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Supporting Information

Contributions from Atomic p(Se), d(Se), and f(Se) Orbitals to Absolute Paramagnetic Shielding Tensors in Neutral and Charged SeH_n and Some Oxides, Together with the Effect of Methyl and Halogen Substitutions on s^p(Se)

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Table S1. Contributions from Each MO to σ^{p}(Se) in Se*H_n (* = null, +, or –).[a–d]

Species	ψ_1, ψ_2	ψ_3–ψ_5	ψ_6	ψ_7	ψ_8	ψ_9	ψ_{10}–ψ_{14}	ψ_{15}	ψ_{16}	ψ_{17}	ψ_{18}	ψ_{19}	ψ_{20}	total
Main AO	1s, 2s	2p	3s	3p	3p	3p	3d	4s	4p	4p	4p	4d	4d	
SeH^{-}(C_v)	0.0	13.2	0.0	–3.2	–41.9	–41.9	–0.4	–10.4	–144.2	–136.3	–136.3			–501.5
SeH_2 (C_{2v})	0.0	22.7	0.0	–42.6	–34.0	–73.0	–1.6	–14.3	–112.9	–228.8	–444.2			–928.8
SeH_3^{+}(C_{3v})	0.0	26.8	0.1	–59.4	–59.4	–55.0	–3.9	–16.8	–229.5	–229.5	–453.2			–1079.9
SeH_3^{+} (pl)	0.0	25.2	0.0	–43.5	–43.5	–83.6	0.6	–2.2	–243.3	–243.3	–441.1			–1074.6
SeH_4 (T_d)	0.0	20.6	0.0	–64.1	–64.1	–64.1	2.4	0.1	–498.9	–498.9	–498.9	–1.1[e]		–1666.8
SeH_4 (TBP)	0.0	29.4	0.1	–58.9	–56.4	–66.4	–27.0	–12.6	–149.0	–163.8	–281.1	–180.5[f]		–966.3
SeH_5^{+} (TBP)	0.0	31.7	0.0	–65.1	–65.1	–58.0	–23.7	0.1	–267.5	–267.5	–253.6	–238.7[f]		–1207.4
SeH_5^{+} (SP)	0.0	35.2	0.0	–71.8	–62.3	–62.3	–25.0	–1.0	–261.1	–261.1	–210.2	–240.3		–1159.9
SeH_5^{-} (SP)	0.0	29.3	0.0	–59.9	–59.9	–72.1	–44.3	–10.3	–160.2	–163.6	–163.6	–117.3	–84.2	–905.9
SeH_6 (O_h)	0.0	47.1	0.0	–76.6	–76.6	–76.6	–63.4	0.1	–107.4	–107.4	–107.4	–207.7	–207.7	–983.6

[a] Calculated with the DFT-GIAO method employing the 6-311+G(3df,3pd) basis sets. [b] A utility program (NMRANAL-NH03G) being employed. [c] In ppm. [d] Half of the contribution from the $\psi_i \rightarrow \psi_j$ (Occ-to-Occ) transitions ($\sigma^{p}_{i\rightarrow j}$(Se)/2) is fractionalized to each of ψ_i and ψ_j, in our treatment. [e] Mainly constructed by 4s(Se). [f] Corresponding to ψ_2 of H_{ax}–Se–H_{ax} 3c–4e.

Table S2. The $<r_{Se}^{-3}>_{kk}$ values evaluated with the Gaussian functions ($^{g}F_k$) of the p_x type.[a–c]

k[d]	Contraction[e]	S_{kk}[f]	$<r_{Se}^{-3}>_{kk}$[g]
9	3	1.000	11268.88
12	3	1.000	586.28
15	3	1.000	25.92
18	1	1.000	3.81
21	1	1.000	1.32
24	1	1.000	0.33
27	1	1.000	0.06
43[h]	1	1.000	0.01

[a] Calculated with the DFT-GIAO method employing the 6-311+G(3df,3pd) basis sets. [b] A utility program (NMRANAL-NH03G) being employed for the evaluation. [c] In ppm. [d] The orbital number for the the p_x type being employed, which appears in the output of MO coeffients. [e] The number of contraction in $^{g}F_k$. [f] Obrital overlap integral: $S_{kk} = <{}^{g}F_k \,|{}^{g}F_k>$. [g] Defined by Equation (S1) with $k = l$. [h] Correspond to the diffusion function.

