

The pivotal Role of Electronics in Preferred Alkene over Alkyne Ni-Carboryne Insertions and Absolute Regioselectivities

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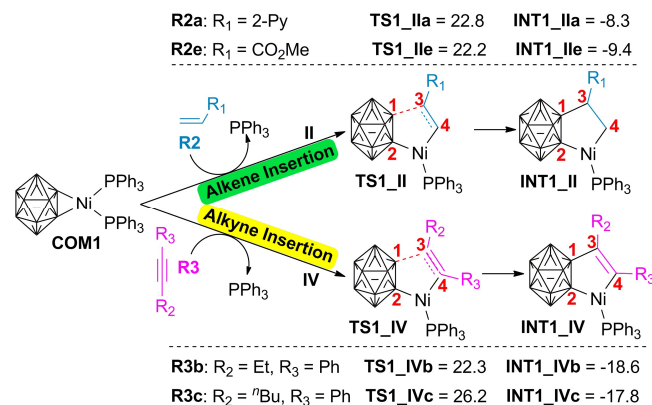


Figure S1 Competing insertion of alkene/alkyne into the Ni-C bond of activated **COM1**.

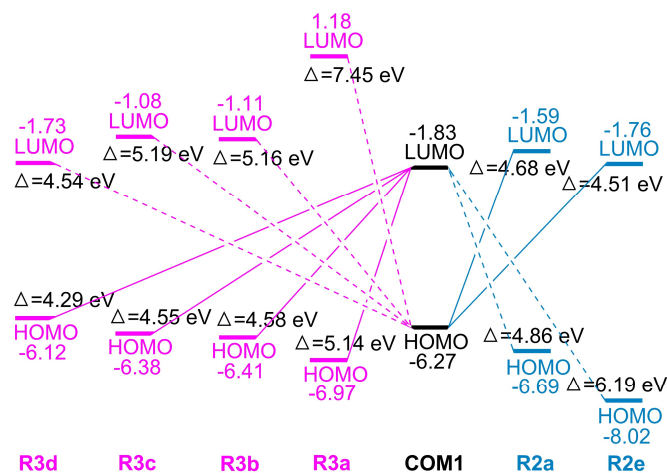


Figure S2 Frontier orbital graphics obtained at IDSCRF-B3LYP/DZVP//DZVP level in THF solvent.

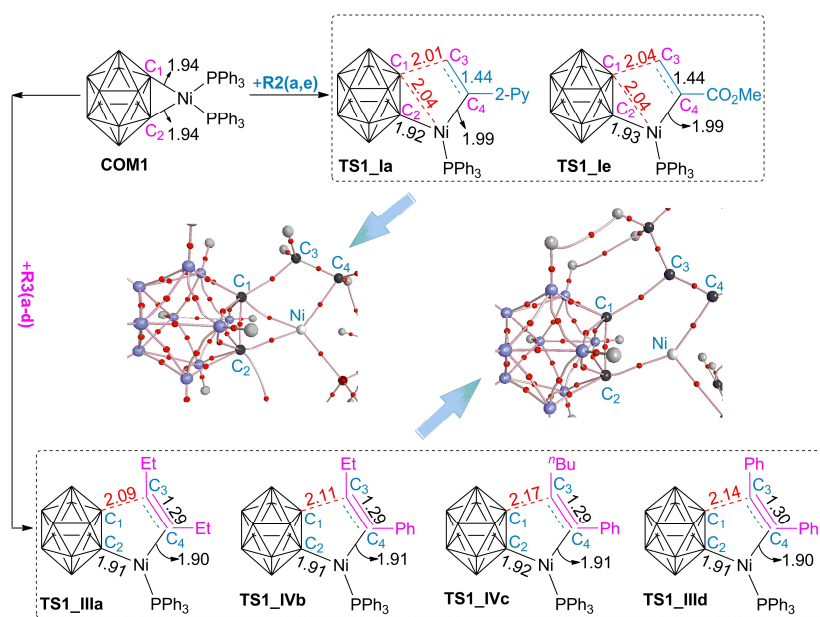


Figure S3 Molecular graphics and key optimized bond lengths (Å) of selected stationary points involved in the alkene/alkyne insertion process.

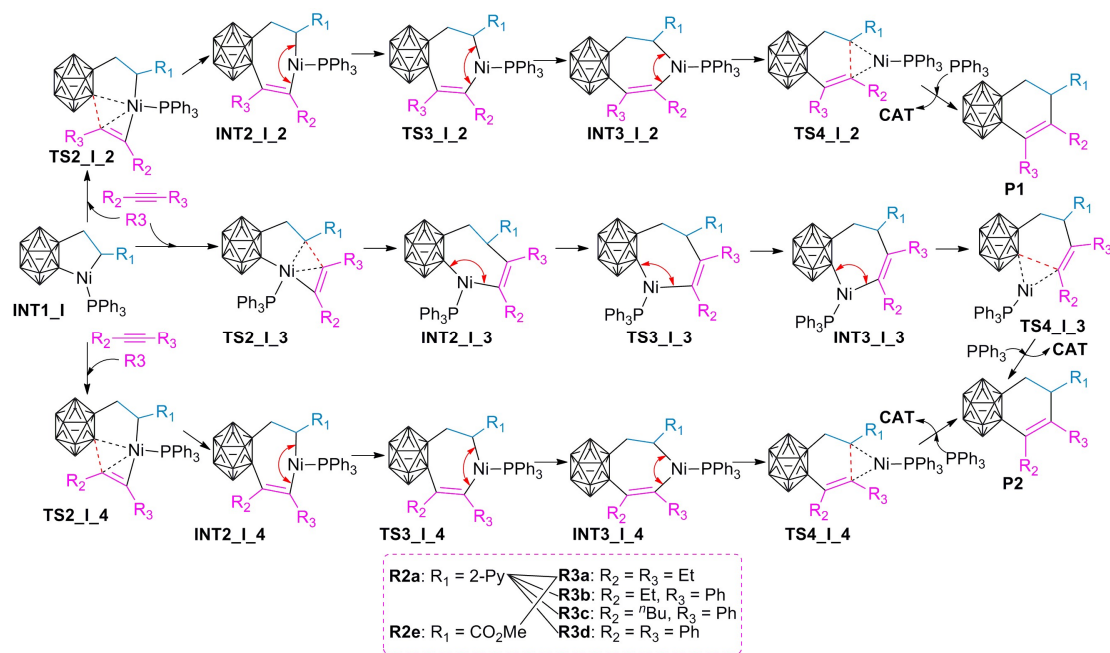


Figure S4 Other plausible reaction channels directing the formation of **P1** and **P2** from **INT1_I** in reactions **a-e**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

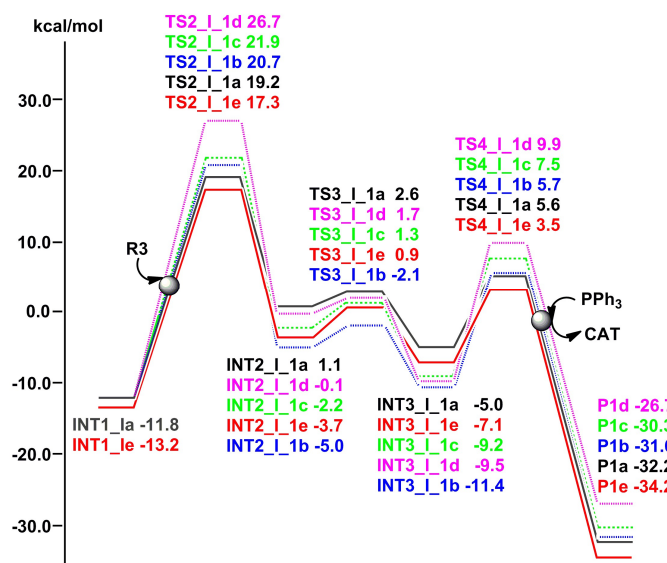


Figure S5 Relative free energies ($\text{kcal}\cdot\text{mol}^{-1}$) for the optimal reaction channel in reactions **a-e** (path **I_1**, after **INT1_I**), obtained at IDSCRF-B3LYP/DZVP level in THF solvent at 383K.

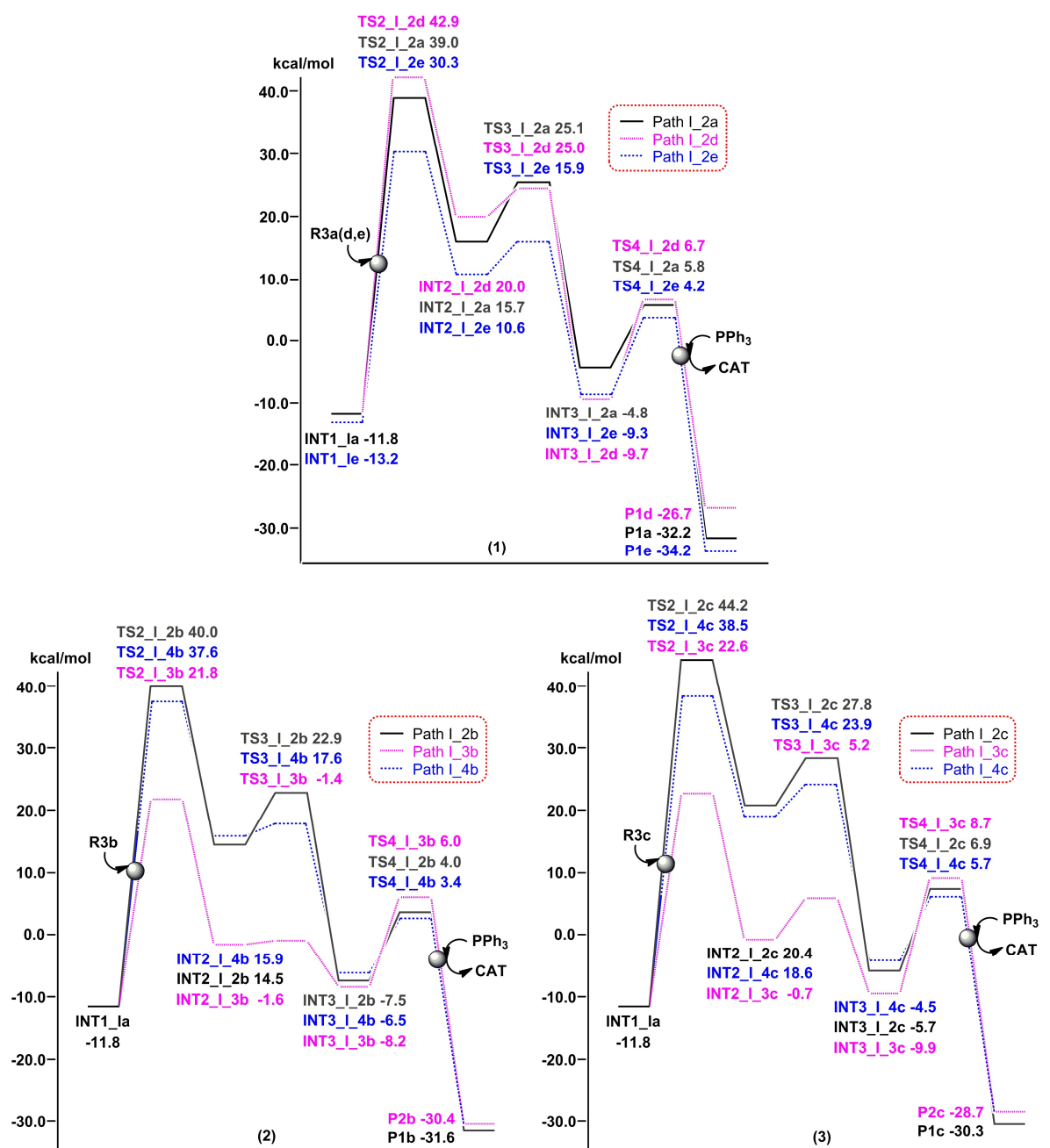


Figure S6 Relative free energies ($\text{kcal} \cdot \text{mol}^{-1}$) for paths **I**₂₋₄ in reactions **a-e**, obtained at IDSCRF-B3LYP/DZVP level in THF solvent at 383 K.

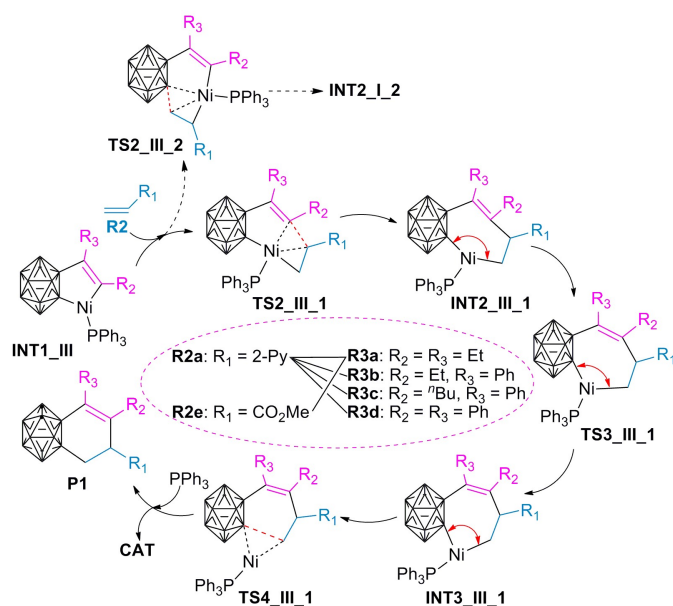


Figure S7 Plausible reaction channels directing the formation of **P1** from **INT1_III** in reactions **a-e**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

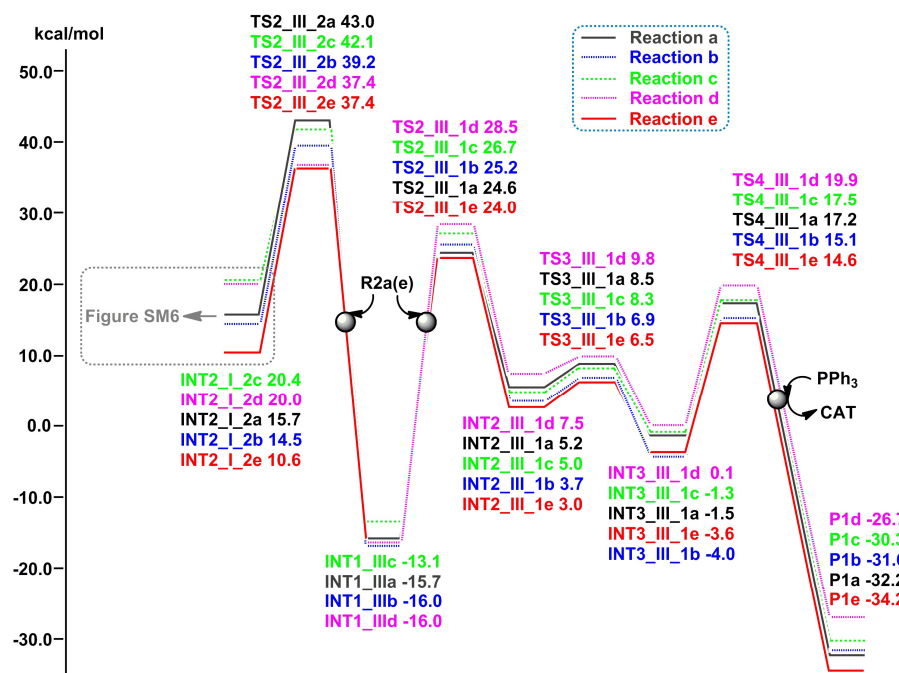


Figure S8 Relative free energies ($\text{kcal}\cdot\text{mol}^{-1}$) for paths **III_1-2** (derived from **INT1_III**) in reactions **a-e**, obtained at IDSCRF-B3LYP/DZVP level in THF solvent at 383 K.

Table S1 NBO charge distributions on C₃ and C₄ in **TS1**, **TS1_III** and **TS1_IV** for reactions **a-e**.

	TS1_Ia	TS1_Ie	TS1_IIIa	TS1_IIIb	TS1_IVb	TS1_IIIc	TS1_IVc	TS1_IIId
C3	-0.292	-0.284	0.047	0.024	0.079	0.024	0.088	0.050
C4	-0.364	-0.435	-0.114	-0.081	-0.135	-0.074	-0.128	-0.110

Table S2 Calculated free energy barriers ($\Delta G_{\text{rel}}(\text{TS1})$ and $\Delta G_{\text{rel}}(\text{TS2})$, 383K, kcal·mol⁻¹), rate constants (k , L·mol⁻¹·s⁻¹), half-lives ($t_{1/2}$, h) and end-product identity for reactions **a-e**, determined at the IDSCRF-B3LYP/DZVP level in THF solvent.

