
	-0.150	1.04	
	-0.100	0.43	
	-0.050	0.10	
	0.000	0.00	
	0.050	0.09	
	0.100	0.32	
	0.150	0.67	
	0.200	1.11	

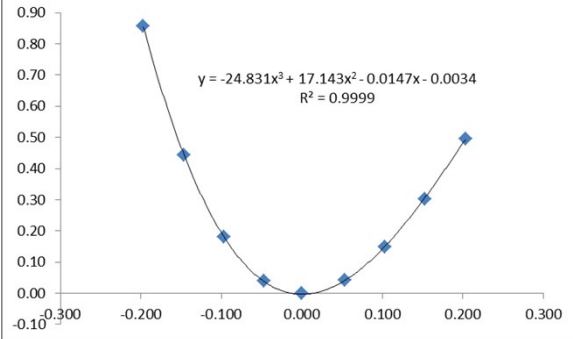
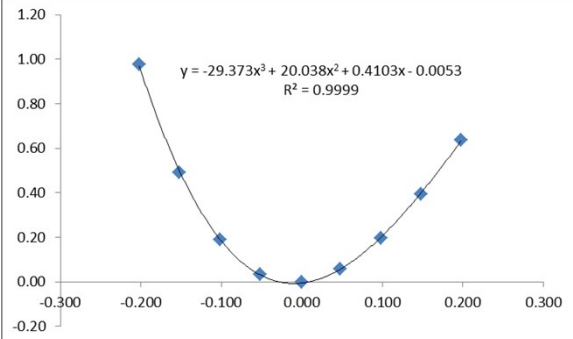
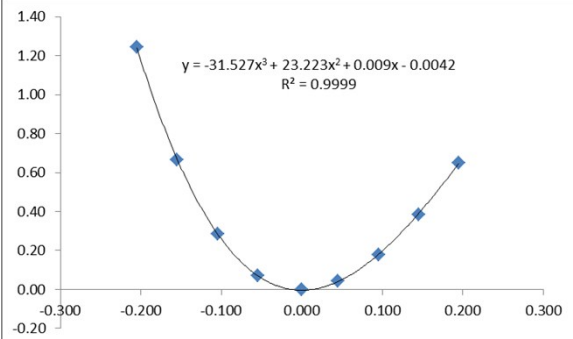
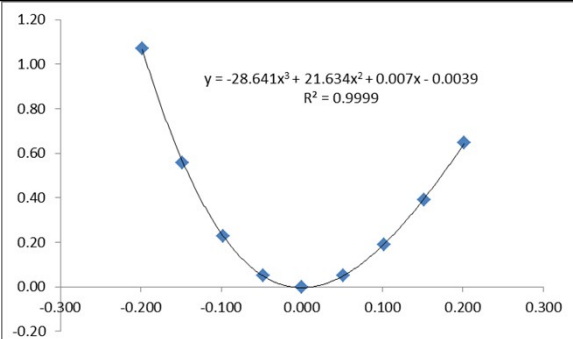
H2O...HCl	-0.204	2.52	
	-0.154	1.33	
	-0.104	0.56	
	-0.054	0.14	
	0.000	0.00	
	0.046	0.09	
	0.096	0.37	
	0.146	0.79	
	0.196	1.33	
H3N...HCl	-0.196	2.43	
	-0.146	1.31	
	-0.096	0.55	
	-0.046	0.12	
	0.000	0.00	
	0.054	0.15	
	0.104	0.52	
	0.154	1.09	
	0.204	1.82	
N2...F2	-0.20	0.51	
	-0.15	0.26	
	-0.10	0.11	
	-0.05	0.02	
	0.00	0.00	
	0.05	0.02	
	0.10	0.07	
	0.15	0.15	
	0.20	0.25	
OC...F2	-0.20	0.59	
	-0.15	0.30	
	-0.10	0.12	
	-0.05	0.03	
	0.00	0.00	
	0.05	0.02	
	0.10	0.09	
	0.15	0.18	
	0.20	0.29	