$$<r_N^{-3}>_{kl} = <{}^{g}F_k \,|\, r_N^{-3} \,|{}^{g}F_l> \qquad \text{(S1)}$$

The expectation values of $<r_N^{-3}>_{kl}$ are evaluated by averaging over Gaussian functions as shown in Equation (S1), where $^{g}F_k$ and $^{g}F_l$ are the k-th and l-th Gaussian functions, respectively. Table S2 shows the $<r_N^{-3}>_{kk}$ values evaluated based on the 6-311+G(3df,3pd) basis sets. The evaluated $<r_N^{-3}>_{kk}$ values are very large for k = 9, which corresponds to the p_x type ^{g}F located nearest to the Se nucleus. The $<r_N^{-3}>_{kk}$ values with k = 12 is second largest. The values with k = 43 is smallest which acts as the diffusion function of the p_x type. The $<r_N^{-3}>_{kk}$ values with k = 21, 24, and 27 are also very small, which correspond to the polarization functions of the p_x type. The value with k = 18 is also small. The values decrease exponentially as k becomes larger. The $^{g}F_k$ functions with k = 18–27 contribute much to construct the vacant orbitals of higher energies, together with the diffusion functions (k = 43). As shown in Table S2, the contributions from p(Se) in vacant orbitals to σ^{p}(Se) should also decrease exponentially as the energies of vacant orbitals become higher, although the cross terms (k ? l) must also be considered. It is strongly suggested that p(Se) of the higher energy levels would not contribute so much to σ^{p}(Se) whereas 4p(Se) should substantially contribute to σ^{p}(Se) for usual selenium compounds.

Optimized structures given by Cartesian coordinates for Se*H_n , R_rSe*X_x (* = null, +, or –), and Some Oxides, together with the total energies, with the DFT-GIAO method employing the 6-311+G(3df,3pd) basis sets.

SeH^-
Total energy: -2402.2070415 a.u

34	0	0.000000	0.000000	0.042181
1	0	0.000000	0.000000	-1.434154

SeH_2 (C_{2v})
Total energy: -2402.7571055 a.u

34	0	0.000000	0.000000	0.057058
1	0	-0.000000	1.050918	-0.969988
1	0	-0.000000	-1.050918	-0.969988

SeH_3^+ (C_{3v})
Total energy: -2403.0372297 a.u

34	0	-0.000000	0.000000	0.066099
1	0	0.000000	1.237878	-0.749121
1	0	1.072034	-0.618939	-0.749121
1	0	-1.072034	-0.618939	-0.749121

SeH_3^+ (pl)
Total energy: -2402.9772012 a.u

34	0	0.000000	0.000000	0.000000
1	0	0.000000	1.454273	0.000000
1	0	1.259437	-0.727136	0.000000
1	0	-1.259437	-0.727136	0.000000

SeH_4 (T_d)
Total energy: -2403.7173966 a.u

34	0	0.000000	0.000000	0.000000
1	0	1.008286	1.008286	1.008286
1	0	-1.008286	-1.008286	1.008286
1	0	-1.008286	1.008286	-1.008286
1	0	1.008286	-1.008286	-1.008286

SeH_4 (TBP)
Total energy: -2403.8233666 a.u

34	0	0.000000	0.000000	0.060940
1	0	0.000000	1.173108	-0.829567
1	0	-0.000000	-1.173108	-0.829567
1	0	-1.675566	0.000000	-0.206414
1	0	1.675566	-0.000000	-0.206414

SeH_5^+ (TBP)
Total energy: -2404.0828123 a.u

34	0	0.000000	0.000000	0.000000
1	0	0.000000	1.512810	-0.000000
1	0	1.310132	-0.756405	-0.000000
1	0	-1.310132	-0.756405	-0.000000
1	0	0.000000	0.000000	1.553804
1	0	0.000000	0.000000	-1.553804

SeH_5^+ (C_{4v} (SP))
Total energy: -2404.0815741 a.u

34	0	0.000000	0.000000	0.013211
1	0	-0.000000	1.527859	0.252050
1	0	-1.527859	0.000000	0.252050
1	0	1.527859	-0.000000	0.252050
1	0	-0.000000	-1.527859	0.252050
1	0	0.000000	0.000000	-1.457370