Reactions	TS1	$\Delta G_{\text{rel}}(\text{TS1})$	k	$t_{1/2}$	TS2	$\Delta G_{\text{rel}}(\text{TS1})$	k	$t_{1/2}$	Product	Yields(%)
a	TS1_Ia	15.9	6.749x10 ³	4.116x10 ⁻⁸	TS2_I_1a	31.0	1.633x10 ⁻⁵	1.701x10 ¹	P1a	57
	TS1_IIa	22.8	7.798x10 ⁻¹	1.562x10 ⁻⁴	TS2_I_2a	50.8	8.217x10 ⁻¹⁷	3.381x10 ¹²		
	TS1_IIIa	24.1	1.413x10 ⁻¹	1.966x10 ⁻³	TS2_III_1a	40.3	8.057x10 ⁻¹¹	3.448x10 ⁶		
					TS2_III_2a	58.7	2.552x10 ⁻²¹	1.089x10 ¹⁷		
					TS2_I_1b	32.5	2.275x10 ⁻⁶	1.221x10 ²	P1b	39
b	TS1_Ib	15.9	6.749x10 ³	4.116x10 ⁻⁸	TS2_I_2b	51.8	2.208x10 ⁻¹⁷	1.258x10 ¹³		
	TS1_IIb	22.8	7.798x10 ⁻¹	1.562x10 ⁻⁴	TS2_I_3b	33.6	5.362x10 ⁻⁷	5.181x10 ²		
	TS1_IIIb	21.8	2.901x10 ⁰	9.575x10 ⁻⁵	TS2_I_4b	49.4	5.171x10 ⁻¹⁶	5.372x10 ¹¹		
					TS2_III_1b	41.2	2.470x10 ⁻¹¹	1.125x10 ⁷		
	TS1_IVb	22.3	1.541x10 ⁰	1.847x10 ⁻⁴	TS2_III_2b	55.2	2.535x10 ⁻¹⁹	1.096x10 ¹⁵		
c					TS2_I_1c	33.7	4.702x10 ⁻⁷	5.908x10 ²	P1c	31
	TS1_Ic	15.9	6.749x10 ³	4.116x10 ⁻⁸	TS2_I_2c	56.0	8.861x10 ⁻²⁰	3.135x10 ¹⁵		
	TS1_IIc	22.8	7.798x10 ⁻¹	1.562x10 ⁻⁴	TS2_I_3c	34.4	1.874x10 ⁻⁷	1.482x10 ³		
	TS1_IIIc	25.6	1.969x10 ⁻²	1.411x10 ⁻²	TS2_I_4c	50.3	1.585x10 ⁻¹⁶	1.753x10 ¹²		
					TS2_III_1c	39.8	1.554x10 ⁻¹⁰	1.787x10 ⁶		
d	TS1_IVc	26.2	8.951x10 ⁻³	3.103x10 ⁻²	TS2_III_2c	55.2	2.535x10 ⁻¹⁹	1.096x10 ¹⁵		
	TS1_Id	15.9	6.749x10 ³	4.116x10 ⁻⁸	TS2_I_1d	38.5	8.576x10 ⁻¹⁰	3.239x10 ⁵	P1d	--
	TS1_IId	22.8	7.798x10 ⁻¹	1.562x10 ⁻⁴	TS2_I_2d	54.7	4.890x10 ⁻¹⁹	5.681x10 ¹⁴		
	TS1_IIId	26.9	3.568x10 ⁻³	7.785x10 ⁻²	TS2_III_1d	44.5	3.233x10 ⁻¹³	8.592x10 ⁸		
					TS2_III_2d	53.4	2.698x10 ⁻¹⁸	1.029x10 ¹⁴		
e	TS1_Ie	14.2	6.299x10 ⁴	4.410x10 ⁻⁹	TS2_I_1e	30.5	3.149x10 ⁻⁵	8.820x10 ⁰	P1e	59
	TS1_IId	22.2	1.715x10 ⁰	1.619x10 ⁻⁴	TS2_I_2e	43.5	1.203x10 ⁻¹²	2.309x10 ⁸		
	TS1_IIIe	24.1	1.413x10 ⁻¹	1.966x10 ⁻³	TS2_III_1e	39.7	1.772x10 ⁻¹⁰	1.567x10 ⁶		
					TS2_III_2e	53.1	4.002x10 ⁻¹⁸	6.941x10 ¹³		

Table S3 The optimized Cartesian coordinates (Å) for active **COM1** generation process, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	Cartesian coordinates				Species	Cartesian coordinates			
R	6	0.005458	0.028304	0.005971	TS1	6	-2.382839	-0.974664	0.992987
	6	0.012885	0.048967	1.634657		6	-1.759685	-0.092390	-0.253243
	5	1.524684	-0.019715	0.814147		5	-3.257827	-0.903689	-0.460580
	5	-1.247460	0.887799	0.815275		5	-1.482339	0.412628	1.360078
	5	-0.430553	1.570615	2.248700		5	-1.928687	1.569778	0.102243
	5	1.270770	1.013654	2.248006		5	-3.023530	0.757740	-1.023433
	5	0.858731	2.634905	-0.112014		5	-4.323326	0.878846	1.558103
	5	1.257587	0.976976	-0.643101		5	-4.068962	-0.837287	1.139835
	5	-0.443738	1.533936	-0.642407		5	-2.958691	-0.017345	2.277066
	5	2.077210	1.665070	0.790248		5	-4.517978	0.318892	-0.142514
	5	0.866897	2.657627	1.678686		5	-3.685119	1.871687	0.213622
	5	-0.696719	2.573169	0.791377		5	-2.708322	1.656535	1.709147
	1	2.111370	-1.044415	0.824501		1	-3.304763	-1.861359	-1.154085
	1	-2.326532	0.408423	0.826309		1	-0.389592	0.284339	1.806863
	1	-1.036047	1.607006	3.264613		1	-1.093940	2.311192	-0.299919
	1	1.781303	0.684678	3.263466		1	-2.940451	0.952740	-2.191025
	1	1.165890	3.574002	-0.768866		1	-5.250157	1.213482	2.223165
	1	1.758879	0.622307	-1.654508		1	-4.684965	-1.784289	1.499422
	1	-1.058465	1.544612	-1.653359		1	-2.840252	-0.423668	3.384651
	1	3.237591	1.908807	0.781870		1	-5.572123	0.258363	-0.687735
	1	1.179930	3.613061	2.308655		1	-4.154371	2.922897	-0.085516
	1	-1.488328	3.455926	0.783791		1	-2.477707	2.539695	2.470419
1	-0.299788	-0.903551	-0.455194	1	-1.883471	-1.916840	1.187394		
1	-0.288032	-0.870847	2.122092	1	-0.672213	-0.580359	-0.863688		
CAT1	6	-1.269178	4.884550	-1.753270	6	0.419021	-1.299243	-1.729475	

Species	Cartesian coordinates			Species	Cartesian coordinates		
	1	-0.245064	4.857264 -2.181724		1	-0.033202 -1.004376 -2.692373	
	1	-1.749575	5.732187 -2.287304		1	1.510065 -1.169245 -1.911028	
	6	-1.135469	5.291938 -0.269827		6	0.167388 -2.801346 -1.503044	
	1	-2.134684	5.359108 0.196799		1	0.665778 -3.129938 -0.576749	
	1	-0.618372	4.495278 0.293468		1	-0.906812 -2.968872 -1.328032	
	6	-0.401425	6.618762 0.028444		6	0.610286 -3.738528 -2.642678	
	1	0.608844	6.567104 -0.403148		1	0.107163 -3.430440 -3.569756	
	1	-0.914515	7.432795 -0.504304		1	1.686073 -3.600913 -2.821760	
	6	-0.302460	6.967369 1.522561		6	0.322527 -5.222941 -2.373233	
	1	0.224445	7.915134 1.691693		1	0.649216 -5.857467 -3.205775	
	1	-1.298767	7.058437 1.974384		1	0.839528 -5.570149 -1.469835	
	1	0.235838	6.187024 2.075977		1	-0.750347 -5.397728 -2.225020	
	3	-2.316082	3.085735 -2.182344		3	1.278677 0.087888 -0.292670	
	6	-2.384675	0.819345 -4.291644		6	2.246293 -1.718820 1.954791	
	8	-1.669207	1.521951 -3.235379		8	2.410700 -0.483817 1.194632	
	6	-0.234581	1.392626 -3.443019		6	3.631644 0.195644 1.612341	
	6	-0.074804	1.003724 -4.911030		6	4.412942 -0.831834 2.430382	
	6	-1.314952	0.123738 -5.142831		6	3.286813 -1.657458 0.193883	
	1	-3.087228	0.120543 -3.828006		1	1.215478 -1.759730 2.316183	
	1	-2.949868	1.559869 -4.868961		1	2.423012 -2.561641 1.277358	
	1	0.220973	2.348721 -3.174970		1	4.153001 0.534704 0.713442	
	1	0.147167	0.609701 -2.775026		1	3.351544 1.066373 2.216903	
	1	-0.107948	1.895035 -5.546963		1	5.023371 -1.460264 1.773169	
	1	0.865334	0.478706 -5.101445		1	5.071841 -0.357932 3.162743	
	1	-1.607015	0.058378 -6.194364		1	3.609110 -2.653685 3.387831	
	1	-1.133663	-0.892107 -4.775923		1	2.880509 -1.136392 3.947231	
	6	-4.664304	1.370058 -1.095462		6	2.002236 3.079662 -0.193385	
	8	-4.167607	2.643772 -1.596888		8	1.794344 1.855208 -0.956081	
	6	-4.977690	3.730882 -1.067429		6	1.681460 2.169258 -2.378271	
	6	-5.689443	3.144848 0.149949		6	2.136449 3.622202 -2.514549	
	6	-5.931153	1.691749 -0.292866		6	1.715688 4.225427 -1.164166	
	1	-4.851244	0.711389 -1.948773		1	1.333402 3.060328 0.671287	
	1	-3.883821	0.924686 -0.468155		1	3.041622 3.093795 0.155427	
	1	-4.303529	4.560631 -0.843543		1	2.301673 1.457756 -2.929524	
	1	-5.692267	4.043671 -1.839745		1	0.635423 2.037359 -2.674863	
	1	-5.034380	3.178493 1.027263		1	3.223640 3.674634 -2.636653	
	1	-6.612885	3.679860 0.388295		1	1.670545 4.118080 -3.370147	
	1	-6.071452	1.003062 0.544609		1	2.271166 5.130721 -0.905041	
	1	-6.816849	1.632708 -0.934360		1	0.647401 4.465303 -1.167248	
INT1	6	-2.759581	0.649806 -1.370634	TS2	6	-1.769803 -0.995925 1.725050	
	6	-3.848293	0.325118 -0.141590		6	-0.199519 -0.315418 1.513855	
	5	-2.883064	-0.934658 -0.811693		5	-1.360941 0.454053 2.491764	
	5	-3.026079	1.837384 -0.205535		5	-0.438136 -2.008942 1.574550	
	5	-3.159700	0.945371 1.306866		5	0.899259 -1.232835 2.448591	
	5	-3.070824	-0.770629 0.931546		5	0.317269 0.319079 3.026517	
	5	-0.533328	0.416854 0.219317		5	-1.202200 -1.751171 4.350986	
	5	-1.297920	-0.212999 -1.263405		5	-2.314910 -0.796578 3.324462	
	5	-1.387491	1.528147 -0.882638		5	-1.725702 -2.357584 2.751802	
	5	-1.455434	-1.128897 0.253540		5	-0.995883 0.029345 4.197435	
	5	-1.626871	0.061657 1.587065		5	0.432621 -1.056982 4.163005	
	5	-1.601785	1.709692 0.874044		5	-0.021498 -2.534926 3.243785	
	1	-3.390394	-1.764184 -1.493121		1	-1.865420 1.468394 2.122198	
	1	-3.625157	2.822147 -0.489487		1	-0.280846 -2.661670 0.590584	
	1	-3.896684	1.352351 2.147774		1	2.013626 -1.355897 2.039422	
	1	-3.745763	-1.560678 1.511048		1	1.013828 1.286053 3.025090	
	1	0.651689	0.454184 0.328559		1	-1.567188 -2.265040 5.364286	
	1	-0.778583	-0.574223 -2.267828		1	-3.475025 -0.604022 3.511340	
	1	-0.927677	2.323684 -1.634169		1	-2.471086 -3.260944 2.539787	
	1	-0.938331	-2.191795 0.392026		1	-1.213619 0.790499 5.089200	
	1	-1.227333	-0.158485 2.687300		1	1.245452 -1.076427 5.036267	
	1	-1.188184	2.663573 1.453191		1	0.465188 -3.602966 3.455573	
	1	-3.199127	0.838785 -2.342393		1	-2.482280 -0.701989 0.585626	
	3	-5.962526	0.278912 -0.369212		3	1.381986 -0.246426 -0.132922	
	6	-8.069877	2.110146 0.791973		6	2.599936 -3.178874 -0.445965	
	8	-7.155695	1.832690 -0.310720		8	2.549525 -1.776760 -0.846213	
	6	-7.015338	3.018738 -1.148912		6	3.624156 -1.497152 -1.787740	
	6	-7.645299	4.162006 -0.353283		6	4.215719 -2.855795 -2.169633	
	6	-8.742533	3.438687 0.445137		6	3.967607 -3.686331 -0.900312	
	1	-8.767130	1.271539 0.873162		1	2.441128 -3.225804 0.632216	
	1	-7.483854	2.180066 1.715893		1	1.783401 -3.711461 -0.948360	
	1	-5.951903	3.161714 -1.356633		1	3.203616 -0.951411 -2.637986	
	1	-7.547125	2.835910 -2.090266		1	4.361513 -0.857962 -1.289243	
	1	-6.908881	4.608116 0.323335		1	3.674719 -3.285652 -3.019527	
	1	-8.035367	4.948773 -1.004335		1	5.272677 -2.781739 -2.439209	
	1	-9.055080	3.984816 1.338976		1	3.965326 -4.763983 -1.084473	
	1	-9.625029	3.269598 -0.181047		1	4.728386 -3.468801 -0.142827	
	6	-8.298255	-1.419577 -1.299312		6	3.109673 2.355632 0.755930	
	8	-7.025364	-1.336795 -0.591916		8	2.817419 1.175540 -0.039943	
	6	-6.594756	-2.672240 -0.187253		6	3.802820 1.047805 1.111036	
	6	-7.487111	-3.640917 -0.962149		6	4.898893 2.065536 0.792303	
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	1	-8.963501	-0.653090 -0.893535		1	3.531517 2.034406 -1.716996	
	1	-8.115362	-1.208634 -2.359508		1	2.171484 2.884980 -0.940020	
	1	-5.531169	-2.765588 -0.415820		1	3.301261 1.264620 2.059256	
	1	-6.738770	-2.764121 0.895609		1	4.153626 0.012474 1.124880	
	1	-7.065585	-3.841394 -1.952985		1	5.399320 2.423530 1.695877	
	1	-7.607332	-4.594234 -0.440808		1	5.655211 1.625821 0.133056	
	1	-9.433714	-3.188461 -1.906511		1	3.601960 3.814490 0.772066	

