

Metal	Name	EE (kJ/mol)	Δ EE(kJ/mol)	Calculated CCS (Å ²)	
				N ₂	He
Mg	Glyphosate_Mg_a	-2863538.716	0.000	127.941	61.2072
	Glyphosate_Mg_b	-2863538.713	0.003	127.938	61.247
	Glyphosate_Mg_c	-2863509.725	28.991	131.074	62.6081
	Glyphosate_Mg_d	-2863502.339	36.376	132.933	62.6085
	Glyphosate_Mg_e	-2863502.334	36.382	132.943	61.2063
	Glyphosate_Mg_f	-2863476.741	61.975	130.973	62.0399
	Glyphosate_Mg_g	-2863476.741	61.975	130.973	62.0635
	Glyphosate_Mg_h	-2863470.369	68.347	133.066	64.359
	Glyphosate_Mg_i	-2863462.075	76.641	128.932	62.9563
	AMPA_Mg_a	-2265287.614	0.000	119.103	52.0235
	AMPA_Mg_b	-2265238.937	48.677	128.557	56.0643
	AMPA_Mg_c	-2265220.094	67.520	129.719	54.7855
	AMPA_Mg_d	-2265217.613	70.001	130.166	57.6498
	AMPA_Mg_e	-2265209.618	77.996	120.001	53.077
Ca	Glyphosate_Ca_a	-4117336.564	0.000	134.281	63.9074
	Glyphosate_Ca_b	-4117316.311	20.253	136.572	64.0529
	Glyphosate_Ca_c	-4117316.277	20.287	136.564	64.0511
	Glyphosate_Ca_d	-4117309.750	26.814	138.062	64.0884
	Glyphosate_Ca_e	-4117283.426	53.137	139.561	65.6726
	Glyphosate_Ca_f	-4117281.029	55.535	139.244	64.8085
	Glyphosate_Ca_g	-4117278.364	58.199	140.190	65.0911
	Glyphosate_Ca_h	-4117271.633	64.931	139.918	64.8218
	Glyphosate_Ca_i	-4117265.447	71.117	144.281	65.1605
	AMPA_Ca_a	-3519124.572	0.000	124.590	54.7011
	AMPA_Ca_b	-3519089.616	34.956	132.364	58.6088
	AMPA_Ca_c	-3519071.799	52.773	133.315	55.7643
	AMPA_Ca_d	-3519071.342	53.229	132.544	59.9555
	AMPA_Ca_e	-3519071.327	53.245	130.643	59.5171
	AMPA_Ca_f	-3519069.268	55.304	131.871	59.7073

Metal	Name	EE (kJ/mol)	$\Delta EE(kJ/mol)$	Calculated CCS (\AA^2)	
				N ₂	He
Sr	Glyphosate_Sr_a	-2418929.370	0.000	125.306	65.9144
	Glyphosate_Sr_b	-2418929.362	0.008	125.060	65.9617
	Glyphosate_Sr_c	-2418912.087	17.284	129.076	66.3817
	Glyphosate_Sr_d	-2418906.639	22.732	129.908	66.8149
	Glyphosate_Sr_e	-2418879.184	50.186	124.240	67.0879
	Glyphosate_Sr_f	-2418876.682	52.689	127.523	67.0853
	Glyphosate_Sr_g	-2418875.364	54.007	124.951	65.9138
	Glyphosate_Sr_h	-2418873.578	55.792	125.852	67.2041
	Glyphosate_Sr_i	-2418868.414	60.956	125.832	67.0483
	Glyphosate_Sr_j	-2418841.849	87.521	125.789	69.6546
	Glyphosate_Sr_k	-2418833.335	96.036	142.332	66.3635
	AMPA_Sr_a	-1820728.657	0.000	130.220	56.7116
	AMPA_Sr_b	-1820728.655	0.003	129.535	60.7748
	AMPA_Sr_c	-1820695.626	33.031	136.387	57.6028
	AMPA_Sr_d	-1820678.704	49.953	138.106	62.1074
	AMPA_Sr_e	-1820678.206	50.452	136.689	61.7096