SeH_5^- (C_{4v} (SP))
Total energy: -2404.3975475 a.u

34	0	0.000000	0.000000	0.053036
1	0	-0.000000	1.764635	-0.101682
1	0	-1.764635	0.000000	-0.101682
1	0	1.764635	-0.000000	-0.101682
1	0	-0.000000	-1.764635	-0.101682
1	0	0.000000	0.000000	-1.396500

SeH_6 (O_h)
Total energy: -2404.92077 a.u

34	0	0.000000	0.000000	0.000000
1	0	0.000000	0.000000	1.560986
1	0	-0.000000	1.560986	-0.000000
1	0	0.000000	-1.560986	0.000000
1	0	0.000000	-0.000000	-1.560986
1	0	1.560986	0.000000	0.000000
1	0	-1.560986	0.000000	-0.000000

SeMe–
Total energy: -2441.5215557 a.u

34	0	0.000004	-0.444512	0.000000
6	0	0.000004	1.552415	0.000000
1	0	1.022133	1.933155	0.000000
1	0	-0.511152	1.932881	0.885216
1	0	-0.511152	1.932881	-0.885216

$SeMe_2$ (C_{2v})
Total energy: -2481.4117621 a.u

34	0	-0.000000	0.000000	0.474310
6	0	-0.000000	1.472944	-0.822478
6	0	-0.000000	-1.472944	-0.822478
1	0	0.000000	-2.395958	-0.248558
1	0	0.893275	-1.429839	-1.439920
1	0	-0.893275	-1.429839	-1.439920
1	0	0.000000	2.395958	-0.248558
1	0	-0.893275	1.429839	-1.439920
1	0	0.893275	1.429839	-1.439920

$SeMe_3^+$ (T_d)
Total energy: -2521.0828618 a.u

34	0	0.000000	0.000000	0.425766
6	0	1.077152	-1.349521	-0.488827
6	0	0.630143	1.607602	-0.488827
1	0	0.000000	2.428294	-0.157842
1	0	1.656427	1.770504	-0.171975
1	0	0.563315	1.462372	-1.562566

1	0	2.102964	-1.214147	-0.157842
1	0	0.705087	-2.319760	-0.171975
1	0	0.984794	-1.219031	-1.562566
6	0	-1.707295	-0.258081	-0.488827
1	0	-2.102964	-1.214147	-0.157842
1	0	-2.361515	0.549256	-0.171975
1	0	-1.548108	-0.243341	-1.562566

$SeMe_3^+$ (C_{3h})
Total energy: -2521.0283454 a.u

34	0	0.000000	0.000000	0.000000
6	0	-0.000000	1.968991	0.000000
1	0	-1.054962	2.229216	0.000000
1	0	0.490120	2.300931	0.906943
1	0	0.490120	2.300931	-0.906943
6	0	-1.705196	-0.984496	0.000000
1	0	-1.403077	-2.028232	0.000000
1	0	-2.237725	-0.726009	0.906943
1	0	-2.237725	-0.726009	-0.906943
6	0	1.705196	-0.984496	0.000000
1	0	1.747605	-1.574922	0.906943
1	0	1.747605	-1.574922	-0.906943
1	0	2.458039	-0.200984	0.000000

$SeMe_4$ (T_d)
Total energy: -2561.0649817 a.u

34	0	0.000000	0.000000	0.000000
6	0	1.330702	1.330702	1.330702
1	0	1.921680	1.921680	0.640887
1	0	0.640887	1.921680	1.921680
1	0	1.921680	0.640887	1.921680
6	0	-1.330702	-1.330702	1.330702
1	0	-1.921680	-0.640887	1.921680
1	0	-1.921680	-1.921680	0.640887
1	0	-0.640887	-1.921680	1.921680
6	0	-1.330702	1.330702	-1.330702
1	0	-0.640887	1.921680	-1.921680
1	0	-1.921680	0.640887	-1.921680
1	0	-1.921680	1.921680	-0.640887
6	0	1.330702	-1.330702	-1.330702
1	0	1.921680	-1.921680	-0.640887
1	0	0.640887	-1.921680	-1.921680
1	0	1.921680	-0.640887	-1.921680