Species	Cartesian coordinates			Species	Cartesian coordinates		
F1	1	-9.375337	-2.916632 -0.154841		1	4.751220	3.792888 -0.579787
	6	-0.172783	1.750323 -0.000001		6	-3.313355	-0.280503 -0.602903
	1	0.166681	2.302493 0.884554		1	-4.031545	0.438678 -0.168924
	1	0.166677	2.302489 -0.884559		1	-3.009615	0.169310 -1.572330
	1	-1.268564	1.763938 0.000001		6	-4.048499	-1.597584 -0.895501
	6	0.369640	0.315164 0.000001		1	-3.360767	-2.308370 -1.382613
	1	-0.016027	-0.221301 -0.877719		1	-4.319236	-2.076660 0.059070
	1	-0.016024	-0.221298 0.877724		6	-5.320719	-1.494114 -1.757618
	6	1.903449	0.244750 -0.000002		1	-6.022462	-0.801564 -1.272025
	1	2.289113	0.781212 -0.877725		1	-5.063471	-1.035729 -2.723310
	1	2.289117	0.781215 0.877717		6	-6.017334	-2.841488 -2.000458
	6	2.445873	-1.190409 -0.000001		1	-6.918515	-2.728690 -2.615286
	1	2.106413	-1.742575 0.884558		1	-5.351191	-3.545393 -2.515027
	1	2.106409	-1.742579 -0.884555		1	-6.317805	-3.307505 -1.053926
	1	3.541653	-1.204024 -0.000003		3	-1.281621	0.670623 -0.259485
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INT2	6	-0.661778	-1.542168 -0.624067		1	-1.600213	0.976440 -3.837645
	6	1.035785	-1.181575 -0.848281		1	-0.233921	1.084590 -4.965987
	5	0.523767	-2.270681 0.342404		1	-1.297811	-1.380949 -4.402721
	5	-0.028734	-1.249478 -2.164287		1	0.459536	-1.195076 -4.489731
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	5	1.939535	-2.628777 -0.670199		8	-1.386028	2.676985 -0.454502
	5	-0.284952	-4.108417 -1.750989		6	-2.626005	3.322877 -0.881586
	5	-0.837386	-3.216460 -0.300565		6	-2.545966	4.767984 -0.380159
	5	-1.186892	-2.568976 -1.891753		6	-1.630785	4.645165 0.849334
	5	0.788117	-3.937716 -0.320185		1	-0.189879	3.006175 1.203769
	5	1.443938	-3.741638 -1.981094		1	0.173260	4.036630 -0.209841
	5	0.210954	-2.865465 -2.950109		1	-2.694475	3.243403 -1.970493
	1	0.621432	-2.008901 1.505727		1	-3.460607	2.776067 -0.432768
	1	-0.318972	-0.267355 -2.782150		1	-2.085184	5.413934 -1.135269
	1	2.433902	-1.444102 -2.918123		1	-3.533610	5.171982 -0.142811
	1	3.031504	-2.560756 -0.190120		1	-1.144534	5.586559 1.119644
	1	-0.771551	-5.153362 -2.070294		1	-2.193258	4.283524 1.716419
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	1	-2.308998	-2.454223 -2.287604				
	1	1.077391	-4.854784 0.389689				
	1	2.209935	-4.521413 -2.466842				
TS3	1	0.085210	-3.012267 -4.129536		6	-2.257495	1.411642 0.719544
	3	-2.033968	-0.305246 0.367538		6	-0.728180	0.512889 0.593962
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	6	-5.192356	0.986825 -2.042939		5	-0.794890	3.601009 1.768483
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	1	-5.069047	0.531598 0.829269		5	-0.143299	3.208236 0.140703
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	1	-5.277028	2.925576 -1.058283		1	-1.290397	1.592181 -1.615606
	1	-5.712724	0.026055 -1.966123		1	-1.919501	-0.094718 2.735309
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	6	-1.659339	-0.003847 4.615309		1	-3.112391	2.660932 2.708855
	6	-2.099803	-1.455541 4.363472		1	0.309593	4.019966 -0.603642
	1	-3.931250	-1.104473 3.215863		1	1.783194	3.117427 1.945004
	1	-2.797833	-2.232105 2.419953		1	-0.379182	2.272498 4.012372
	1	-0.324023	0.233502 2.901942		3	-4.028882	0.453744 -0.070196
	1	-1.510851	1.559618 3.061739		3	-1.255117	-1.242042 -0.610904
	1	-0.792987	0.073829 5.277606		6	-4.992742	-0.824332 2.574351
	1	-2.479164	0.577727 5.050566		6	-6.690702	-0.840171 0.904809
					6	-7.247711	-1.485641 2.175917
					6	-6.353088	-0.877904 3.268209
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					1	-7.173831	0.119435 0.689924
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					1	-7.122946	-2.573303 2.140952
					1	-6.691796	0.131329 3.526459
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Species	Cartesian coordinates				Species	Cartesian coordinates			
	1	-1.226903	-2.103907	4.236646	1	-7.250516	4.438747	-0.243960	
	1	-2.717161	-1.863006	5.168507	1	-7.992782	2.831476	-0.140734	
	8	-3.449443	0.759166	-0.451523	8	-5.279884	-0.594150	1.163422	
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	8	1.247035	2.446631	-0.484963	8	-3.255687	-0.950958	-1.511151	
	6	-0.027324	2.727582	-1.130257	6	-3.151677	-0.350642	-2.856628	
	6	0.211532	3.993514	-1.949053	6	-4.000793	-1.226697	-3.789919	
	6	1.192448	4.769668	-1.053921	6	-4.922780	-1.996368	-2.827843	
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	1	2.959303	3.467015	-1.062947	1	-4.532220	-2.338963	-0.668347	
	1	-0.298331	1.850247	-1.721058	1	-3.524971	0.672954	-2.776675	
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	1	0.676045	3.743813	-2.909027	1	-4.551568	-0.628323	-4.520570	
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	1	1.786680	5.504748	-1.603023	1	-5.798443	-1.395975	-2.558303	
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	8	3.810711	0.795808	0.342690	8	-1.466339	-3.066670	0.181843	
	6	4.901744	0.179806	-0.406041	6	-1.399962	-3.242621	1.623656	
	6	5.930542	-0.243513	0.641944	6	-1.275154	-4.749404	1.838705	
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	1	3.933039	2.064088	1.980875	1	-1.735102	-4.706304	-1.058456	
	1	3.708876	0.337099	2.370208	1	-0.132627	-3.920153	-1.161585	
	1	4.487895	-0.653176	-0.978795	1	-0.525339	-2.703981	2.003254	
	1	5.307797	0.930305	-1.095224	1	-2.305321	-2.805684	2.052563	
	1	5.689979	-1.238261	1.031419	1	-0.810825	-4.991644	2.798770	
	1	6.945123	-0.268918	0.235390	1	-2.261705	-5.225305	1.802691	
	1	6.098788	0.502471	2.715885	1	0.637039	-4.981158	0.830615	
	1	6.268806	1.745779	1.462220	1	-0.539848	-6.228539	0.371345	
CAT2	28	0.000472	0.004475	-0.005669	8	1.657727	-0.291616	-0.307434	
	17	0.000334	-0.914595	-2.016913	7	0.421195	-1.063824	-2.349701	
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	6	4.355248	1.549424	-1.220551	6	5.438525	-1.197943	1.750264	
	6	2.133244	1.883715	-2.127059	6	4.523943	0.209401	3.989005	
	6	4.858073	2.516422	-2.094888	1	3.291000	1.311133	2.618759	
	1	5.031595	1.066279	-0.519998	6	5.923181	-1.513945	3.023909	
	6	2.638042	2.856276	-2.997638	1	5.789611	-1.763364	0.892521	
	1	1.076506	1.636843	-2.150642	6	5.471396	-0.809753	4.144906	
	6	4.000281	3.172668	-2.986348	1	4.159547	0.756546	4.855555	
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	1	1.963869	3.366288	-3.682175	1	5.850039	-1.056674	5.134339	
	1	4.391611	3.929253	-3.663040	6	4.832809	-0.583168	-1.328296	
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	1	3.909768	-1.738871	1.818935	6	6.990402	-0.843146	-2.420053	
	6	3.966624	1.902729	3.157763	1	6.650428	0.450469	-0.739409	
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	1	5.163233	1.115376	4.778767	6	4.183539	2.021915	-0.353474	
	6	2.915567	-1.691431	-0.608800	6	3.665331	2.611480	-1.520808	
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	1	5.226340	-3.283339	-2.550303	1	5.987413	4.677140	0.804135	
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	1	-1.064488	-1.588409	2.188075					
	6	-3.991508	-3.077760	3.093534					
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	1	-4.381917	-3.812326	3.794583					
	6	-3.256263	-0.358776	-1.456595					
	6	-3.957477	0.617296	-2.181584					
	6	-3.257631	-1.685615	-1.926219					
	6	-4.653442	0.273189	-3.347575					
	1	-3.979348	1.647836	-1.840989					
	6	-3.957813	-2.028203	-3.084132					
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Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -5.201206 -1.316128 -4.704831 6 -2.910979 1.706706 0.551007 6 -2.297413 2.815206 -0.058693 6 -3.947969 1.920061 1.470399 6 -2.730418 4.112314 0.227070 1 -1.471951 2.666699 -0.752329 6 -4.373324 3.221205 1.765144 1 -4.422088 1.082033 1.972385 6 -3.770906 4.318767 1.141661 1 -2.248304 4.960235 -0.254422 1 -5.174210 3.373599 2.485375 1 -4.103415 5.328520 1.372182		
INT3	6 -2.574391 1.548835 -0.754897 6 -1.057940 1.758204 -0.215980 5 -1.282954 1.523515 -1.875296 5 -2.266461 2.566661 0.599906 5 -0.669183 3.331286 0.327941 5 -0.051907 2.639547 -1.195994 5 -2.389414 4.159889 -1.805767 5 -2.719622 2.455236 -2.231627 5 -3.329867 3.096195 -0.707276 5 -1.090215 3.165320 -2.547190 5 -0.723883 4.294719 -1.173042 5 -2.133192 4.251481 -0.034548 1 -0.954753 0.503086 -2.388672 1 -2.619477 2.234128 1.682449 1 0.077001 3.460447 1.242971 1 1.101142 2.266695 -1.203047 1 -2.904984 5.049831 -2.405876 1 -3.464874 2.073549 -3.075179 1 -4.500447 3.163245 -0.510415 1 -0.678001 3.339220 -3.649230 1 -0.039044 5.257241 -1.315583 1 -2.464260 5.184842 0.624977 3 -3.057166 -0.424329 0.039486 6 -4.152003 -0.701514 2.908459 6 -5.743965 0.012614 1.284467 6 -6.407332 0.033341 2.664596 6 -5.200002 0.163229 3.608334 1 -4.254812 -1.759765 3.180232 1 -3.121285 -0.386747 3.085698 1 -5.616958 1.021480 0.876193 1 -6.277283 -0.602851 0.553684 1 -7.122523 0.854345 2.763354 1 -6.937577 -0.907014 2.850260 1 -4.863121 1.204056 3.660143 1 -5.409260 -0.182375 4.624495 6 -3.413376 -1.795904 -2.672376 8 -3.507331 -1.875997 -1.223783 6 -4.039103 -3.172758 -0.830349 6 -4.125991 -4.000162 -2.117106 6 -4.306198 -2.919447 -3.196600 1 -3.729129 -0.794396 -2.972871 1 -2.366183 -1.941604 -2.964975 1 -3.371666 -3.605191 -0.079355 1 -5.024061 -3.011798 -0.378047 1 -3.194111 -4.551327 -2.282777 1 -4.947286 -4.721197 -2.086836 1 -4.008059 -3.253533 -4.194147 1 -5.349687 -2.589052 -3.241462 8 -4.422088 -0.565084 1.485475 28 0.406180 0.657245 0.073343 17 -0.742128 -0.853577 1.198876 15 2.532239 -0.259311 0.159475 6 3.000221 -0.703586 1.879499 6 2.487655 0.089429 2.920945 6 3.846829 -1.779784 2.190645 6 2.833993 -0.175323 4.249164 1 1.812477 0.912765 2.696222 6 4.183939 -2.050173 3.521341 1 4.241381 -2.415077 1.402308 6 3.682314 -1.246920 4.552057 1 2.432983 0.447644 5.045520 1 4.837270 -2.889011 3.751148 1 3.945675 -1.459017 5.585974 6 2.776766 -1.781332 -0.845542 6 1.670885 -2.618953 -1.073935 6 4.027751 -2.136178 -1.380419 6 1.818469 -3.796574 -1.814201 1 0.697917 -2.353064 -0.669344 6 4.170642 -3.311694 -2.124303 1 4.892327 -1.495434 -1.226603 6 3.067121 -4.145285 -2.341466 1 0.956084 -4.437673 -1.983310 1 5.143463 -3.574236 -2.534166 1 3.179466 -5.058553 -2.921746 6 3.863041 0.877968 -0.418717 6 3.816597 1.333413 -1.750075	TS4	6 -1.963154 1.337717 0.748661 6 -0.316980 1.338912 0.492990 5 -1.283663 2.333829 -0.467416 5 -0.890210 1.118184 2.059933 5 0.546142 2.135121 1.733701 5 0.305751 2.894498 0.141185 5 -1.724949 3.879497 1.926825 5 -2.526900 2.956944 0.623085 5 -2.283119 2.200311 2.196400 5 -1.104282 3.971081 0.243847 5 0.028313 3.835483 1.633103 5 -0.703143 2.726111 2.845260 1 -1.460633 2.081571 -1.614001 1 -0.808905 0.063906 2.599607 1 1.605642 1.726084 2.067726 1 1.203233 3.004134 -0.623882 1 -2.273987 4.798084 2.450865 1 -3.622088 3.145449 0.199661 1 -3.209033 1.866857 2.864481 1 -1.189495 4.946310 -0.433660 1 0.775491 4.711353 1.939223 1 -0.499333 2.815864 4.014831 28 0.247749 -0.190371 -0.463792 17 -1.381932 -1.453428 -1.430004 3 -3.097471 -0.298139 -0.114184 15 2.438682 -0.225623 -0.198777 6 3.042333 -0.787501 1.434127 6 4.390145 -0.670369 1.815299 6 2.131296 -1.415038 2.300739 6 4.816147 -1.171933 3.048960 1 5.110069 -0.193125 1.156013 6 2.562190 -1.920182 3.530146 1 1.084874 -1.505144 2.018688 6 3.904441 -1.796950 3.907619 1 5.860438 -1.074669 3.336823 1 1.848326 -2.400844 4.194993 1 4.238080 -2.183408 4.868067 6 2.688178 -1.654269 -1.335634 6 3.400205 -2.805760 -0.956031 6 2.103511 -1.600189 -2.616382 6 3.539485 -3.872240 -1.848912 1 3.848436 -2.875297 0.030688 6 2.247398 -2.667673 -3.506362 1 1.535825 -0.724616 -2.927116 6 2.965797 -3.805724 -3.124380 1 4.097003 -4.755748 -1.546368 1 1.790989 -2.610991 -4.491684 1 3.074404 -4.639296 -3.814605 6 3.609272 1.075030 -0.767084 6 4.211560 1.013555 -2.035508 6 3.893727 2.170344 0.069972 6 5.078356 2.027340 -2.457513 1 4.024779 0.174953 -2.698071 6 4.764735 3.176416 -0.353165 1 3.444190 2.242511 1.054561 6 5.357307 3.111320 -1.619553 1 5.538600 1.961971 -3.440781 1 4.975090 4.013667 0.308340 1 6.033156 3.897498 -1.948494 6 -3.703752 -1.757308 2.510351 8 -4.030759 -1.570194 1.105211 6 -4.645929 -2.776914 0.574170 6 -4.440652 -3.853817 1.641603 6 -4.438619 -3.028392 2.939157 1 -2.617018 -1.865562 2.603813 1 -4.015771 -0.860250 3.050857 1 -5.709914 -2.572377 0.403645 1 -4.169827 -3.009421 -0.382099 1 -5.225053 -4.615256 1.615645 1 -3.474624 -4.350960 1.502356 1 -5.463854 -2.794101 3.246011 1 -3.939273 -3.532914 3.770869 6 -5.799058 0.797787 -0.935606 8 -4.565762 0.176535 -1.391227 6 -4.357785 0.461431 -2.802303 6 -5.694851 0.999502 -3.313557

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 4.883337 1.344250 0.424745 6 4.779796 2.223365 -2.229478 1 3.034565 0.986063 -2.422610 6 5.843716 2.243678 -0.055945 1 4.939492 1.008946 1.456464 6 5.796030 2.684145 -1.381805 1 4.733124 2.561748 -3.262194 1 6.628769 2.596104 0.609507 1 6.542777 3.382164 -1.753656		6 -6.249037 1.718701 -2.072288 1 -6.530455 0.003643 -0.741164 1 -5.592412 1.327226 -0.001665 1 -3.558984 1.206410 -2.892939 1 -4.035121 -0.463349 -3.286897 1 -5.570927 1.660982 -4.175399 1 -6.354335 0.174737 -3.605560 1 -5.789657 2.707171 -1.966556 1 -7.334961 1.845541 -2.094966
F2	3 -0.193160 0.068345 -1.178971 17 -1.143064 -1.957952 -1.556438 6 1.948995 -0.832556 0.643362 8 1.463207 0.269852 -0.180670 6 2.548433 1.212088 -0.434369 6 3.746717 0.706172 0.376957 6 3.466993 -0.802169 0.490487 1 1.642804 -0.650599 1.680903 1 1.472143 -1.745879 0.280552 1 2.751053 1.210074 -1.511029 1 2.214687 2.209878 -0.135273 1 4.696561 0.932187 -0.114615 1 3.758639 1.166552 1.370430 1 3.768722 -1.322885 -0.424612 1 3.976764 -1.269104 1.337546 6 -2.002797 1.674985 -2.871620 8 -0.979290 1.722518 -1.832134 6 -1.016788 3.018029 -1.161221 6 -2.059513 3.853791 -1.912408 6 -2.988248 2.781913 -2.507996 1 -1.522264 1.862596 -3.839737 1 -2.425911 0.667941 -2.867116 1 -1.301357 2.848131 -0.116989 1 -0.012673 3.450711 -1.192258 1 -2.577145 4.551825 -1.249284 1 -1.583855 4.431573 -2.711783 1 -3.701793 2.425906 -1.757200 1 -3.549354 3.136978 -3.376615	COM1	6 -0.762030 2.655873 -0.106539 6 0.776420 2.601217 -0.144449 5 -0.016638 3.134404 -1.568221 5 0.055845 3.009819 1.357212 5 1.523534 3.822482 0.787372 5 1.479905 3.898172 -1.001541 5 -0.785196 5.392886 0.012640 5 -1.413427 4.009431 -0.928221 5 -1.372341 3.928766 0.858823 5 0.055210 4.894183 -1.491668 5 1.006246 5.325096 -0.033016 5 0.123661 4.769416 1.426256 1 -0.077797 2.430219 -2.521509 1 0.041461 2.229860 2.249891 1 2.554939 3.627944 1.337708 1 2.484447 3.755760 -1.616487 1 -1.396970 6.411877 0.069406 1 -2.453186 3.950179 -1.494172 1 -2.386682 3.810333 1.461945 1 0.054577 5.546660 -2.486286 1 1.693506 6.296180 -0.009435 1 0.170849 5.335059 2.471578 28 -0.055514 0.850581 -0.129349 15 1.771282 -0.493749 -0.052853 15 -1.856710 -0.471428 -0.003315 6 1.648823 -2.318218 0.254576 6 2.029097 -2.917921 1.464743 6 1.162198 -3.138389 -0.780470 6 1.930431 -4.304255 1.634409 1 2.419508 -2.317117 2.279616 6 1.068475 -4.521488 -0.612227 1 0.874838 -2.707192 -1.734847 6 1.452703 -5.111068 0.598331 1 2.234283 -4.749776 2.579115 1 0.698597 -5.137377 -1.429132 1 1.382616 -6.188624 0.729815 6 2.866061 0.116366 1.301499 6 4.210222 0.465497 1.098496 6 2.312319 0.267656 2.585530 6 4.986950 0.942301 2.161159 1 4.659693 0.380271 0.113988 6 3.091722 0.731463 3.648099 1 1.268918 0.021251 2.763182 6 4.433421 1.071803 3.438650 1 6.025260 1.214823 1.984992 1 2.647028 0.837594 4.635150 1 5.039048 1.442422 4.262723 6 2.809506 -0.459112 -1.577630 6 3.857917 -1.380467 -1.764806 6 2.560404 0.495932 -2.574637 6 4.641650 -1.337490 -2.919994 1 4.064045 -2.136933 -1.012061 6 3.344166 0.536431 -3.733934 1 1.755776 1.211319 -2.450606 6 4.386348 -0.378457 -3.909123 1 5.449890 -2.054099 -3.048583 1 3.136214 1.283224 -4.496983 1 4.994932 -0.348533 -4.810293 6 -2.174888 -1.467983 -1.518549 6 -1.326972 -1.307821 -2.625556 6 -3.295958 -2.310227 -1.634607 6 -1.576606 -1.993600 -3.819959 1 -0.477001 -0.632477 -2.562371 6 -3.539553 -3.003044 -2.822613 1 -3.991049 -2.416580 -0.805105 6 -2.678857 -2.848114 -3.917810 1 -0.913001 -1.855046 -4.670594 1 -4.406893 -3.655204 -2.897938 1 -2.875265 -3.382186 -4.844871 6 -1.743303 -1.614043 1.434888 6 -1.493251 -1.024128 2.689046 6 -1.870946 -3.007846 1.353734 6 -1.404487 -1.810331 3.840102 1 -1.385159 0.055876 2.773327 6 -1.771011 -3.795139 2.507006 1 -2.036097 -3.492095 0.396732 6 -1.545310 -3.200947 3.751822 1 -1.222994 -1.337155 4.802687 1 -1.866380 -4.875525 2.426732
PPh₃	15 -0.078834 -0.221546 0.119180 6 -0.038394 -0.122507 1.968840 6 0.788118 -0.906583 2.792023 6 -0.872568 0.837600 2.573371 6 0.772294 -0.742910 4.183057 1 1.449378 -1.648222 2.351780 6 -0.899399 0.992735 3.963059 1 -1.507035 1.469603 1.953610 6 -0.073569 0.202915 4.773151 1 1.420395 -1.357671 4.804465 1 -1.555377 1.736225 4.411041 1 -0.085110 0.328591 5.853700 6 1.415478 -1.245651 -0.269601 6 1.401339 -2.638633 -0.456734 6 2.635770 -0.559505 -0.421711 6 2.577956 -3.328187 -0.776135 1 0.471722 -3.192385 -0.355258 6 3.813963 -1.248440 -0.727195 1 2.666478 0.522343 -0.300336 6 3.787702 -2.637186 -0.908008 1 2.547624 -4.406496 -0.919121 1 4.747751 -0.700491 -0.834723 1 4.700841 -3.174187 -1.155640 6 -1.475006 -1.397464 -0.198075 6 -2.090395 -2.189743 0.786428 6 -1.966275 -1.461643 -1.516229 6 -3.160453 -3.032182 0.459000 1 -1.738486 -2.152652 1.814004 6 -3.025714 -2.312539 -1.847335 1 -1.517344 -0.842130 -2.291309 6 -3.628472 -3.099932 -0.858083 1 -3.625734 -3.637114 1.234687 1 -3.386630 -2.351928 -2.872987 1 -4.459302 -3.755155 -1.110902		