	AMPA_Sr_f	-1820674.068	54.589	136.744	56.9309
Ba	Glyphosate_Ba_a	-2405263.206	0.000	141.387	67.7866
	Glyphosate_Ba_b	-2405263.188	0.018	142.000	68.1276
	Glyphosate_Ba_c	-2405247.975	15.231	143.011	68.9312
	Glyphosate_Ba_d	-2405247.970	15.236	143.293	68.0907
	Glyphosate_Ba_e	-2405213.818	49.388	146.408	68.8987
	Glyphosate_Ba_f	-2405210.609	52.597	146.861	69.3972
	Glyphosate_Ba_g	-2405209.864	53.342	147.137	68.946
	Glyphosate_Ba_h	-2405206.527	56.679	148.080	72.0218
	Glyphosate_Ba_i	-2405185.152	78.053	153.785	72.126
	Glyphosate_Ba_j	-2405185.147	78.059	153.244	77.295
	Glyphosate_Ba_k	-2405181.836	81.370	155.057	71.7288
	Glyphosate_Ba_l	-2405176.349	86.857	154.602	73.3259
	AMPA_Ba_a	-1807074.224	0.000	132.208	59.0567
	AMPA_Ba_b	-1807074.213	0.011	132.193	62.6589
	AMPA_Ba_c	-1807045.537	28.686	138.402	63.8489
	AMPA_Ba_d	-1807029.207	45.017	140.108	63.4883
	AMPA_Ba_e	-1807028.466	45.757	139.653	59.7211
	AMPA_Ba_f	-1807020.632	53.592	138.934	59.0569

Metal	Name	EE (kJ/mol)	Δ EE(kJ/mol)	Calculated CCS (\AA^2)	
				N ₂	He
Mn	Glyphosate_Mn_a	-5360016.524	0.000	128.559	60.9314
	Glyphosate_Mn_b	-5359974.839	41.685	128.710	61.9878
	Glyphosate_Mn_c	-5359968.769	47.755	135.180	60.6789
	Glyphosate_Mn_d	-5359968.375	48.149	131.103	60.7037
	Glyphosate_Mn_e	-5359967.834	48.690	128.698	62.1057
	Glyphosate_Mn_f	-5359953.229	63.296	132.398	61.6563
	Glyphosate_Mn_g	-5359942.049	74.475	133.252	61.5644
	Glyphosate_Mn_h	-5359941.144	75.381	131.844	63.146
	Glyphosate_Mn_i	-5359935.861	80.663	130.830	61.801
	AMPA_Mn_a	-4761776.599	0.000	116.199	50.7531
	AMPA_Mn_b	-4761776.578	0.021	116.023	51.7713
	AMPA_Mn_c	-4761724.336	52.263	124.026	54.1786
	AMPA_Mn_d	-4761722.464	54.135	122.672	51.9068
	AMPA_Mn_e	-4761720.624	55.976	115.358	55.9332
	AMPA_Mn_f	-4761707.160	69.439	127.385	50.7704
Co	Glyphosate_Co_a	-5968379.254	0.000	125.670	60.5005
	Glyphosate__i	-5968355.530	23.724	125.426	61.2875
	Glyphosate__c	-5968344.768	34.486	128.068	60.7714
	Glyphosate__b	-5968337.336	41.919	130.540	61.4614
	Glyphosate__f	-5968330.788	48.467	132.012	59.7654
	Glyphosate__d	-5968330.286	48.968	130.402	61.4587
	Glyphosate__e	-5968325.159	54.096	124.744	59.8132
	Glyphosate__g	-5968320.674	58.580	125.748	61.1172
	Glyphosate__h	-5968312.493	66.761	126.498	62.6619
	Glyphosate__j	-5968295.422	83.832	126.086	60.7718
	Glyphosate__k	-5968294.375	84.880	126.317	66.6002
	AMPA_Co_a	-5370133.204	0.000	112.659	49.6795
	AMPA_Co_b	-5370121.741	11.463	110.787	51.0384