H_2SeF_2 (TBP)
Total energy: -2602.4857626 a.u

34	0	0.000000	0.000000	0.103763
1	0	1.092456	-0.000000	-0.882160
1	0	-1.092456	0.000000	-0.882160
9	0	0.000000	1.854752	-0.097979
9	0	-0.000000	-1.854752	-0.097979

Me_2SeF_2 (TBP)
Total energy: -2681.1671853 a.u

34	0	0.000000	0.000000	0.365331
6	0	0.000000	1.491834	-0.883741

6	0	-0.000000	-1.491834	-0.883741
1	0	0.000000	-2.402540	-0.292463
1	0	0.906698	-1.418009	-1.473233
1	0	-0.906698	-1.418009	-1.473233
1	0	0.000000	2.402540	-0.292463
1	0	-0.906698	1.418009	-1.473233
1	0	0.906698	1.418009	-1.473233
9	0	-1.888284	0.000000	0.258972
9	0	1.888284	-0.000000	0.258972

Me_2SeCl_2 (TBP)
Total energy: -3401.8867711 a.u

34	0	0.000000	0.000000	0.272060
6	0	0.000000	1.489677	-1.004834
6	0	-0.000000	-1.489677	-1.004834
1	0	0.000000	-2.397003	-0.408954
1	0	0.906395	-1.410273	-1.592755
1	0	-0.906395	-1.410273	-1.592755
1	0	0.000000	2.397003	-0.408954
1	0	-0.906395	1.410273	-1.592755
1	0	0.906395	1.410273	-1.592755
17	0	-2.409123	0.000000	0.294026
17	0	2.409123	-0.000000	0.294026

Me_2SeBr_2 (TBP)
Total energy: -7629.7363451 a.u

34	0	0.000000	0.000000	0.156048
6	0	0.000000	1.488037	-1.128367
6	0	-0.000000	-1.488037	-1.128367
1	0	0.000000	-2.396961	-0.535072
1	0	0.905706	-1.407690	-1.717429
1	0	-0.905706	-1.407690	-1.717429
1	0	0.000000	2.396961	-0.535072
1	0	-0.905706	1.407690	-1.717429
1	0	0.905706	1.407690	-1.717429
35	0	-2.591541	0.000000	0.231066
35	0	2.591541	-0.000000	0.231066

$Me_3SeF_2^+$(C_{3h})
Total energy: -2720.7844178 a.u

34	0	0.000000	0.000000	0.000000
6	0	1.941487	0.000000	0.000000
1	0	2.234991	1.047350	0.000000
1	0	2.242635	-0.500030	0.913994
1	0	2.242635	-0.500030	-0.913994
6	0	-0.970743	1.681377	0.000000
1	0	-2.024527	1.411884	0.000000
1	0	-0.688279	2.192194	0.913994
1	0	-0.688279	2.192194	-0.913994
6	0	-0.970743	-1.681377	0.000000
1	0	-1.554356	-1.692164	0.913994
1	0	-1.554356	-1.692164	-0.913994
1	0	-0.210464	-2.459234	0.000000
9	0	0.000000	0.000000	1.804018
9	0	0.000000	0.000000	-1.804018

SeF_5^+ (C_{3h})
Total energy: -2900.4563575 a.u

34	0	0.000000	0.000000	0.000000
9	0	0.000000	1.659600	-0.000000
9	0	1.437256	-0.829800	-0.000000
9	0	-1.437256	-0.829800	-0.000000
9	0	0.000000	0.000000	1.677430
9	0	0.000000	0.000000	-1.677430

$SeMe_5^+$ (C_{4v} (SP))
Total energy: -2600.8196598 a.u

34	0	0.042359	0.001789	0.000000
6	0	0.436307	-1.413634	1.428388
1	0	1.516896	-1.443966	1.546728
1	0	-0.039940	-1.102229	2.352032
1	0	0.061307	-2.370682	1.082822
6	0	0.436307	1.429976	1.417555
1	0	0.054666	1.085929	2.372725
1	0	1.517471	1.541294	1.454190
1	0	-0.031395	2.357257	1.103799
6	0	0.436307	-1.413634	-1.428388
1	0	1.516896	-1.443966	-1.546728
1	0	-0.039940	-1.102229	-2.352032
1	0	0.061307	-2.370682	-1.082822
6	0	0.436307	1.429976	-1.417555
1	0	0.054666	1.085929	-2.372725
1	0	1.517471	1.541294	-1.454190
1	0	-0.031395	2.357257	-1.103799
6	0	-1.898381	-0.040511	0.000000
1	0	-2.197538	-1.083400	0.000000
1	0	-2.240892	0.467174	0.895534
1	0	-2.240892	0.467174	-0.895534