Species	Cartesian coordinates	Species	Cartesian coordinates
			1 -1.472364 -3.815554 4.646329
			6 -3.500100 0.349581 0.219961
			6 -4.375673 0.052026 1.275303
			6 -3.900016 1.280600 -0.754518
			6 -5.625503 0.679896 1.357055
			1 -4.098066 -0.669741 2.037292
			6 -5.148600 1.899489 -0.676265
			1 -3.237761 1.524485 -1.580759
			6 -6.016031 1.603286 0.383284
			1 -6.291993 0.440737 2.182972
			1 -5.441296 2.617934 -1.438730
			1 -6.987072 2.089361 0.447667

Table S4 The first three vibration frequencies for stationary points corresponding to the generation of active **COM1**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)
R	449 458 507	INT1	14 19 21	INT2	-9 11 13	INT3	7 8 12
CAT1	13 17 19	F1	118 223 259	CAT2	9 17 21	F2	18 24 26
TS1	-1271i 10 15	TS2	-1398i 6 15	TS3	-51i 15 17	TS4	-36i 9 10
PPh₃	25 26 45	COM1	17 18 24				

Table S5 The total energies (*E*: a.u.), zero-point energies (*ZPE*: kcal·mol⁻¹) and Gibbs free energies [*G* and *G*(sol,298K): a.u.] for stationary points corresponding to the generation of **COM1**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	<i>E</i>	<i>ZPE</i>	<i>G</i>	<i>G</i> (sol,298K)
R	-332.10394	110.34233	-331.95895	-331.94707
CAT1	-630.36758	223.56864	-630.06822	-630.05801
TS1	-962.46867	332.11422	-962.00726	-961.99665
INT1	-804.06442	252.19498	-803.71982	-803.70928
F1	-158.47286	82.93258	-158.36874	-158.35829
TS2	-1434.41746	474.41160	-1433.74625	-1433.73591
INT2	-1275.99937	393.50106	-1275.45312	-1275.44317
CAT2	-4501.20600	346.29956	-4500.73170	-4500.71869
TS3	-4740.86056	569.20927	-4740.05633	-4740.04519
INT3	-3808.09625	417.39800	-3807.52070	-3807.50985
TS4	-3808.10139	418.09296	-3807.52083	-3807.50949
F2	-932.80480	150.01709	-932.61432	-932.60275
PPh₃	-1036.32562	171.02850	-1036.09936	-1036.08737
COM1	-3911.65455	440.55338	-3911.03221	-3911.02141

Table S6 The optimized Cartesian coordinates (Å) for stationary points on potential energy surfaces from **COM1** and **R2** (or **R3**) to **INT1_I-IV**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	Cartesian coordinates	Species	Cartesian coordinates
R2a	6 -2.951471 0.326615 -0.000154	R2e	6 -2.812824 0.389871 -0.027474
	1 -2.817089 1.406054 -0.000349		1 -2.536563 1.438794 -0.088788
	1 -3.977638 -0.031471 -0.000096		1 -3.873193 0.149722 -0.014625
	6 -1.925154 -0.539796 0.000082		6 -1.888846 -0.579146 0.030566
	1 -2.130522 -1.609585 0.000288		1 -2.167966 -1.628183 0.091878
	6 -0.482902 -0.216793 0.000129		6 -0.422119 -0.349054 0.018782
	6 0.016051 1.100921 0.000094		8 0.396929 -1.258239 0.073121
	6 1.665904 -1.072699 -0.000092		8 -0.078238 0.954832 -0.057359
	6 1.393528 1.309002 0.000020		6 1.339510 1.233860 -0.072088
	1 -0.663425 1.948784 0.000136		1 1.420390 2.318857 -0.135700
	6 2.246038 0.198829 -0.000058		1 1.809559 0.867244 0.843533
	1 2.295155 -1.962865 -0.000128		1 1.811637 0.762672 -0.937416
	1 1.797315 2.319274 0.000019		
	1 3.327126 0.311620 -0.000098		
	7 0.342445 -1.288327 0.000015		
R3a	6 -0.431664 1.879154 0.000193	R3b	6 -0.010793 0.003778 0.043457
	6 0.784664 1.870846 -0.000193		6 -0.015518 0.002727 1.261230
	6 2.257552 1.839613 -0.000750		6 0.015752 0.005234 -1.426731
	1 2.626651 2.403627 -0.866348		1 -0.524776 -0.876396 -1.792637
	1 2.626590 2.367256 0.887511		1 -0.538250 0.879080 -1.791108
	6 2.837933 0.412228 -0.030340		6 1.442847 0.016647 -2.011105
	1 2.513163 -0.123999 -0.927250		1 2.004791 -0.865216 -1.689305
	1 3.932440 0.448897 -0.029590		1 1.400414 0.017250 -3.105208
	1 2.513167 -0.160739 0.843554		1 1.991251 0.906443 -1.687790

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 -1.904552 1.910387 0.000750 1 -2.273590 1.382744 -0.887511 1 -2.273651 1.346373 0.866348 6 -2.484933 3.337772 0.030340 1 -2.160167 3.910739 -0.843554 1 -3.579440 3.301103 0.029590 1 -2.160163 3.873999 0.927250		6 -0.026515 0.001497 2.697095 6 -0.009086 -1.213736 3.414330 6 -0.056607 1.215481 3.416026 6 -0.021597 -1.211219 4.811034 1 0.014195 -2.153767 2.868515 6 -0.069006 1.210534 4.812720 1 -0.070123 2.156461 2.871517 6 -0.051556 -0.000955 5.515865 1 -0.007808 -2.155237 5.351369 1 -0.092163 2.153616 5.354368 1 -0.061193 -0.001903 6.603482
R3c	6 0.793945 0.005425 0.746012 6 -0.394590 0.003544 0.480662 6 2.229053 -0.010056 1.061726 1 2.742505 0.721158 0.423543 1 2.371164 0.333416 2.095108 6 2.881893 -1.398126 0.885700 1 2.734976 -1.733868 -0.148228 1 2.362126 -2.121320 1.526174 6 -1.796237 0.002425 0.168770 6 -2.501716 1.216383 0.026768 6 -2.493014 -1.213004 -0.001104 6 -3.865203 1.211134 -0.276413 1 -1.973091 2.157663 0.155825 6 -3.856432 -1.210694 -0.304467 1 -1.957553 -2.153130 0.106510 6 -4.548208 -0.000481 -0.443355 1 -4.396621 2.154306 -0.382989 1 -4.380957 -2.155022 -0.432815 1 -5.609918 -0.001590 -0.679501 6 4.379311 -1.389261 1.221320 1 4.517990 -1.043577 2.254512 1 4.890709 -0.657591 0.581529 6 5.037511 -2.764581 1.050668 1 4.946124 -3.122955 0.018603 1 6.104387 -2.727109 1.296810 1 4.571021 -3.511495 1.703713	R3d	6 -0.219398 0.577329 0.002720 6 1.000862 0.577272 0.002655 6 -1.650610 0.577397 0.002788 6 -2.368036 0.619590 -1.212920 6 -2.367926 0.535272 1.218562 6 -3.764035 0.619494 -1.208176 1 -1.822664 0.652157 -2.152816 6 -3.763925 0.535501 1.213950 1 -1.822469 0.502654 2.158408 6 -4.467408 0.577531 0.002920 1 -4.305470 0.652215 -2.150989 1 -4.305275 0.502831 2.156813 1 -5.555008 0.577582 0.002971 6 2.432061 0.577204 0.002587 6 3.149373 0.619329 -1.213183 6 3.149483 0.535010 1.218290 6 4.545371 0.619100 -1.208574 1 2.603923 0.651948 -2.153032 6 4.545480 0.535104 1.213551 1 2.604117 0.502442 2.158190 6 5.248857 0.577068 0.002455 1 5.086722 0.651769 -2.151438 1 5.086917 0.502382 2.156364 1 6.336457 0.577016 0.002404
TSI_1a	6 2.733704 -1.035053 -0.666087 6 2.459062 0.314648 0.106840 5 3.156112 0.417923 -1.466616 5 2.902699 -1.072079 1.037837 5 3.555841 0.534245 1.390513 5 3.713515 1.443391 -0.139531 5 5.437908 -0.876145 -0.296716 5 4.188992 -1.028396 -1.561356 5 4.032958 -1.942597 -0.024294 5 4.894553 0.581078 -1.192923 5 5.148229 0.655810 0.582942 5 4.640129 -0.905070 1.310321 1 2.489983 0.783888 -2.376550 1 2.079665 -1.623556 1.684952 1 3.210937 1.093357 2.378251 1 3.474975 2.603184 -0.166324 1 6.517603 -1.343397 -0.465429 1 4.254754 -1.625864 -2.583045 1 3.998780 -3.126676 -0.058486 1 5.578407 1.156287 -1.975901 1 6.023607 1.304650 1.057609 1 5.145912 -1.368126 2.280432 28 0.791397 -0.437467 -0.487488 15 -0.901394 0.857597 -0.014556 6 -0.015940 -1.966738 -1.464306 6 1.401007 -2.216491 -1.589984 1 1.777597 -3.097706 -1.080697 1 1.838414 -2.028192 -2.565466 1 -0.509017 -1.563174 -2.346422 6 -0.855394 -2.879307 -0.651358 6 -2.230484 -3.015415 -0.927507 6 -2.995943 -3.895766 -0.165089 1 -2.681611 -2.441726 -1.732551 6 -1.005805 -4.427730 1.057842 6 -2.375261 -4.624396 0.855383 1 -4.058497 -4.015641 -0.366097 1 -0.483242 -4.977570 1.840926 1 -2.928661 -5.325250 1.474757 7 -0.257858 -3.582978 0.335030 6 -2.336279 0.682257 -1.153801 6 -3.650208 0.474945 -0.708030 6 -2.086206 0.743438 -2.537830 6 -4.696875 0.340813 -1.629229 1 -3.867049 0.409073 0.354054 6 -3.132306 0.619571 -3.455055 1 -1.071532 0.893205 -2.903203 6 -4.442543 0.415770 -3.001988 1 -5.710117 0.176575 -1.269210 1 -2.923888 0.675995 -4.521132 1 -5.257044 0.312542 -3.715476 6 -1.545848 0.573672 1.683817	INT1_1a	6 -3.536598 -1.122100 0.250261 6 -2.690571 0.264183 -0.050895 5 -3.522078 0.099958 1.446188 5 -3.481057 -0.523336 -1.355129 5 -3.532765 1.234833 -1.185115 5 -3.553968 1.620785 0.543587 5 -5.969346 0.145621 -0.068459 5 -5.001295 -0.821777 1.074372 5 -4.975180 -1.210626 -0.663514 5 -5.060143 0.955805 1.252294 5 -5.076218 1.667635 -0.395402 5 -5.021790 0.322068 -1.582966 1 -2.898489 -0.084074 2.434051 1 -2.828424 -1.111979 -2.146618 1 -2.904576 1.894131 -1.945921 1 -2.943638 2.545800 0.967125 1 -7.156835 0.086894 -0.071012 1 -5.376171 -1.627987 1.858831 1 -5.333160 -2.276316 -1.040653 1 -5.582924 1.466892 2.189166 1 -5.624608 2.695767 -0.631441 1 -5.517309 0.381564 -2.661374 28 -0.809050 0.029529 -0.018074 15 1.412946 0.603521 -0.019226 6 -1.144909 -1.743363 0.737454 6 -2.576503 -2.272639 0.493781 1 -2.904405 -2.865773 1.355816 1 -2.575240 -2.931059 -0.375600 1 -1.007486 -1.463494 1.788514 6 -0.084618 -2.706570 0.319755 6 1.034269 -2.949283 1.142593 6 1.987624 -3.888746 0.750981 1 1.138351 -2.418954 2.084916 6 0.672171 -4.263181 -1.216650 6 1.808459 -4.566925 -0.457671 1 2.850524 -4.092108 1.381394 1 0.496397 -4.770976 -2.165338 1 2.519880 -5.311165 -0.805952 7 -0.249799 -3.364323 -0.851805 6 2.532215 0.174033 -1.408350 6 2.217549 -0.933087 -2.212111 6 3.666017 0.949010 -1.714972 6 3.034806 -1.272794 -3.296673 1 1.330051 -1.522865 -2.001890 6 4.480202 0.607396 -2.797310 1 3.910414 1.825017 -1.118386 6 4.166981 -0.505896 -3.589065 1 2.780355 -2.130681 -3.914886 1 5.354195 1.212818 -3.027097 1 4.799357 -0.767130 -4.434757 6 2.338125 0.334413 1.542698

Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 -2.803689 1.295190 3.636169		6 2.274525 0.317215 3.976571
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	6 -1.728353 -0.875374 3.628029		6 4.302286 -0.320072 2.816862
	1 -0.633130 -1.382075 1.844957		1 4.224573 -0.273706 0.667569
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	1 -1.486810 -1.812195 4.124943		1 5.336031 -0.658003 2.837085
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	6 -0.533099 2.666778 -0.028573		6 1.220467 2.433510 -0.169295
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	1 -3.471085 5.540602 -0.305618		1 3.040192 3.372944 4.601845
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	6 -3.936416 -1.417431 -0.797524		6 1.962955 2.005884 -2.113646
	6 -3.022461 -1.823207 -3.411183		6 4.537484 1.492131 -3.076598
	1 -1.279152 -0.711067 -2.815493		1 4.680297 0.029777 -1.504356
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 4.786010 0.853453 0.296337		1 -5.367964 0.697857 -0.645090
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	1 4.268698 -4.074978 0.817225		1 -4.375157 -4.183939 -0.921807
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	5 -2.753406 2.290486 0.904251		5 3.027913 2.016336 -1.221581
	5 -2.618864 2.346434 -0.873931		5 2.935878 2.179260 0.539394
	5 -5.164512 1.154415 -0.211758		5 5.594295 1.256181 -0.123774
	5 -4.190896 -0.069826 -1.075038		5 4.793994 -0.006715 0.849720
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	5 -4.120823 1.652649 -1.579908		5 4.521273 1.721291 1.237755
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	1 -4.845542 -1.043579 1.248132		1 5.459249 -1.088215 -1.407323
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15	1.313442 0.232122 -0.026999	15	-1.727144 0.121899 0.034482
6	-0.721663 -2.303795 -0.172814	6	1.299877 -1.593231 -0.134308
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6	0.258704 -3.439323 -0.289433	6	3.530148 -3.547830 1.565257
1	-0.233520 -4.295375 -0.763214	1	2.552171 -3.709301 2.030934
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -1.384365 1.221552 2.362314		1 2.346236 0.871263 -2.489414
	1 -0.122515 3.809273 1.469477		1 0.964307 3.491432 -1.932149
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	15 1.783093 -0.166471 -0.043556		15 -2.129528 -0.152415 0.033297
	6 -1.072872 -1.694101 0.018296		6 1.269023 -0.854433 -0.119815
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Species	Cartesian coordinates	Species	Cartesian coordinates
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Species	Cartesian coordinates	Species	Cartesian coordinates
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TS1_IIIc	6 2.259565 -1.230654 0.094794 6 0.973126 -2.143149 0.229188 5 1.883749 -2.258616 -1.228697 5 1.874404 -1.813973 1.661979 5 1.205759 -3.420269 1.329972 5 1.211363 -3.692609 -0.434882 5 3.950379 -3.361529 0.428481 5 3.560262 -2.023935 -0.687528 5 3.554118 -1.750311 1.088193 5 2.918862 -3.672315 -1.005141 5 2.501710 -4.398193 0.582482 5 2.908407 -3.228195 1.881632 1 1.455006 -1.783799 -2.225963 1 1.438029 -1.062735 2.467116 1 0.299928 -3.812186 1.987761 1 0.307814 -4.262126 -0.947380 1 5.064123 -3.771788 0.495810 1 4.318394 -1.426694 -1.368018 1 4.307299 -0.974339 1.563302 1 3.280658 -4.310300 -1.940252 1 2.562288 -5.571583 0.763546 1 3.261313 -3.555206 2.968308 28 0.403237 -0.340962 -0.057454 6 2.200106 0.888543 -0.235621 6 1.031081 1.432097 -0.310365 15 -1.756437 -0.205991 -0.139840 6 0.598942 2.853866 -0.535252 1 1.453767 3.421565 -0.928035 1 -0.183079 2.880498 -1.300690 6 0.076920 3.550729 0.735748 1 0.845707 3.501762 1.517811 1 -0.795158 3.009474 1.119785 6 -0.304710 5.016089 0.482374 1 0.567574 5.556831 0.091487 1 -1.070540 5.058945 -0.303351 6 -0.822573 5.725906 1.740193 1 -0.066174 5.729544 2.533921 1 -1.086389 6.767944 1.527923 1 -1.716521 5.230155 2.136604 6 -2.362957 1.048842 -1.340583 6 -3.334859 2.012470 -1.033588 6 -1.797762 1.033275 -2.629676 6 -3.742957 2.938044 -2.002546 1 -3.774413 2.056294 -0.041396 6 -2.216292 1.947617 -3.598979 1 -1.023628 0.308624 -2.875936 6 -3.190635 2.904778 -3.286640 1 -4.493385 3.683758 -1.749543 1 -1.774515 1.919892 -4.592535 1 -3.510866 3.623150 -4.037989 6 -2.499480 0.195863 1.494261 6 -3.874203 0.022580 1.739046 6 -1.673229 0.657727 2.531187 6 -4.411799 0.326882 2.992100 1 -4.527001 -0.360288 0.958198 6 -2.212513 0.958802 3.786712 1 -0.605771 0.772812 2.361904 6 -3.582203 0.797465 4.018305 1 -5.476295 0.190233 3.169063 1 -1.560437 1.311661 4.582559 1 -4.001589 1.027829 4.995202 6 -2.646367 -1.751090 -0.620739 6 -3.503569 -1.825362 -1.729415 6 -2.466114 -2.892469 0.180783 6 -4.167226 -3.021483 -2.031775 1 -3.667814 -0.957313 -2.360379 6 -3.136146 -4.080193 -0.116375 1 -1.805792 -2.855966 1.042453 6 -3.987288 -4.150019 -1.227173 1 -4.827568 -3.064319 -2.895186	INT1_IIIc	6 -2.538375 -1.616395 -0.145863 6 -0.867437 -1.682452 -0.215160 5 -1.677822 -2.353597 1.156461 5 -1.773896 -1.836994 -1.676825 5 -0.374791 -2.868280 -1.348742 5 -0.316710 -3.185945 0.393885 5 -2.770508 -4.326625 -0.628919 5 -3.201296 -3.035747 0.525548 5 -3.259455 -2.719404 -1.226371 5 -1.789526 -4.090767 0.856158 5 -0.983540 -4.427181 -0.709203 5 -1.886095 -3.571375 -1.998720 1 -1.630031 -1.781589 2.188285 1 -1.789186 -0.938297 -2.442484 1 0.619056 -2.685271 1.965537 1 0.716702 -3.219952 0.973785 1 -3.469835 -5.276203 -0.778457 1 -4.180055 -2.941379 1.158658 1 -4.278303 -2.422482 -1.749991 1 -1.791050 -4.853537 1.767304 1 -0.402601 -5.443956 -0.913762 1 -1.959172 -3.965465 -3.117403 28 -0.079443 0.005253 0.071780 15 2.264439 0.141608 0.095301 6 -1.822487 0.604405 0.240250 6 -2.907893 -0.187221 0.149982 6 -1.726804 2.085639 0.507889 1 -2.304168 2.346792 1.405245 1 -0.680049 2.343889 0.765062 6 -2.159625 2.971302 -0.679530 1 -1.580225 2.690184 -1.568250 1 -3.209071 2.756405 -0.913191 6 -1.986116 4.470678 -0.402147 1 -2.557225 4.741292 0.496088 1 -0.932689 4.678113 -0.171621 6 -2.435408 5.351372 -1.575485 1 -2.300464 6.414772 -1.348640 1 -1.860399 5.128777 -2.482187 1 -3.494922 5.192472 -1.807996 6 2.567830 1.898534 -0.370848 6 3.464499 2.740498 0.306872 6 1.826677 2.415485 -1.451277 6 3.624519 4.070794 -0.096421 1 4.036962 2.367033 1.151411 6 1.995219 3.742110 -1.858211 1 1.123543 1.777144 -1.986074 6 2.894211 4.573334 -1.179619 1 4.321004 4.713764 0.437190 1 1.421322 4.125885 -2.698607 1 3.021615 5.607912 -1.490267 6 2.996473 -0.064719 1.767529 6 4.363630 -0.317637 1.974276 6 2.145134 0.051397 2.880018 6 4.868895 -0.442681 3.272029 1 5.035978 -0.423632 1.126477 6 2.652970 -0.067268 4.177506 1 1.080143 0.227396 2.734156 6 4.016064 -0.315229 4.375334 1 5.928124 -0.640525 3.420623 1 1.983512 0.023030 5.029917 1 4.411123 -0.415831 5.383810 6 3.353443 -0.845041 -1.013760 6 4.106650 -0.263857 -2.045938 6 3.405666 -2.238790 -0.828593 6 4.901721 -1.063238 -2.876543 1 4.085457 0.810205 -2.206693 6 4.206084 -3.032089 -1.653386 1 2.829021 -2.709777 -0.036617 6 4.954808 -2.446944 -2.682569 1 5.481417 -0.599521 -3.671666

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -2.988065 -4.953174 0.515370 1 -4.504973 -5.077519 -1.461784 6 3.609566 1.269973 -0.327040 6 4.305286 1.705339 0.816362 6 4.244973 1.333801 -1.581532 6 5.609432 2.193927 0.705682 1 3.818114 1.666629 1.787177 6 5.548892 1.823992 -1.688251 1 3.711256 1.005123 -2.469580 6 6.235757 2.252137 -0.545508 1 6.135620 2.530782 1.596053 1 6.027885 1.872179 -2.663618 1 7.251474 2.632223 -0.629930		1 4.239084 -4.107781 -1.495573 1 5.574068 -3.066154 -3.327742 6 -4.324420 0.227033 0.366523 6 -5.248617 0.270853 -0.693413 6 -4.758807 0.601969 1.650785 6 -6.567860 0.679954 -0.474842 1 -4.930979 -0.003109 -1.696265 6 -6.078304 1.012099 1.870683 1 -4.059141 0.562778 2.482914 6 -6.988279 1.052223 0.807989 1 -7.266706 0.711991 -1.308151 1 -6.395466 1.296023 2.872006 1 -8.014751 1.370251 0.977170
TSI_IVc	6 -2.326961 -1.169521 -0.580490 6 -1.109164 -2.122215 -0.321520 5 -2.236157 -1.915500 0.966332 5 -1.752126 -2.074947 -1.921544 5 -1.245363 -3.596273 -1.170732 5 -1.536490 -3.496973 0.588602 5 -4.085859 -3.265295 -0.762700 5 -3.786625 -1.742552 0.116652 5 -3.487755 -1.837377 -1.654239 5 -3.310394 -3.309815 0.854622 5 -2.699444 -4.357019 -0.467478 5 -2.827855 -3.468921 -2.022091 1 -1.938552 -1.258030 1.903264 1 -1.152185 -1.515687 -2.776815 1 -0.276889 -4.146260 -1.574657 1 -0.759465 -3.978601 1.342240 1 -5.200504 -3.643433 -0.927724 1 -4.605016 -0.999499 0.534404 1 -4.102441 -1.148646 -2.395298 1 -3.854540 -3.729917 1.823608 1 -2.804949 -5.539889 -0.420318 1 -3.028727 -4.000107 -3.065629 28 -0.500579 -0.298452 -0.353334 6 -2.188737 0.990907 -0.681508 6 -1.018988 1.520741 -0.605135 15 1.622922 -0.344025 0.157057 6 -3.620509 1.423971 -0.733325 1 -3.645413 2.253530 -1.453366 1 -4.280722 0.653818 -1.129626 6 -4.141949 1.928914 0.629017 1 -3.502167 2.751492 0.971157 1 -4.052766 1.131300 1.374662 6 -5.599650 2.403117 0.550704 1 -6.233213 1.573096 0.210990 1 -5.686636 3.188716 -0.211884 6 -6.126348 2.932131 1.891163 1 -5.534865 3.786362 2.241019 1 -7.167816 3.261073 1.805544 1 -6.084139 2.158637 2.666912 6 2.599433 1.216233 0.244981 6 2.752338 1.954669 -0.942107 6 3.226469 1.667751 1.415684 6 3.528145 3.114232 -0.959669 1 2.269895 1.622696 -1.858942 6 3.999662 2.835637 1.397409 1 3.130087 1.111098 2.343173 6 4.154802 3.558933 0.211554 1 3.636493 3.675261 -1.884869 1 4.484167 3.172313 2.311451 1 4.757882 4.464151 0.198362 6 1.733219 -1.074877 1.843260 6 2.510210 -2.203179 2.145938 6 0.956249 -0.487958 2.859597 6 2.523622 -2.724047 3.445683 1 3.100498 -2.689338 1.375140 6 0.980554 -1.001506 4.158254 1 0.327863 0.372527 2.638181 6 1.765480 -2.122964 4.455093 1 3.126971 -3.602285 3.664544 1 0.378429 -0.533576 4.933927 1 1.778502 -2.529100 5.464081 6 2.692745 -1.365942 -0.939755 6 4.089985 -1.381216 -0.765690 6 2.128968 -2.108930 -1.986512 6 4.899317 -2.143999 -1.610029 1 4.551900 -0.792460 0.022994 6 2.941731 -2.868026 -2.836801 1 1.057542 -2.090785 -2.145402 6 4.326512 -2.890658 -2.648452 1 5.976896 -2.150346 -1.461673 1 2.489404 -3.437272 -3.645789 1 4.958557 -3.479813 -3.309321 6 -0.505848 2.889097 -0.696546 6 -0.509346 3.562115 -1.933860 6 -0.039672 3.567225 0.444775	INTI_IVc	6 2.881976 -1.278643 0.513526 6 1.211557 -1.524807 0.403760 5 2.216548 -1.851733 -0.964486 5 2.021942 -1.843037 1.897266 5 0.792529 -2.944291 1.268240 5 0.910515 -2.950217 -0.497284 5 3.397055 -3.991774 0.560516 5 3.759159 -2.480210 -0.313282 5 3.638239 -2.471921 1.462481 5 2.516090 -3.596427 -0.954926 5 1.636014 -4.290881 0.442071 5 2.320978 -3.585721 1.940133 1 2.186673 -1.114993 -1.887738 1 1.870970 -1.102549 2.805024 1 -0.257592 -2.988461 1.811069 1 -0.060509 -2.996034 -1.173954 1 4.192898 -4.873312 0.617757 1 4.769950 -2.177411 -0.851094 1 4.565811 -2.158095 2.130253 1 2.684316 -4.179147 -1.977080 1 1.170394 -5.384470 0.415359 1 2.350983 -4.161513 2.979536 28 0.272307 0.133047 0.301058 15 -2.015118 -0.056609 -0.125964 6 1.953982 0.872917 0.495401 6 3.115678 0.208223 0.555493 6 4.503680 0.802251 0.639342 1 4.449143 1.749676 1.187400 1 5.151508 0.138305 1.224425 6 5.155351 1.066063 -0.736270 1 5.190972 0.135140 -1.313836 1 4.517999 1.758511 -1.301504 6 6.570911 1.648169 -0.618396 1 6.534482 2.575110 -0.030155 1 7.203455 0.950963 -0.052787 6 7.217415 1.933256 -1.980491 1 6.626409 2.654702 -2.557093 1 8.225400 2.346753 -1.863828 1 7.300193 1.018744 -2.579582 6 -2.300218 0.659117 -1.801737 6 -3.397616 1.473643 -2.124546 6 -1.346606 0.373559 -2.797000 6 -3.542705 1.984287 -3.419388 1 -4.139491 1.721221 -1.730755 6 -1.498279 0.875996 -4.093040 1 -0.483057 -0.245834 -2.562138 6 -2.597080 1.684611 -4.406768 1 -4.395803 2.616884 -3.654850 1 -0.755613 0.641467 -4.852388 1 -2.713116 2.082388 -5.412506 6 -3.066448 0.923346 1.025883 6 -4.453966 0.720888 1.138557 6 -2.455771 1.908827 1.819530 6 -5.213443 1.496561 2.018934 1 -4.944737 -0.048578 0.547779 6 -3.216875 2.686607 2.698683 1 -1.382117 2.071278 1.759873 6 -4.597047 2.482406 2.799769 1 -6.285370 1.328667 2.096923 1 -2.729267 3.443992 3.308130 1 -5.188886 3.082323 3.487635 6 -2.853919 -1.697024 -0.170112 6 -3.326944 -2.271994 -1.359474 6 -2.990536 -2.409205 1.035030 6 -3.930524 -3.535474 -1.343335 1 -3.234514 -1.741467 -2.302779 6 -3.599726 -3.665689 1.049898 1 -2.632332 -1.981834 1.968916 6 -4.069814 -4.234719 -0.140671 1 -4.293297 -3.968272 -2.273102 1 -3.701474 -4.202456 1.990545 1 -4.540016 -5.215541 -0.129198 6 1.488319 2.243159 0.624175 6 1.578686 2.961354 1.846213 6 0.739581 2.814287 -0.436569

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 -0.070738 4.886735 -2.021092		6 0.987458 4.213840 1.975194
	1 -0.858008 3.043725 -2.824259	1	2.121258 2.520654 2.679132
	6 0.388867 4.893284 0.353957	6	0.133682 4.070440 -0.290876
	1 -0.021832 3.054640 1.403223	1	0.683958 2.293702 -1.390356
	6 0.376800 5.559501 -0.877828	6	0.260282 4.773157 0.907873
	1 -0.081843 5.394040 -2.983581	1	1.082428 4.761392 2.910460
	1 0.740896 5.405462 1.246713	1	-0.427760 4.496192 -1.119107
	1 0.716232 6.590564 -0.946577	1	-0.203681 5.750338 1.020258
TSI_IIIa	6 -2.021601 -1.539020 -0.217165	INT1_IIIa	6 -2.718189 1.476228 0.147138
	6 -0.636441 -2.280860 -0.082228	6	-1.024591 1.609868 0.168506
	5 -1.732039 -2.390180 1.243640	5	-1.899547 2.018055 -1.268750
	5 -1.342551 -2.196926 -1.653162	5	-1.925574 1.965645 1.596741
	5 -0.543851 -3.665617 -1.069358	5	-0.576041 2.985432 1.079324
	5 -0.779697 -3.783304 0.698476	5	-0.557955 3.016250 -0.690543
	5 -3.379496 -3.892299 -0.562192	5	-3.036476 4.222365 0.188389
	5 -3.325296 -2.428266 0.454479	5	-3.440614 2.745444 -0.729386
	5 -3.083763 -2.302325 -1.322177	5	-3.452200 2.720844 1.051484
	5 -2.543660 -3.942404 1.024619	5	-2.074626 3.777083 -1.259574
	5 -1.811365 -4.737605 -0.409211	5	-1.255798 4.396048 0.209554
	5 -2.158358 -3.746731 -1.865081	5	-2.100060 3.727979 1.640889
	1 -1.512047 -1.777374 2.232603	1	-1.850065 1.289962 -2.197733
	1 -0.884393 -1.463551 -2.463729	1	-1.896451 1.206522 2.501723
	1 0.491207 -3.983658 -1.548378	1	0.428930 2.949506 1.700995
	1 0.097187 -4.185983 1.387011	1	0.462473 2.994728 1.291863
	1 -4.414768 -4.449716 -0.736610	1	-3.770959 5.157084 0.199892
	1 -4.244165 -1.885605 0.958054	1	-4.424426 2.510673 -1.345811
	1 -3.842921 -1.670756 -1.971650	1	-4.443550 2.498272 1.655556
	1 -2.962508 -4.542578 1.960718	1	-2.122082 4.377741 -2.283926
	1 -1.705017 -5.919723 -0.473616	1	-0.713305 5.453523 0.233831
	1 -2.304551 -4.207599 -2.950487	1	-2.170967 4.294798 2.683076
	28 -0.317323 -0.399908 -0.043228	28	-0.178866 -0.095988 0.119140
	6 -2.251059 0.584841 -0.074707	15	2.152706 -0.016489 -0.007179
	6 -1.171939 1.300080 -0.120492	6	-1.908675 -0.728805 0.090032
	15 1.826014 -0.065968 0.055897	6	-3.037719 0.000322 0.084385
	6 -3.685689 0.751415 0.157330	6	-4.411642 -0.546206 -0.068093
	6 -4.581173 0.891875 -0.918000	6	-4.663081 -1.505296 -1.069397
	6 -4.166658 0.884053 1.474168	6	-5.476670 -0.164646 0.769948
	6 -5.931527 1.159980 -0.679563	6	-5.932807 -2.067805 -1.224928
	1 -4.216583 0.801923 -1.937513	1	-3.857932 -1.800385 -1.737415
	6 -5.517233 1.150988 1.707745	6	-6.746780 -0.727795 0.614372
	1 -3.478450 0.779003 2.309026	1	-5.313116 0.560863 1.559486
	6 -6.404109 1.286625 0.632122	6	-6.982444 -1.681082 -0.383156
	1 -6.614135 1.271855 -1.518951	1	-6.103885 -2.802766 -2.008685
	1 -5.877324 1.253939 2.728931	1	-7.553015 -0.422806 1.278183
	1 -7.456190 1.493367 0.815383	1	-7.972267 -2.115583 -0.504360
	6 -0.951840 2.748460 -0.180035	6	-1.531939 -2.127810 0.179499
	6 -1.731080 3.541805 -1.048118	6	-0.653029 -2.658131 -0.799690
	6 0.012444 3.383058 0.624498	6	-1.836990 -2.923677 1.315326
	6 -1.557226 4.926818 -1.097465	6	-0.125213 -3.950571 -0.661900
	1 -2.469550 3.066635 -1.688392	1	-0.440509 -2.080750 -1.697316
	6 0.171763 4.770376 0.586601	6	-1.319710 -4.208698 1.433989
	1 0.630428 2.792196 1.292827	1	-2.488073 -2.517089 2.085124
	6 -0.608801 5.549107 -0.276158	6	-0.459271 -4.727074 0.447411
	1 -2.165243 5.521325 -1.776117	1	0.537014 -4.345422 -1.428617
	1 0.914393 5.243041 1.225712	1	-1.578431 -4.816122 2.298649
	1 -0.476081 6.628106 -0.312155	1	-0.056112 -5.731608 0.552690
	6 2.430341 1.342600 -0.961448	6	2.987292 -1.133351 1.196355
	6 3.520564 2.148357 -0.596898	6	2.218785 -2.103138 1.861448
	6 1.785227 1.578497 -2.187638	6	4.363877 -1.047039 1.474274
	6 3.963187 3.165168 -1.449657	6	2.814367 -2.979195 2.775361
	1 4.026408 1.998419 0.352109	1	1.150079 -2.176444 1.675161
	6 2.236268 2.586478 -3.044263	6	4.958073 -1.921593 2.388052
	1 0.925153 0.976277 -2.472711	1	4.974565 -0.290536 0.987632
	6 3.326771 3.383052 -2.676739	6	4.185024 -2.891048 3.039494
	1 4.805227 3.786531 -1.152761	1	2.205185 -3.722645 3.284234
	1 1.729385 2.755215 -3.991699	1	6.023366 -1.843190 2.593674
	1 3.673906 4.173213 -3.338851	1	4.648141 -3.568015 3.754033
	6 2.382453 0.213991 1.787943	6	2.615867 -0.633857 -1.682368
	6 3.732607 0.088175 2.163792	6	1.809614 -0.231945 -2.763907
	6 1.430212 0.541295 2.767504	6	3.707319 -1.483099 -1.926687
	6 4.121705 0.311633 3.487045	6	2.100880 -0.654220 -4.064767
	1 4.482451 -0.200988 1.431516	1	0.951681 0.415503 -2.593026
	6 1.820910 0.763480 4.092374	6	3.991677 -1.913113 -3.227607
	1 0.378386 0.608772 2.499669	1	4.335714 -1.821168 -1.107921
	6 3.167538 0.653663 4.453685	6	3.192943 -1.497797 -4.299310
	1 5.168886 0.211933 3.763840	1	1.471185 -0.329951 -4.890283
	1 1.071622 1.012631 4.840412	1	4.838092 -2.573871 -3.401817
	1 3.471975 0.822106 5.484297	1	3.417072 -1.833328 -5.309442
	6 2.870308 -1.484374 -0.495376	6	3.079090 1.566252 0.181585
	6 3.632897 -1.441232 -1.672559	6	3.137797 2.159347 1.455665
	6 2.876102 -2.657807 0.279754	6	3.692029 2.214829 -0.901187
	6 4.392610 -2.550902 -2.064656	6	3.809272 3.369254 1.643584
	1 3.648701 -0.546338 -2.287422	1	2.669113 1.674537 2.309242
	6 3.641429 -3.758692 -0.107713	6	4.357414 3.432339 -0.712090
	1 2.288392 -2.715246 1.192165	1	3.662073 1.776852 -1.894763
	6 4.401510 -3.710033 -1.283683	6	4.419895 4.011611 0.558838
	1 4.979457 -2.502491 -2.979335	1	3.849794 3.812850 2.635973
	1 3.638670 -4.657359 0.505117	1	4.828895 3.922916 -1.560854