	AMPA_Co_c	-5370074.201	59.003	118.358	50.531
	AMPA_Co_d	-5370066.839	66.365	119.016	52.6578
	AMPA_Co_e	-5370060.094	73.110	120.393	54.0024
	AMPA_Co_f	-5370054.016	79.188	120.747	54.2523
	AMPA_Co_g	-5370053.124	80.080	120.080	54.1488
	AMPA_Co_h	-5370045.276	87.928	116.045	51.8454
	AMPA_Co_i	-5370041.789	91.415	115.878	52.203

Metal	Name	EE (kJ/mol)	Δ EE(kJ/mol)	Calculated CCS (Å ²)	
				N ₂	He
Cu	Glyphosate_Cu_a	-6645032.717	0.000	125.220	60.3003
	Glyphosate_Cu_b	-6645028.086	4.631	126.492	62.2656
	Glyphosate_Cu_c	-6645000.082	32.635	124.904	62.3996
	Glyphosate_Cu_d	-6645000.069	32.648	124.935	62.5396
	Glyphosate_Cu_e	-6644988.084	44.634	129.821	60.9261
	Glyphosate_Cu_f	-6644986.068	46.650	127.523	60.0027
	Glyphosate_Cu_g	-6644983.523	49.194	128.503	62.9184
	Glyphosate_Cu_h	-6644977.613	55.104	124.650	62.4775
	Glyphosate_Cu_i	-6644975.707	57.010	126.937	62.8899
	Glyphosate_Cu_j	-6644975.665	57.052	128.386	63.2962
	Glyphosate_Cu_k	-6644964.124	68.594	129.359	61.3875
	Glyphosate_Cu_l	-6644940.969	91.748	127.435	62.2566
	AMPA_Cu_a	-6046818.730	0.000	109.550	51.1997
	AMPA_Cu_b	-6046764.608	54.122	113.436	49.5142
	AMPA_Cu_c	-6046758.448	60.281	113.556	55.0807
	AMPA_Cu_d	-6046757.695	61.035	111.227	55.3725
	AMPA_Cu_e	-6046755.920	62.810	113.581	51.6603
	AMPA_Cu_f	-6046753.544	65.186	110.659	52.176
	AMPA_Cu_g	-6046735.063	83.667	116.237	50.8455
	AMPA_Cu_h	-6046735.050	83.680	116.474	50.8702
	AMPA_Cu_i	-6046733.272	85.457	119.112	53.2385
	AMPA_Cu_j	-6046733.272	85.457	115.987	51.0365
Zn	Glyphosate_Zn_a	-7009701.654	0.000	124.436	59.9886
	Glyphosate_Zn_b	-7009677.187	24.467	127.923	60.783
	Glyphosate_Zn_c	-7009671.388	30.267	128.357	61.5815
	Glyphosate_Zn_d	-7009658.512	43.142	123.752	59.0071
	Glyphosate_Zn_e	-7009657.914	43.741	123.823	59.0128
	Glyphosate_Zn_f	-7009652.628	49.026	120.862	60.2384
	Glyphosate_Zn_g	-7009650.103	51.552	121.886	60.5125
	Glyphosate_Zn_h	-7009648.333	53.321	121.127	62.008
	Glyphosate_Zn_i	-7009636.356	65.299	124.842	62.1803
	Glyphosate_Zn_j	-7009614.732	86.922	122.630	60.1661
	Glyphosate_Zn_k	-7009614.333	87.322	142.332	60.9631
	Glyphosate_Zn_l	-7009602.988	98.666	125.040	62.8352
	AMPA_Zn_a	-6411447.956	0.000	115.316	50.5465
	AMPA_Zn_b	-6411447.956	0.000	115.153	51.5984
	AMPA_Zn_c	-6411429.121	18.835	113.906	52.3093
	AMPA_Zn_d	-6411413.150	34.806	122.533	53.5933
	AMPA_Zn_e	-6411383.151	64.805	122.341	55.0527
	AMPA_Zn_f	-6411370.648	77.308	124.098	55.1545
	AMPA_Zn_g	-6411367.805	80.151	123.778	50.3958