SeF_5^+ (C_{4v} (SP))
Total energy: -2900.4519873 a.u

34	0	0.000000	0.000000	0.026497
9	0	0.000000	1.636816	0.379177
9	0	-1.636816	0.000000	0.379177
9	0	1.636816	0.000000	0.379177
9	0	0.000000	-1.636816	0.379177
9	0	0.000000	0.000000	-1.616806

$SeMe_5^-$ (C_{4v} (SP))
Total energy: -2601.05371023 a.u

34	0	0.281733	0.005727	0.000000
6	0	0.177464	-1.577502	1.680924
1	0	1.143364	-1.493877	2.184576
1	0	-0.629166	-1.393533	2.395962
1	0	0.071534	-2.568743	1.235471
6	0	0.177464	1.614968	1.546454
1	0	-0.017039	1.160980	2.518680
1	0	1.165752	2.078338	1.537799
1	0	-0.581946	2.362813	1.309743
6	0	0.177464	-1.577502	-1.680924
1	0	1.143364	-1.493877	-2.184576
1	0	-0.629166	-1.393533	-2.395962

1	0	0.071534	-2.568743	-1.235471
6	0	0.177464	1.614968	-1.546454
1	0	-0.017039	1.160980	-2.518680
1	0	1.165752	2.078338	-1.537799
1	0	-0.581946	2.362813	-1.309743
6	0	-1.682405	-0.096602	0.000000
1	0	-1.947525	-1.147881	0.000000
1	0	-2.050553	0.395620	0.895298
1	0	-2.050553	0.395620	-0.895298

SeF_5^- (C_{4v} (SP))
Total energy: -2901.0502238 a.u

34	0	0.000000	0.000000	0.272303
9	0	-0.000000	1.862354	0.109811
9	0	-1.862354	0.000000	0.109811
9	0	1.862354	-0.000000	0.109811
9	0	-0.000000	-1.862354	0.109811
9	0	0.000000	0.000000	-1.467945

$SeMe_6$ (C_i)
Total energy: -2640.9274949 a.u

34	0	0.000000	0.000000	0.000000
6	0	-0.008716	-0.013264	-2.072863
1	0	0.236171	0.978360	-2.443628
1	0	0.732430	-0.732675	-2.409841
1	0	-0.996343	-0.309474	-2.416463
6	0	0.008716	0.013264	2.072863
1	0	-0.236171	-0.978360	2.443628
1	0	-0.732430	0.732675	2.409841
1	0	0.996343	0.309474	2.416463
6	0	0.013474	2.072867	0.007052
1	0	-0.978199	2.443553	-0.237751
1	0	0.310115	2.417238	0.994282
1	0	0.732630	2.409154	-0.734656
6	0	-0.013474	-2.072867	-0.007052
1	0	0.978199	-2.443553	0.237751
1	0	-0.310115	-2.417238	-0.994282
1	0	-0.732630	-2.409154	0.734656
6	0	-2.072887	-0.006933	-0.011705
1	0	-2.417547	-0.994237	-0.307766
1	0	-2.409762	0.734570	-0.730797
1	0	-2.442723	0.238174	0.980210
6	0	2.072887	0.006933	0.011705
1	0	2.417547	0.994237	0.307766
1	0	2.442723	-0.238174	-0.980210
1	0	2.409762	-0.734570	0.730797

$HSeF_5$ (C_{4v})
Total energy: -2901.4732309 a.u

34	0	0.000000	0.000000	0.186840
1	0	0.000000	0.000000	1.661540
9	0	0.000000	1.730327	0.158519
9	0	-0.000000	-1.730327	0.158519
9	0	0.000000	0.000000	-1.524529
9	0	1.730327	-0.000000	0.158519
9	0	-1.730327	0.000000	0.158519