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 4.994485 -4.569987 -1.587280		1 4.939102 4.956260 0.704726

Table S7 The first three vibration frequencies for stationary points on potential energy surfaces from **COM1** and **R2** (or **R3**) to **INT1_I-IV**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)
R2a	59 197 239	R2e	92 152 176	R3a	11 98 151	R3b	-4 69 83
R3c	4 40 56	R3d	14 44 50	TS1_Ia	-224i 7 25	INT1_Ia	9 14 21
TS1_Ia	-247i 10 14	INT1_Ia	8 14 17	TS1_Ie	-204i 12 17	INT1_Ie	9 14 24
TS1_Ie	-258i 11 18	INT1_Ie	10 13 17	TS1_IIIa	-196i 16 23	INT1_IIIa	14 17 21
TS1_IIIb	-188i 6 16	INT1_IIIb	14 15 17	TS1_IVb	-172i 12 15	INT1_IVb	13 14 19
TS1_IIIc	-179i 9 14	INT1_IIIc	10 17 19	TS1_IVc	-158i 10 15	INT1_IVc	13 17 23
TS1_IIId	-162i 12 16	INT1_IIId	12 15 22				

Table S8 The total energies (E : a.u.), zero-point energies (ZPE : kcal·mol⁻¹) and Gibbs free energies [G and $G(\text{sol}, 383\text{K})$: a.u.] for stationary points on potential energy surfaces from **COM1** and **R2** (or **R3**) to **INT1_I-IV**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	E	ZPE	G	$G(\text{sol}, 383\text{K})$
R2a	-325.71802	76.04080	-325.62803	-325.62519
R3a	-234.62734	89.17045	-234.51889	-234.51846
TS1_Ia	-3201.02189	345.72535	-3200.53764	-3200.55409
INT1_Ia	-3201.06507	347.16313	-3200.58052	-3200.59825
TS1_Ia	-3201.01038	345.41795	-3200.52723	-3200.54314
INT1_Ia	-3201.05900	347.03841	-3200.57522	-3200.59277
TS1_IIIa	-3109.92155	358.71270	-3109.41680	-3109.43440
INT1_IIIa	-3109.98457	360.03206	-3109.47930	-3109.49783
R3b	-387.06468	104.43522	-386.93242	-386.93188
TS1_IIIb	-3262.35490	373.29035	-3261.83168	-3261.85138
INT1_IIIb	-3262.41732	374.88319	-3261.89187	-3261.91167
TS1_IVb	-3262.35616	373.35948	-3261.83190	-3261.85070
INT1_IVb	-3262.42263	375.09429	-3261.89661	-3261.91584
R3c	-465.69913	140.19201	-465.51786	-465.51984
TS1_IIIc	-3340.98934	409.09230	-3340.41282	-3340.43340
INT1_IIIc	-3341.05053	410.21039	-3340.47341	-3340.49494
TS1_IVc	-3340.98790	409.21176	-3340.41025	-3340.43239
INT1_IVc	-3341.05953	410.63686	-3340.48095	-3340.50253
R3d	-539.50227	119.67041	-539.35135	-539.35117
TS1_IIId	-3414.78892	388.32590	-3414.24318	-3414.26264
INT1_IIId	-3414.85759	390.03406	-3414.31064	-3414.33102
R2e	-306.51731	59.78178	-306.45255	-306.44975
TS1_Ie	-3181.82166	329.41509	-3181.36356	-3181.38144
INT1_Ie	-3181.86694	330.95351	-3181.40775	-3181.42505
TS1_Ie	-3181.80922	329.00778	-3181.35180	-3181.36862
INT1_Ie	-3181.85939	330.63477	-3181.40195	-3181.41902

Table S9 The optimized Cartesian coordinates (Å) for stationary points on potential energy surfaces from **INT1_I** and **R3** to products **P1** and **P2**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	Cartesian coordinates	Species	Cartesian coordinates
TS2_I_1a	6 -2.286294 2.433000 0.286967	INT2_I_1a	6 -2.284882 2.172417 -0.108998
	6 -0.669871 2.002196 0.028798		6 -0.571693 2.076491 -0.353706
	5 -1.596463 2.712220 -1.245668		5 -1.614135 2.739161 -1.566531
	5 -1.179504 2.621214 1.555560		5 -1.231039 2.391624 1.207806
	5 0.316241 3.177471 0.807161		5 0.156865 3.297121 0.586817
	5 0.054025 3.233677 -0.935336		5 -0.089691 3.516374 -1.147023
	5 -1.741228 5.145540 0.290703		5 -2.198790 4.931404 0.223270
	5 -2.721384 3.883253 -0.501146		5 -2.932744 3.620616 -0.739592
	5 -2.455990 3.831218 1.254066		5 -2.685594 3.410376 1.006101
	5 -1.219741 4.445579 -1.276142		5 -1.546311 4.515194 -1.395446
	5 -0.018429 4.745461 0.017264		5 -0.434264 4.868222 -0.032695
	5 -0.785508 4.353186 1.587346		5 -1.142550 4.162037 1.454434
	1 -1.925635 2.046158 -2.162348		1 -1.804438 2.128701 -2.560536
	1 -1.262796 1.888793 2.481732		1 -1.175033 1.553284 2.040328

Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -2.140691 6.261778 0.387266		1 -2.794729 5.940187 0.429571
	1 -3.820747 3.961438 -0.940320		1 -4.022301 3.567261 -1.205605
	1 -3.375154 3.874277 2.002502		1 -3.608922 3.212111 1.723346
	1 -1.241402 5.045127 -2.302703		1 -1.657115 5.217783 -2.348412
	1 0.826926 5.576362 -0.082743		1 0.257087 5.836221 -0.010156
	1 -0.498140 4.885344 2.611019		1 -0.968715 4.612876 2.540833
	6 -3.227959 1.243852 0.406054	28	-0.096288 0.173629 -0.779126
	6 -2.464404 -0.067256 0.554883	6	-0.664605 -1.355347 -1.606232
28	-0.557032 0.000849 -0.314573	6	-1.971947 -1.027253 -1.408772
6	-1.968389 -0.840744 -1.457550	15	1.799267 -0.298543 0.171493
6	-0.892563 -1.551376 -1.392506	6	-3.181936 0.922562 -0.136723
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6	-3.199586 -0.581222 -2.266279	6	-3.048384 -1.328619 -2.461968
1	-4.094152 -0.775764 -1.666511	1	-2.942540 -2.373714 -2.775637
1	-3.240076 0.474094 -2.550702	1	-4.036191 -1.255743 -1.996894
1	-3.902424 1.213550 -0.449629	6	-0.113981 -2.310725 -2.624043
1	-3.868437 1.373731 1.286149	1	-0.700628 -2.234765 -3.549247
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1	-2.380007 -1.241228 -4.189882	1	0.263454 -4.440076 -2.898876
1	-3.244274 -2.512127 -3.304339	1	0.442728 -3.900221 -1.223509
6	-3.08451 -2.763801 -2.054372	1	-1.174910 -4.092114 -1.920782
1	0.776141 -2.794841 -1.939419	6	-3.024974 -0.430360 -3.712336
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6	-0.910943 -4.078374 -1.523421	1	-3.785385 -0.764620 -4.427223
1	-1.994645 -4.106445 -1.673202	1	-3.236268 0.612333 -3.462102
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1	3.885476 -1.631879 -1.576412	1	2.089031 -2.744282 1.969527
6	2.338635 -4.337789 0.737941	6	3.660692 -4.539417 -0.453588
1	0.992772 -2.802343 1.406910	1	4.140262 -3.801063 -2.429103
6	3.406113 -4.665783 -0.108643	1	3.067272 -4.963570 1.579823
1	4.783794 -3.926979 -1.599142	1	4.101329 -5.519902 -0.619639
1	1.907087 -5.093330 1.390924	6	1.631571 -0.053649 1.989881
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1	4.536046 2.722019 -3.866436	6	4.499714 0.566295 0.156283
6	2.311803 0.038377 1.755487	6	3.043930 1.594726 -1.485266
6	3.681178 -0.083416 2.058722	6	5.577240 1.302509 -0.338966
6	1.413366 0.325720 2.791354	1	4.664727 -0.135799 0.970149
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1	4.395505 -0.346785 1.282757	1	2.064563 1.700853 -1.939216
6	1.868634 0.511712 4.101925	6	5.392658 2.186515 -1.411412
1	0.353163 0.406348 2.579245	1	6.562331 1.180902 0.106008
6	3.232737 0.413997 4.389652	1	3.977474 3.002310 -2.825930
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1	1.156070 0.735952 4.892613	1	-3.815650 0.971238 -1.024360
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6	-3.307951 -1.266279 0.874509	6	-3.438191 -1.520055 0.550013
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6	-3.549881 -3.453207 1.878903	6	-3.754852 -3.658430 1.626324
1	-1.675578 -2.389323 1.748249	1	-1.825337 -2.873518 1.052219
6	-5.397588 -2.250226 0.940378	6	-5.577478 -2.207827 1.067858
6	-4.916794 -3.394544 1.578131	6	-5.131620 -3.408119 1.622710
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1	-5.592410 -4.205714 1.836573	1	-5.840987 -4.120050 2.036630
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TS3_I_1a	5 1.232590 -3.384775 0.871936	INT3_I_1a	6 1.950597 2.254974 0.441606
	5 2.284828 -4.643218 0.155642	6	0.610527 2.016094 -0.493495
	5 3.955717 -2.493276 1.090745	5	0.402976 2.447828 1.163971
	5 3.974686 -4.079515 0.286406	5	2.021011 2.759677 -1.196605
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	1 1.983105 -5.793581 0.192280	5	0.100696 4.191374 1.209091
	1 4.806194 -1.988610 1.745526	5	0.096036 4.771495 -0.487273
	1 4.901719 -4.814405 0.413732	5	1.726751 4.498581 -1.169814
	1 5.084358 -2.142740 -1.209114	1	0.043254 1.618192 1.923554
	1 2.412970 -1.568072 -2.362438	1	2.690508 2.184634 -1.971138

Species	Cartesian coordinates	Species	Cartesian coordinates
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	5 1.400974 -3.486989 -0.881841		1 1.905372 6.073272 0.921966
	1 0.469347 -3.729642 -1.575991		1 2.248669 3.459459 2.616946
	5 3.092809 -3.907662 -1.266735		1 3.913159 3.784765 0.187907
	1 3.374957 -4.516369 -2.248671		1 -0.578841 4.651076 2.068555
	6 3.049108 -1.464398 0.054914		1 -0.596578 5.667265 -0.849377
	6 1.429323 -1.976132 -0.072908		1 2.206029 5.186234 -2.012045
	28 0.087073 -0.474459 -0.483687		28 0.040143 0.217947 -0.670219
	6 0.393865 0.973131 -1.600467		15 -2.093890 -0.498155 0.205014
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	6 3.429823 0.027809 0.031572		6 2.670244 0.983026 0.898965
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	6 4.458173 3.880013 1.149499		6 -2.904879 -1.127363 4.233187
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	1 1.588649 4.995623 2.575826		6 -3.188033 0.164340 4.687114
	1 5.511617 4.125567 1.015833		1 -3.376226 2.245509 4.127666
	1 4.011677 5.652594 2.301015		1 -2.931001 -1.967806 4.923416
	7 4.046291 2.729584 0.592196		1 -3.432698 0.335818 5.733007
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	5 -1.240313 1.956140 1.562701		5 3.910776 -1.330689 -0.524423
	5 -2.859825 2.672338 -0.727036		5 2.397035 -0.073211 1.462688
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	5 -2.691151 2.786748 2.154507		5 4.402053 -2.073641 1.037025
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	5 -1.141794 3.660588 2.042477		5 5.442063 -0.846128 0.273470
	5 -1.188585 4.653694 0.547004		5 5.139819 0.715514 1.103048
	5 -2.772420 4.378965 -0.253071		5 3.867505 0.452699 2.327752
	1 -0.813366 1.015829 2.147857		1 3.800166 -1.992269 -1.496149
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -3.209606 2.366401 3.133223		1 4.616353 -3.238514 1.052126
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	6 -2.554605 -1.457789 -2.187983		6 1.989236 0.638396 -1.872017
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	1 -3.753318 0.251514 1.841987		1 1.243065 -2.048407 -1.519990
	1 -4.346886 0.455068 0.203701		6 -0.490742 -2.890665 -0.744829
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	1 -1.646402 -0.732511 0.985679		6 -2.706771 -4.519377 -1.121206
	6 -3.204190 -2.085566 0.630658		1 -2.826206 -3.674774 -3.116151
	6 -2.411689 -3.203185 0.942964		1 -2.258823 -5.116077 0.904398
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	1 -2.427909 -5.302526 1.455537		6 0.603506 2.827110 -2.163340
	1 -6.219027 -3.350515 0.826301		1 -0.354308 3.114989 -1.724063
	1 -4.949211 -5.428891 1.372994		1 0.428322 2.681316 -3.238167
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	6 -1.543672 1.356386 -3.818887		6 2.188789 0.724703 -4.388956
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	6 4.632101 2.838873 -0.953274		6 -2.871020 0.364163 4.217259
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	6 5.832635 1.503411 0.669910		6 -1.826194 -1.759852 3.729422
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -5.208367 -2.343320 0.061956		1 -4.826601 -2.591354 -0.202990
	1 -3.005124 -2.090873 2.094304		1 -2.447497 -2.448736 1.596726
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	1 -5.735251 2.070205 2.285824		1 -5.581542 1.199225 2.919286
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	6 -2.353538 -1.819056 -0.832993		6 -2.211095 -1.501210 -1.279877
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	6 -2.260566 1.455560 -1.437838	28	-0.217280 0.058688 -0.640649
	6 -0.711092 1.418996 -1.295398	6	-2.548391 1.806863 -1.169860
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -5.125329 -1.578163 -1.252870		1 5.346801 -2.340131 1.346157
	1 -2.779835 -2.682481 0.288101		1 3.100420 -1.351760 3.005595
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	1 3.476227 -3.783845 -3.292383		1 -6.604972 0.063510 0.959711
	1 -0.502170 -4.611710 -1.853233		1 -4.836677 -2.521444 -2.002011
	1 1.424619 -5.199107 -3.325303		1 -6.844889 -1.731972 -0.752340
CAT	28 -0.000187 0.002034 -0.001716	Pla	6 1.400021 0.432751 0.139363
	15 2.140865 0.000788 -0.000769		6 1.056921 -0.867405 -0.819210
	15 -2.141162 0.000704 -0.001010		5 2.331948 0.197735 -1.309033
	6 2.922830 1.546369 -0.656025		5 0.919589 -1.059471 0.888794
	6 4.088255 2.123122 -0.125126		5 1.611498 -2.335092 -0.126933
	6 2.290113 2.175753 -1.744173		5 2.473711 -1.564623 -1.479919
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	1 4.588358 1.663625 0.723487		5 3.116854 0.680452 0.198862
	6 2.822127 3.341875 -2.302290		5 2.243569 -0.081324 1.551188
	1 1.372250 1.750639 -2.147632		5 3.822957 -0.607288 -0.814501
	6 3.986870 3.907959 -1.767752		5 3.386596 -2.181819 -0.076296
	1 5.516659 3.734752 -0.251589		5 2.412101 -1.856284 1.393287
	1 2.322322 3.813977 -3.145558		1 2.105051 0.925468 -2.210057
	1 4.397119 4.820625 -2.194776		1 -0.154451 -1.103514 1.363936