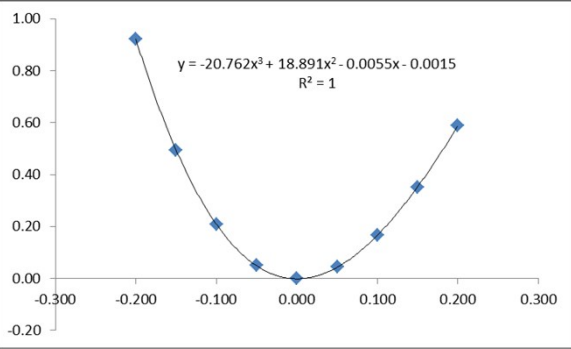
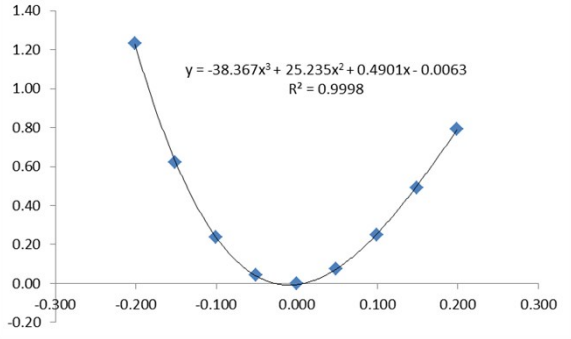
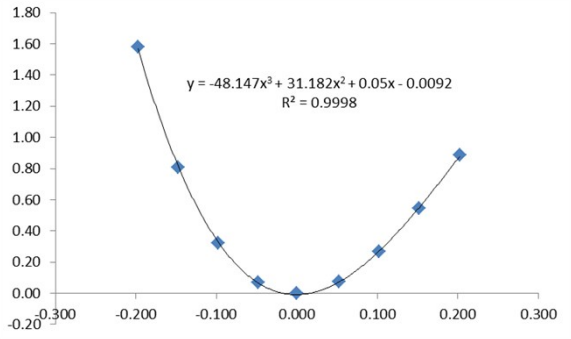
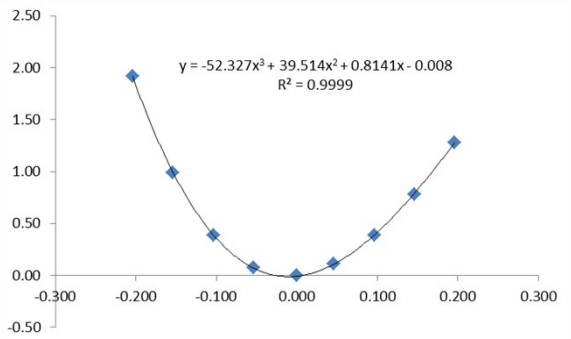
C2H2...F2	-0.20	0.60	
	-0.15	0.31	
	-0.10	0.13	
	-0.05	0.03	
	0.00	0.00	
	0.05	0.02	
	0.10	0.09	
	0.15	0.19	
	0.20	0.31	
C2H4...F2	-0.20	0.64	
	-0.15	0.33	
	-0.10	0.14	
	-0.05	0.03	
	0.00	0.00	
	0.05	0.03	
	0.10	0.10	
	0.15	0.21	
	0.20	0.35	
H2S...F2	-0.20	0.56	
	-0.15	0.29	
	-0.10	0.12	
	-0.05	0.03	
	0.00	0.00	
	0.05	0.02	
	0.10	0.09	
	0.15	0.19	
	0.20	0.31	
H3P...F2	-0.20	0.50	
	-0.15	0.26	
	-0.10	0.11	
	-0.05	0.03	
	0.00	0.00	
	0.05	0.02	
	0.10	0.08	
	0.15	0.17	
	0.20	0.29	

HCN...F2	-0.20	0.83	
	-0.15	0.43	
	-0.10	0.17	
	-0.05	0.04	
	0.00	0.00	
	0.05	0.03	
	0.10	0.12	
	0.15	0.25	
	0.20	0.42	
H2O...F2	-0.20	0.98	
	-0.15	0.50	
	-0.10	0.20	
	-0.05	0.05	
	0.00	0.00	
	0.05	0.04	
	0.10	0.15	
	0.15	0.30	
	0.20	0.49	
H3N...F2	-0.20	1.01	
	-0.15	0.53	
	-0.10	0.22	
	-0.05	0.05	
	0.00	0.00	
	0.05	0.04	
	0.10	0.16	
	0.15	0.33	
	0.20	0.55	
N2...ClF	-0.197	1.08	
	-0.147	0.55	
	-0.097	0.22	
	-0.047	0.05	
	0.000	0.00	
	0.053	0.05	
	0.103	0.18	
	0.153	0.36	
	0.203	0.59	