$MeSeF_5$ (C_s)
Total energy: -2940.8200536 a.u

34	0	0.001553	0.002593	0.000000
9	0	0.079174	-1.226282	1.236921
9	0	1.721342	0.001585	0.000000
9	0	0.079174	1.239175	-1.228996
9	0	0.079174	-1.226282	-1.236921
9	0	0.079174	1.239175	1.228996
6	0	-1.945076	-0.034319	-0.000000
1	0	-2.256204	0.477735	-0.902525
1	0	-2.256204	0.477735	0.902525
1	0	-2.212247	-1.084058	-0.000000

SeF_6 (O_h)
Total energy: -3000.7537733 a.u

34	0	0.000000	0.000000	0.000000
9	0	0.000000	0.000000	1.707137
9	0	0.000000	1.707137	-0.000000
9	0	0.000000	-1.707137	0.000000
9	0	0.000000	-0.000000	-1.707137
9	0	1.707137	0.000000	0.000000
9	0	-1.707137	0.000000	-0.000000

H_2SeO (C_s)
Total energy: -2477.9354666 a.u

34	0	-0.046336	-0.281300	0.000000
1	0	0.973049	-0.692969	1.044476
1	0	0.973049	-0.692969	-1.044476
8	0	-0.046336	1.368769	-0.000000

Me_2SeO (C_s)
Total energy: -2556.6168008 a.u

34	0	0.377675	-0.138561	-0.000000
6	0	-0.460716	0.901757	1.451139
6	0	-0.460716	0.901757	-1.451139
1	0	-0.163391	0.431248	-2.383918
1	0	-0.112464	1.932103	-1.414547
1	0	-1.537452	0.837118	-1.319397
1	0	-0.163391	0.431248	2.383918
1	0	-1.537452	0.837118	1.319397
1	0	-0.112464	1.932103	1.414547
8	0	-0.460716	-1.563868	-0.000000

H_4SeO (C_{2v})
Total energy: -2479.010111 a.u

34	0	0.000000	0.000000	0.241624
1	0	-0.000000	1.128751	1.258005
1	0	-0.000000	-1.128751	1.258005
1	0	1.551190	-0.000000	0.267625
1	0	-1.551190	0.000000	0.267625
8	0	0.000000	0.000000	-1.408310

H_2SeF_2O (C_{2v})
Total energy: -2677.6557282 a.u

34	0	-0.000000	-0.000000	0.088803

1	0	-1.257254	0.000000	0.863968
1	0	1.257254	-0.000000	0.863968
9	0	0.000000	1.782364	0.405417
9	0	-0.000000	-1.782364	0.405417
8	0	0.000000	0.000000	-1.505593

Me_2SeF_2O
Total energy: -2756.3481288 a.u

34	0	0.000000	0.000000	0.118384
6	0	0.000000	1.684775	-0.861579
6	0	-0.000000	-1.684775	-0.861579
1	0	0.000000	-2.435743	-0.075651
1	0	0.910682	-1.720887	-1.445104
1	0	-0.910682	-1.720887	-1.445104
1	0	0.000000	2.435743	-0.075651
1	0	-0.910682	1.720887	-1.445104
1	0	0.910682	1.720887	-1.445104
9	0	-1.835560	0.000000	-0.084400
9	0	1.835560	-0.000000	-0.084400
8	0	0.000000	0.000000	1.720603

H_2SeO_2 (C_{2v})
Total energy: -2553.1272576 a.u

34	0	0.000000	0.000000	0.200577
1	0	1.147945	-0.000000	1.172194
1	0	-1.147945	0.000000	1.172194
8	0	0.000000	1.414686	-0.572750
8	0	-0.000000	-1.414686	-0.572750

Me_2SeO_2 (C_{2v})
Total energy: -2631.8229099 a.u

34	0	0.000000	0.000000	0.142903
6	0	0.000000	1.536212	-1.051458
6	0	-0.000000	-1.536212	-1.051458
1	0	-0.000000	-2.406327	-0.401553
1	0	0.902733	-1.499374	-1.653962
1	0	-0.902733	-1.499374	-1.653962
1	0	0.000000	2.406327	-0.401553
1	0	-0.902733	1.499374	-1.653962
1	0	0.902733	1.499374	-1.653962
8	0	1.404928	-0.000000	0.948609
8	0	-1.404928	0.000000	0.948609