Species	Cartesian coordinates	Species	Cartesian coordinates
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TS2_I_1b	6 3.436314 1.160619 -0.364475 6 2.425489 -0.185336 -0.523551 5 3.091235 0.577698 -1.926895 5 3.520367 -0.068068 0.802213 5 3.341309 -1.579294 -0.086609 5 3.073235 -1.173966 -1.779927 5 5.715368 -0.239524 -1.060107 5 4.718327 1.173766 -1.490402 5 4.990881 0.764725 0.217260 5 4.531325 -0.342186 -2.404533 5 4.696265 -1.697641 -1.246605 5 4.970891 -1.007195 0.382556 1 2.381529 1.199776 -2.636031 1 3.095828 0.154363 1.883018 1 2.790588 -2.490669 0.421910 1 2.330099 -1.799931 -2.455661 1 6.890068 -0.240698 -1.246372 1 5.061692 2.226151 -1.917606 1 5.520601 1.540964 0.941048 1 4.841475 -0.415711 -3.549937 1 5.135956 -2.755059 -1.568045 1 5.598547 -1.554723 1.230622 28 0.488109 0.421246 -0.343982 6 2.712958 2.428918 0.064228 6 1.298809 2.133617 0.549186 6 -0.046810 2.108103 -1.231325 6 -1.060835 1.338809 -1.016568 1 2.718423 3.141796 -0.762950 1 3.274110 2.899233 0.881401 1 1.308771 1.350138 1.317634 6 0.549014 3.267444 1.182145 6 0.948685 4.610882 1.062305 7 -0.495599 2.909536 1.960805	INT2_I_1b	6 2.605102 -2.098378 -0.585118 6 0.879609 -2.086330 -0.480542 5 1.676281 -2.229831 -2.007902 5 1.844511 -2.820553 0.747161 5 0.384316 -3.598876 0.128932 5 0.280542 -3.232953 -1.597031 5 2.662978 -4.812222 -1.174609 5 3.156360 -3.202290 -1.767376 5 3.257619 -3.583596 -0.036521 5 1.688056 -3.965050 -2.419704 5 0.880760 -4.831404 -1.071690 5 1.854472 -4.574506 0.410941 1 1.646949 -1.317959 -2.760007 1 1.955256 -2.297338 1.803102 1 -0.578342 -3.633711 0.817666 1 -0.755115 -3.004704 -2.122421 1 3.314487 -5.776129 -1.421935 1 4.129273 -2.903876 -2.377041 1 4.299002 -3.538140 0.529089 1 1.626966 -4.316600 -3.553701 1 0.237055 -5.816327 -1.245258 1 1.914440 -5.359618 1.301644 6 3.419873 -0.821076 -0.312502 6 2.651391 0.402430 0.253779 28 0.266498 -0.188829 -0.362940 6 1.992803 1.311776 -0.822486 6 0.654548 1.554172 -0.848473 15 -1.739873 -0.208165 0.465429 6 2.957750 1.979228 -1.810778 1 2.813965 3.063271 -1.751669 1 3.990035 1.799654 -1.495509 1 3.943295 -0.547424 -1.232194 1 4.190427 -1.105592 0.407791

Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 -0.855270 5.228690 2.529242		1 1.794787 1.742207 -3.649304
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	6 0.385927 3.268980 -2.069660		6 -4.710918 2.698024 0.261836
	1 0.576360 4.142009 -1.437088		1 -4.515332 0.659965 -0.391389
	1 1.328135 3.037963 -2.574638		6 -2.773845 3.666157 1.341020
	6 -0.675447 3.639497 -3.121615		1 -1.045761 2.395930 1.504043
	1 -0.321905 4.489967 -3.714241		6 -4.095485 3.783647 0.891928
	1 -0.869022 2.805856 -3.802852		1 -5.737379 2.778741 -0.089377
	1 -1.622643 3.918999 -2.652298		1 -2.285162 4.506793 1.828345
	6 -2.481440 1.250615 -1.337074		1 -4.639668 4.715150 1.031765
	6 -3.416735 2.020231 -0.617241		6 -2.817735 -1.367508 -0.472987
	6 -2.939488 0.446615 -2.398915		6 -3.353048 -2.534104 0.093885
	6 -4.770653 1.991560 -0.958191		6 -3.062157 -1.098929 -1.832596
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	1 -3.431411 -1.726256 -0.516716		1 5.449417 0.837245 0.264152
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	1 -1.404223 -0.618295 3.133290		6 4.912168 2.957189 2.857409
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	1 -3.566262 -0.252970 4.218875		1 5.414823 3.624242 3.552882
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	6 -0.511319 -2.446197 -2.234001		6 -0.936961 2.410547 -2.587501
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	6 -2.592626 -5.647044 -1.538857		1 -0.182288 6.072948 -1.543889
	1 -0.405455 -3.133251 -4.275080		1 -2.245821 3.258495 -4.073690
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	5 4.673141 -1.691372 0.443231		5 0.782681 2.770232 0.560654
	5 4.997977 -3.040865 -0.669498		5 1.828920 1.968777 -1.978703
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	5 2.894554 -1.404463 -1.789184		5 -0.474970 3.028925 -0.645637
	5 3.983684 -3.287842 0.791974		5 1.734338 4.766017 -1.291293
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	1 3.531593 -5.203664 -0.950642		5 0.482818 4.411917 -0.059501
	1 5.442731 -1.090619 1.116831		5 0.097885 4.256598 -1.802335
	1 6.093782 -3.492398 -0.772722		5 1.538892 3.588918 -2.628941
	1 5.348346 -0.638984 -1.821559		1 0.614823 2.369592 1.656843
	1 2.487842 -0.653253 -2.606073		1 2.309528 1.065474 -2.558136
	1 4.336686 -3.920570 1.734776		1 -0.505739 1.950434 -3.005690
	1 2.629419 -1.333120 2.027703		1 -1.600159 2.822957 -0.349796
	5 2.224544 -3.006295 -1.474199		1 2.161483 5.861874 -1.466921
	1 1.304766 -3.376448 -2.127244		1 2.888779 4.144561 1.047318
	5 3.898678 -2.855229 -2.076000		1 3.974292 3.311286 -1.580048
	1 4.192939 -3.175730 -3.182619		1 0.006317 5.236214 0.651768
	6 3.402189 -0.794018 -0.280106		1 -0.667551 4.981287 -2.352923
	6 1.958476 -1.720327 -0.374127		1 1.810103 3.826614 -3.761632
	28 0.291737 -0.537323 -0.426268		28 -0.025727 -0.114283 -0.456650
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	6 1.207880 1.756810 -0.985846		6 3.747831 0.108692 -0.308159
	6 3.393142 0.727889 -0.019347		6 3.001565 1.207500 0.472079
	6 2.038906 1.425206 0.276861		6 4.864582 -0.428259 0.591725
	15 -1.617925 -0.627927 0.584542		6 4.582798 -1.027828 1.830931
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -4.447236 -0.236417 -0.348361		1 8.137780 -0.542878 0.538790
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	1 -1.292771 2.141331 1.414936		1 7.800871 -1.614553 2.768869
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	1 1.552406 1.814898 -3.837942		6 -3.899246 -4.245155 1.665325
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	1 4.042871 0.881110 0.845830		1 -4.296719 -5.223019 1.928232
	1 1.449863 0.763330 0.922183		6 -2.230909 0.941480 2.008928
	6 2.202024 2.688285 1.131278		6 -3.167921 1.941159 2.311407
	6 3.372631 3.461147 1.158822		6 -1.195880 0.683503 2.926930
	6 3.422733 4.598891 1.968894		6 -3.085727 2.649196 3.516281
	1 4.236944 3.186730 0.561132		1 -3.958713 2.185978 1.609211
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	1 0.284771 4.329116 3.222790		1 -3.816049 3.426170 3.731529
	1 2.293771 5.806377 3.379794		1 -0.321321 1.158735 4.837646
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	6 -0.910340 1.368180 -2.333077		6 -3.654416 0.556509 -0.562319
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	6 -1.121252 0.424902 -3.361548		6 -3.415602 1.059690 -1.849632
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	5 -3.145846 -2.251199 -0.670389		5 -1.498041 0.084036 -2.406581
	5 -1.751472 -3.347975 -0.701507		5 -2.772950 1.256522 -2.012066
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	5 -2.780639 -3.131117 -3.393096		5 -3.871096 -0.665194 -3.876654
	5 -2.507599 -1.372520 -3.347936		5 -3.442479 -1.991904 -2.761344
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	1 -0.385575 -2.524099 -4.329448		1 -5.852679 -1.201168 -2.206297
	1 -1.090589 -4.992530 -2.603600		1 -5.043399 1.593124 -3.229033
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	15 2.096847 0.218680 -0.139002		6 -0.483361 -2.036368 -0.075212
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 -2.040013 0.423817 0.966512	15	1.707396 0.591615 -0.066086
	1 -2.247791 2.051019 2.339186	1	-1.304754 -2.095946 0.647961
	1 -2.109464 0.483906 3.110660	6	0.594755 -2.912353 0.454699
	6 -1.361902 -0.763265 0.903517	6	0.838559 -2.977329 1.846533
	1 -3.300154 1.041545 -2.223865	6	1.817527 -3.830257 2.341122
	1 -4.181671 0.373240 -0.863078	1	0.251046 -2.361415 2.522789
	6 -4.104278 0.964718 2.427828	6	2.248726 -4.496373 0.083952
	1 -4.610520 1.509994 1.627954	6	2.549527 -4.617068 1.440693
	1 -4.386686 1.423453 3.382513	1	2.009609 -3.885684 3.410600
	1 -4.481091 -0.062360 2.427712	1	2.790411 -5.092222 -0.651588
	1 -1.262489 1.266658 -0.826707	1	3.323368 -5.302261 1.776949
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	6 -1.704162 3.653391 0.074053	1	-1.441330 -3.454724 -1.424519
	6 -2.098114 4.985208 0.202981	1	-0.191953 -2.488967 -2.177927
	1 -0.656555 3.375430 0.161977	6	-0.906844 2.772043 1.744583
	6 -4.344529 4.259659 -0.203364	1	0.167499 2.920850 1.877430
	6 -3.453230 5.301071 0.063626	1	-1.342391 2.617718 2.743336
	1 -1.362397 5.761867 0.400644	6	-1.512358 4.052487 1.133060
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	1 -3.811861 6.323529 0.150147	1	-1.293490 4.910254 1.777865
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	6 -1.208276 -1.695082 2.068771	6	-3.234269 0.317803 1.832681
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	1 -3.043757 -3.448474 4.369251	1	-4.307038 -2.210732 3.867010
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	6 5.736882 -2.493170 -1.214623	6	2.353557 5.196826 -0.440944
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	1 4.541698 -4.081231 -0.363017	1	1.026549 5.035072 -2.141921
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INT2_I_2b	6 2.911271 -0.553837 0.641460	TS3_I_2b	6 2.713469 -0.552545 0.600692
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	5 3.486696 -3.307406 0.154217	5	3.360001 -3.313373 0.684990
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	5 4.445557 -0.847026 1.341729	5	4.182759 -0.665401 1.486848
	5 2.978249 -0.750336 2.339955	5	2.629181 -0.425180 2.310552
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	1 4.386716 -1.293405 -1.251190	1	4.385697 -1.574272 -0.970638
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	1 1.109071 -3.951974 0.995199	1	0.919274 -3.855551 1.394979
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 1.206401 2.924530 0.092490		6 -2.697625 -0.086442 1.453715
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	1 -3.983005 -3.099656 -3.079352		6 1.361937 3.761709 -0.630779
	1 -3.636100 -5.298324 -1.875331		1 0.836508 3.874274 0.319001
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	6 3.610892 1.455558 -0.820535		6 3.640391 1.249683 -0.993530
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	1 4.719389 2.313304 0.825600		1 4.266119 2.466206 0.679081
	6 4.468251 2.025247 -3.034823		6 5.012698 1.477856 -2.997994
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INT3_I_2b	6 2.843422 -0.652401 0.305339	TS4_I_2b	6 2.564532 -2.187480 0.310172
	6 2.531717 -2.269011 -0.192091		6 2.858075 -0.546335 0.389880
	5 4.108001 -1.623358 -0.378998		5 4.131408 -1.635058 -0.105182
	5 1.739628 -1.640034 1.190805		5 1.807595 -1.271822 1.557872
	5 2.368665 -3.295243 1.169132		5 3.009790 -0.068355 2.041510
	5 3.847354 -3.291560 0.188332		5 4.448786 -0.293793 1.011583
	5 4.300258 -1.630868 2.496235		5 4.093464 -2.697628 2.573273
	5 4.400451 -0.604095 1.044925		5 3.905334 -3.112768 0.851184
	5 2.916809 -0.607266 2.023580		5 2.466318 -2.885830 1.871147
	5 5.047661 -2.259640 0.990761		5 5.126072 -1.914800 1.331024
	5 3.960486 -3.300699 1.967745		5 4.432796 -0.941556 2.669718
	5 2.633316 -2.270736 2.594904		5 2.785456 -1.553395 3.007943
	1 4.465976 -1.370215 -1.474990		1 4.419078 -1.635018 -1.251389
	1 0.587118 -1.395538 1.133388		1 0.653622 -1.052280 1.450285
	1 1.587687 -4.181435 1.075510		1 2.638545 1.014157 2.334929
	1 4.069165 -4.172879 -0.571776		1 5.066471 0.633243 0.625986
	1 4.941487 -1.369349 3.461176		1 4.522530 -3.491361 3.345432