OC...CIF	-0.204	1.34	
	-0.154	0.72	
	-0.104	0.31	
	-0.054	0.08	
	0.000	0.00	
	0.046	0.05	
	0.096	0.22	
	0.146	0.46	
	0.196	0.78	
C2H2...CIF	-0.205	1.89	
	-0.155	1.01	
	-0.105	0.44	
	-0.055	0.11	
	0.000	0.00	
	0.045	0.06	
	0.095	0.25	
	0.145	0.56	
	0.195	0.95	
C2H4...CIF	-0.20	1.89	
	-0.15	1.00	
	-0.10	0.42	
	-0.05	0.10	
	0.00	0.00	
	0.05	0.09	
	0.10	0.33	
	0.15	0.70	
	0.20	1.18	
H2S...CIF	-0.200	2.08	
	-0.150	1.10	
	-0.100	0.47	
	-0.050	0.11	
	0.000	0.00	
	0.050	0.08	
	0.100	0.32	
	0.150	0.69	
	0.200	1.17	

HCN...ClF	-0.205	2.04	
	-0.155	1.04	
	-0.105	0.41	
	-0.055	0.08	
	0.000	0.00	
	0.045	0.12	
	0.095	0.41	
	0.145	0.82	
	0.195	1.33	
H2O...ClF	-0.196	2.70	
	-0.146	1.38	
	-0.096	0.55	
	-0.046	0.12	
	0.000	0.00	
	0.054	0.14	
	0.104	0.47	
	0.154	0.96	
	0.204	1.56	
H3N...ClF	-0.20	5.24	
	-0.15	2.71	
	-0.10	1.11	
	-0.05	0.25	
	0.00	0.00	
	0.05	0.22	
	0.10	0.80	
	0.15	1.66	
	0.20	2.74	
N2...Cl2	-0.202	0.70	
	-0.152	0.36	
	-0.102	0.15	
	-0.052	0.04	
	0.000	0.00	
	0.048	0.03	
	0.098	0.10	
	0.148	0.21	
	0.198	0.35	

OC...Cl2	-0.197	0.86	
	-0.147	0.44	
	-0.097	0.18	
	-0.047	0.04	
	0.000	0.00	
	0.053	0.04	
	0.103	0.15	
	0.153	0.30	
	0.203	0.50	
C2H2...Cl2	-0.202	0.98	
	-0.152	0.49	
	-0.102	0.19	
	-0.052	0.03	
	0.000	0.00	
	0.048	0.06	
	0.098	0.20	
	0.148	0.39	
	0.198	0.64	
C2H4...Cl2	-0.205	1.24	
	-0.155	0.66	
	-0.105	0.28	
	-0.055	0.07	
	0.000	0.00	
	0.045	0.04	
	0.095	0.18	
	0.145	0.39	
	0.195	0.65	
H2S...Cl2	-0.198	1.07	
	-0.148	0.56	
	-0.098	0.23	
	-0.048	0.05	
	0.000	0.00	
	0.052	0.05	
	0.102	0.19	
	0.152	0.39	
	0.202	0.65	

H3P...Cl2	-0.200	0.92	
	-0.150	0.49	
	-0.100	0.21	
	-0.050	0.05	
	0.000	0.00	
	0.050	0.04	
	0.100	0.17	
	0.150	0.35	
	0.200	0.59	
HCN...Cl2	-0.201	1.23	
	-0.151	0.62	
	-0.101	0.24	
	-0.051	0.04	
	0.000	0.00	
	0.049	0.08	
	0.099	0.25	
	0.149	0.49	
	0.199	0.79	
H2O...Cl2	-0.198	1.58	
	-0.148	0.81	
	-0.098	0.32	
	-0.048	0.07	
	0.000	0.00	
	0.052	0.08	
	0.102	0.27	
	0.152	0.54	
	0.202	0.88	
H3N...Cl2	-0.204	1.92	
	-0.154	0.99	
	-0.104	0.39	
	-0.054	0.08	
	0.000	0.00	
	0.046	0.11	
	0.096	0.38	
	0.146	0.78	
	0.196	1.28	