Species	Cartesian coordinates				Species	Cartesian coordinates			
	1	5.048443	0.371724	0.920764	1	4.090876	-4.151878	0.313074	
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	1	6.212267	-2.456763	0.872757	1	6.288396	-2.125615	1.212999	
	1	4.347622	-4.263702	2.544902	1	5.115213	-0.457445	3.512699	
	1	2.062018	-2.477548	3.614820	1	2.273067	-1.517180	4.078146	
28	-0.330951	-0.626653	-0.799549		6	1.673800	-2.746996	-0.794711	
15	-1.882128	0.432796	0.526092		6	1.016047	-1.764201	-1.785203	
6	1.064668	0.652522	-0.953298		6	2.291590	0.316698	-0.703134	
6	2.332626	0.540596	-0.485494		6	1.178623	-0.043902	-1.434645	
6	1.738953	-2.632287	-1.463262		28	-0.528232	-0.750846	-0.678289	
6	0.731669	-1.657859	-2.074589		15	-1.897307	0.480407	0.482707	
6	-0.633522	-2.102671	-2.319638		1	2.269907	-3.461851	-1.370968	
6	-1.368070	-2.718688	-1.267222		1	0.883848	-3.315395	-0.302262	
6	-2.534967	-2.037931	-3.640697		6	0.818593	0.747409	-2.706652	
6	-2.737245	-3.002964	-1.455429		1	0.065752	0.181528	-3.263341	
1	-0.848965	-3.123470	-0.401611		1	1.695756	0.801871	-3.363949	
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1	-4.385229	-2.858780	-2.850106		1	-0.665964	2.146230	-1.937733	
1	1.235400	-3.571822	-1.221015		1	1.627000	-1.681113	-2.687372	
1	2.477198	-2.882351	-2.231757		6	-0.334924	-2.276574	-2.234935	
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6	0.651484	1.874432	-1.765996		6	-1.950301	-2.897467	-3.923729	
1	-0.334813	2.212081	-1.430649		1	0.006445	-2.101822	-4.370948	
1	1.333255	2.711177	-1.579083		6	-2.431251	-3.079597	-1.576056	
6	0.584581	1.628632	-3.286223		6	-2.837501	-3.259287	-2.893430	
1	1.564249	1.343131	-3.684561		1	-2.233217	-3.025647	-4.966259	
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7	-1.249241	-1.749461	-3.497567		7	-1.208992	-2.614912	-1.235276	
6	3.347066	1.638370	-0.703612		6	3.116565	1.523818	-1.047872	
6	3.485071	2.688928	0.220081		6	3.972312	1.505912	-2.164514	
6	4.154603	1.657159	-1.853549		6	3.076960	2.691279	-0.264960	
6	4.402092	3.722896	0.006253		6	4.754046	2.618274	-2.494329	
1	2.864504	2.697223	1.112368		1	4.038257	0.608696	-2.776079	
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6	-4.734611	0.547952	0.218658		6	-3.410592	1.011330	-1.801197	
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -1.736963 2.631371 1.656245		1 1.547955 2.988386 -2.181699
	1 0.501773 6.623247 -0.297740		1 -1.144752 6.518721 0.031481
	1 2.660118 4.580550 0.724274		1 -3.027415 4.245210 -1.018157
	1 2.025116 4.635015 -2.182119		1 -2.294774 4.268339 1.872227
	1 0.033210 5.062400 2.324352		1 -0.560868 5.145296 -2.670938
	1 -2.252425 5.365237 0.280790		1 1.737237 5.689451 -0.687153
	1 -1.024989 5.135908 -2.533330		1 0.653399 5.171037 2.153086
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6	2.470980 1.920426 -0.832527	6	-0.878446 -1.236610 -1.009138
6	1.948334 0.529075 -1.147867	6	-2.044960 -0.667777 -0.599584
6	1.888895 -0.681626 0.803779	15	2.055055 -0.635581 0.081075
6	0.857024 -1.451558 0.837874	6	-2.580052 1.675457 0.437291
15	-1.943447 -0.657257 0.050983	6	-2.163170 0.204859 0.686416
1	3.170148 1.888493 0.005723	6	2.138935 -2.462315 0.383909
1	3.049898 2.286097 -1.687735	6	2.354871 -3.332987 -0.700232
6	-2.171384 -2.222261 -0.921008	6	1.937915 -3.015642 1.659700
6	-3.456438 -2.739210 -1.178845	6	2.378152 -4.717997 -0.510959
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6	-2.502772 -4.580555 -2.437351	1	1.806554 -4.809041 2.844471
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TS3_I_3b	5 0.745430 3.763434 0.520673	INT3_I_3b	6 1.190288 2.650572 0.492924
	5 0.142529 5.257830 -0.261071		6 0.077818 2.093146 -0.591637
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	5 -1.576104 5.450989 0.183945		5 1.509198 2.892782 -1.175657
	5 -2.467275 4.050571 -0.473770		5 -0.075628 3.200946 -1.889328
	5 -1.294533 2.990949 -1.306315		5 -1.298213 3.133680 -0.609640
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -3.607253 3.988323 -0.795145		1 -0.885177 2.009266 1.729327
	1 1.632637 2.251529 -2.166322		1 2.363396 2.292802 -1.713017
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	1 -0.465807 2.330856 2.371708		1 -2.359537 2.653572 -0.826069
	5 0.299722 3.739011 -1.187436		1 0.665271 6.456059 0.262475
	1 1.100934 3.505736 -2.031410		1 0.955098 4.215200 2.434210
	5 -1.139926 4.767918 -1.416350		1 2.998026 4.366747 0.293933
	1 -1.345760 5.328694 -2.444518		1 -1.829328 4.918395 1.221282
	6 -1.793724 2.676811 0.294329		1 -1.410801 5.445469 -1.794094
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	6 -1.895530 -0.657146 -0.634898		6 3.013414 0.735776 0.554955
	6 -2.726041 1.484120 0.582641		6 1.941642 1.574700 1.282405
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	6 3.328241 -2.766454 -1.438455		6 3.914520 -1.994558 3.093605
	6 1.450004 -3.357434 -0.025640		1 2.381617 -1.765007 1.583415
	6 3.437355 -4.102831 -1.843756		6 5.038466 -1.396178 3.670472
	1 4.019043 -2.032167 -1.842517		1 6.313175 0.349562 3.603877
	6 1.566422 -4.689869 -0.424372		1 3.561603 -2.963646 3.440257
	1 0.661356 -3.077252 0.669266		1 5.590179 -1.876554 4.474463
	6 2.561212 -5.066623 -1.336894		6 2.599655 -0.111718 -0.651925
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	6 3.583747 0.265543 -0.652455		1 3.771678 1.439723 0.189474
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	6 3.431564 1.105801 -1.766900		6 1.130732 -0.756159 -2.620005
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	6 4.534117 1.781696 -2.299900		6 0.377212 -2.098777 -2.689512
	1 2.450289 1.245683 -2.212673		1 0.921585 -2.887481 -2.161470
	6 5.796391 1.629542 -1.717483		1 -0.622802 -2.038927 -2.248682
	1 6.931668 0.686368 -0.136862		1 0.256462 -2.411907 -3.732787
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	1 3.564538 -2.587995 4.393703		6 -2.140894 -2.448749 0.283274
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	6 0.010435 -0.652105 -3.653114		6 -0.681634 -4.203775 1.138120
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	6 -2.299201 -1.824089 2.400247		6 -5.109380 -0.688347 -0.897338
	6 -3.061312 -2.622227 3.253432		6 -3.358618 -0.115865 -2.472683
	1 -1.227514 -1.982161 2.303012		6 -6.060512 -0.567662 -1.914566
	6 -4.972307 -1.339350 2.588081		1 -5.432468 -0.946873 0.108146
	6 -4.435246 -2.379141 3.350405		6 -4.310319 -0.001269 -3.491313
	1 -2.593004 -3.413571 3.834962		1 -2.311380 0.082533 -2.692479
	1 -6.037216 -1.113010 2.640206		6 -5.662889 -0.227311 -3.213721
	1 -5.073746 -2.970615 4.001593		1 -7.111519 -0.738300 -1.692110
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	6 -3.762314 -0.336794 -2.320453		6 -3.283489 -0.155204 1.680873
	6 -3.671057 -2.404921 -1.075556		6 -3.807118 1.147036 1.785203
	6 -4.903666 -0.790623 -2.992174		6 -3.381716 -1.018234 2.783795
	1 -3.352885 0.640798 -2.561243		6 -4.424435 1.570381 2.964262
	6 -4.807749 -2.862178 -1.749758		1 -3.746022 1.832638 0.944232
	1 -3.193025 -3.042059 -0.335413		6 -3.994482 -0.588274 3.967442
	6 -5.431288 -2.054816 -2.708918		1 -2.992548 -2.030629 2.728120
	1 -5.375254 -0.156827 -3.740272		6 -4.517430 0.704897 4.061697
	1 5.205650 -3.849891 -1.526052		1 -4.828505 2.578413 3.025960
	1 -6.316073 -2.409810 -3.232876		1 -4.065725 -1.270141 4.812066
	1 0.231739 -1.247186 -4.545925		1 -4.994982 1.036656 4.980948
TS4_I_3b	6 1.881809 2.712963 -0.680528	TS2_I_4b	6 2.446811 -2.323083 0.267322
	6 0.705733 2.243156 0.421227		6 2.686426 -0.579465 -0.172430
	5 0.259880 2.651260 -1.257409		5 3.608056 -1.848817 -0.881187
	5 2.025722 3.197541 0.968386		5 2.252067 -1.074596 1.435642
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Species	Cartesian coordinates			Species	Cartesian coordinates				
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	5	1.351250	3.966832	-1.733724	5	3.920594	-3.128300	0.339736	
	5	2.436815	4.298375	-0.368936	5	3.052850	-2.635741	1.809844	
	5	-0.317985	4.329057	-1.227853	5	5.168882	-1.906651	-0.004754	
	5	-0.254233	4.900736	0.474014	5	5.093996	-0.669502	1.291480	
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	1	-0.022201	1.799289	-2.034679	1	3.431261	-2.139592	-2.012349	
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	1	-1.831363	2.787969	0.302958	1	4.793821	0.439472	-1.089066	
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	1	1.781362	3.955524	-2.837282	1	3.943049	-4.252730	-0.031682	
	1	3.586140	4.511645	-0.560846	1	2.448170	-3.410427	2.471224	
	1	-1.138127	4.683947	-2.009895	1	6.168488	-2.198361	-0.575105	
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	1	3.822515	1.797160	-0.697758	1	3.654798	1.408229	-2.743669	
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	6	3.328682	-0.786779	-1.634479	1	1.157369	-1.798035	-2.083959	
	6	2.861194	-2.049286	-2.033675	6	-0.763738	-2.549500	-1.869875	
	6	3.735979	-2.940109	-2.653712	6	-1.183782	-2.066906	-3.131960	
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	6	5.434784	-1.264982	-2.446273	1	-0.610735	-1.285568	-3.625023	
	6	5.060234	-2.542698	-2.865869	6	-2.540346	-4.041303	-1.846264	
	1	3.391593	-3.922140	-2.970969	6	-3.015475	-3.622308	-3.089592	
	1	6.454741	-0.912920	-2.600917	1	-2.633861	-2.240086	-4.717278	
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	6	5.127050	-1.635467	2.156150	6	-0.359490	5.064464	-1.215169	
	1	4.729359	0.148114	1.025877	1	-1.099965	3.053073	-1.054093	
	6	4.602273	-2.811848	2.705295	6	0.768269	5.895438	-1.229736	
	1	2.825867	-4.020165	2.937615	1	2.926782	5.966206	-1.121149	
	1	6.180041	-1.394548	2.287641	1	-1.354221	5.496401	-1.300880	
	1	5.242815	-3.491268	3.263496	1	0.653781	6.972851	-1.325912	
	6	-2.068167	-2.225137	0.621484	6	-1.633294	-1.003700	2.103492	
	6	-2.929944	-2.767228	1.587997	6	-1.845118	-2.364784	1.818002	
	6	-0.972068	-2.991406	0.186172	6	-1.661983	-0.584108	3.444861	
	6	-2.703903	-4.050581	2.102353	6	-2.089857	-3.277379	2.847916	
	1	-3.783302	-2.197056	1.943737	1	-1.822823	-2.727440	0.794459	
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	6	-1.621825	-4.811750	1.649834	6	-2.116591	-2.851850	4.181433	
	1	-3.380089	-4.454453	2.852871	1	-2.254210	-4.325067	2.604319	
	1	0.089629	-4.861199	0.328171	1	-1.918046	-1.155978	5.505923	
	1	-1.451148	-5.810652	2.045171	1	-2.302902	-3.564404	4.982108	
	6	-3.832299	0.081416	0.700699	6	-1.326894	1.800184	1.587850	
	6	-5.117724	-0.169646	0.192176	6	-2.506199	2.547717	1.736247	
	6	-3.705557	0.838430	1.878828	6	-0.145433	2.275136	2.181898	
	6	-6.250344	0.321043	0.851609	6	-2.503583	3.742550	2.465526	
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	6	-6.113996	1.063779	2.030056	6	-1.325632	4.199528	3.065253	
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	1	-6.995565	1.445270	2.540597	1	-1.325036	5.126794	3.634084	
	6	-2.822257	-0.896829	-1.838335	6	-2.838289	0.173967	-0.282777	
	6	-2.782407	0.159362	-2.766028	6	-4.082643	-0.210365	0.245600	
	6	-3.281447	-2.154181	-2.264749	6	-2.776236	0.642979	-1.605551	
	6	-3.201027	-0.032522	-4.085652	6	-5.241645	-0.113145	-0.530965	
	1	-2.427020	1.139428	-2.456133	1	-4.153033	-0.583748	1.263661	
	6	-3.689591	-2.350025	-3.589532	6	-3.936914	0.753083	-2.376672	
	1	-3.322870	-2.987603	-1.568844	1	-1.816933	0.914912	-2.039403	
	6	-3.652380	-1.290813	-4.502876	6	-5.173106	0.375966	-1.840860	
	1	-3.167108	0.797371	-4.788194	1	-6.198075	-0.415051	-0.109640	
	1	-4.039414	-3.330854	-3.904576	1	-3.872788	1.121011	-3.398332	
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	5 2.418207 -0.601462 1.006531		5 2.423588 -0.980410 1.135212
	5 3.379722 -2.098116 0.941640		5 2.848122 -2.641048 0.672509
	5 4.699624 -1.799625 -0.208673		5 4.105455 -2.524204 -0.574095
	5 5.033973 0.012896 2.014707		5 5.172274 -1.406552 1.860371
	5 4.741654 0.990717 0.555452		5 5.095916 -0.105479 0.646101
	5 3.416721 0.698173 1.701584		5 3.840708 -0.215158 1.899065
	5 5.723052 -0.486228 0.435431		5 5.536537 -1.747873 0.136516
	5 5.013286 -1.706240 1.544572		5 4.564365 -2.900134 1.103234
	5 3.566131 -0.968479 2.309929		5 3.495132 -1.942125 2.176182
	1 4.691307 0.142892 -1.941188		1 4.577192 -0.343473 -1.926401
	1 1.236619 -0.646419 1.112219		1 1.314114 -0.674166 1.402056
	1 2.807096 -3.127725 0.976496		1 1.985530 -3.439820 0.614405
	1 5.049487 -2.629916 -0.977137		1 4.103965 -3.239309 -1.517751
	1 5.704536 0.440839 2.896480		1 6.012474 -1.399231 2.699864
	1 5.123127 2.087868 0.333196		1 5.824693 0.818637 0.564548
	1 2.879417 1.593514 2.256674		1 3.660455 0.656622 2.679589
	1 6.880063 -0.431076 0.176365		1 6.627401 -1.983331 -0.268292
	1 5.668842 -2.533241 2.088976		1 4.953956 -3.983520 1.395000
	1 3.175622 -1.256393 3.392952		1 3.113209 -2.323077 3.233856
	6 2.334658 1.623204 -0.716823		6 2.878437 1.487845 -0.109619
	6 1.022924 1.895622 -0.390624		6 1.535175 1.694322 -0.208621
	6 2.292862 -1.548336 -1.652245		28 0.274664 0.154853 -0.286263
	6 0.736401 -1.498301 -1.604365		6 1.875315 -1.277032 -1.691038
	28 0.419975 0.134739 -0.468835		6 0.322732 -1.254613 -1.591434
	15 -1.587436 -0.027479 0.394016		15 -1.758159 0.055001 0.422043
	6 -1.714082 -1.334769 1.700295		6 -2.316665 -1.366771 1.448719
	6 -1.893376 -2.681772 1.337084		6 -1.525737 -2.521672 1.538554
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	6 -1.938154 -3.682135 2.311498		6 -1.922950 -3.589334 2.351928
	1 -2.013062 -2.958188 0.295482		1 -0.597109 -2.591596 0.983462
	6 -1.596630 -2.024899 4.035387		6 -3.899642 -2.355261 3.010377
	1 -1.429058 0.008245 3.380837		1 -4.112410 -0.386632 2.177006
	6 -1.787739 -3.359670 3.664532		6 -3.110736 -3.511075 3.084664
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	6 -2.185419 1.483168 1.283707		6 -2.995602 0.312320 -0.910641
	6 -3.525977 1.901049 1.241476		6 -2.696177 1.284525 -1.884571
	6 -1.278293 2.204906 2.078250		6 -4.189287 -0.418398 -1.017218
	6 -3.950533 3.005344 1.988837		6 -3.585950 1.532503 2.932449
	1 -4.249221 1.376953 0.625242		1 -1.768887 1.850736 -1.822890
	6 -1.705607 3.298195 2.836360		6 -5.074590 -0.173269 -2.073872
	1 -0.230646 1.917422 2.098841		1 -4.431750 -1.188239 -0.291065
	6 -3.044420 3.703160 2.793993		6 -4.777697 0.802485 -3.030797
	1 -4.991524 3.317454 1.939334		1 -3.345575 2.290322 -3.674766
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	1 -3.376459 4.559785 3.376536		1 -5.467222 0.990892 -3.850709
	6 -2.937691 -0.412694 -0.796842		6 -1.992669 1.470805 1.580057
	6 -4.148208 -1.011656 -0.405407		6 -1.155271 1.529626 2.709486
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	6 -5.168395 -1.222783 -1.337963		6 -1.301905 2.553946 3.646039
	1 -4.301586 -1.315567 0.626669		1 -0.389732 0.772180 2.863541
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	1 -6.098141 -1.689768 -1.020468		1 -0.651167 2.584656 4.517175
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	6 0.111665 -2.840132 -1.504354		6 -0.379975 -2.561136 -1.722609
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	6 0.164934 -4.999262 -0.657488		6 -2.281421 -3.850961 -2.495608
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	1 -1.504605 -2.407463 -2.887301		6 -0.390996 -4.853931 -1.421173
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	1 0.686520 -5.713889 -0.019221		1 -3.252247 -3.911888 -2.982903
	1 -2.495714 -4.682303 -2.735338		1 0.145069 -5.727641 -1.049197
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	7 0.708981 -3.776416 -0.731123		7 0.233184 -3.677791 -1.278138
	6 0.391367 3.194927 -0.651505		6 3.902493 2.609096 -0.300991
	6 0.906019 4.355107 -0.028526		1 3.361583 3.549865 -0.176620
	6 -0.754909 3.335290 -1.459540		1 4.645036 2.580741 0.503193
	6 0.304378 5.600703 -0.214874		6 4.635370 2.661244 -1.655973
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	6 -1.340698 4.585115 -1.668718		1 5.306488 1.812033 -1.803463
	1 -1.175753 2.458048 -1.941352		6 1.017593 3.030863 -0.589565
	6 -0.817880 5.724794 -1.044041		6 0.658622 3.987980 0.382846
	1 0.715168 6.477359 0.281818		6 0.799059 3.365724 -1.944305
	1 -2.213555 4.669427 -2.312779		6 0.126676 5.228399 0.017113
	1 -1.281976 6.696452 -1.197976		1 0.797957 3.752606 1.435485
	6 3.052233 2.459362 -1.789063		6 0.266735 4.606519 -2.309870
	1 2.818773 3.512848 -1.615874		1 1.058708 2.645212 -2.718155
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Species	Cartesian coordinates			Species	Cartesian coordinates		
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	5	-4.535106	-0.589906 -0.869991		5	4.676811	0.602936 -0.362543
	5	-2.698105	1.341519 0.100032		5	2.574858	-1.360787 -0.433042
	5	-3.703307	2.137729 -1.125958		5	3.459258	-1.575328 1.081458
	5	-4.858217	0.937386 -1.732687		5	4.764320	-0.363271 1.124406
	5	-5.414148	1.378570 1.053664		5	5.268160	-2.119423 -1.108817
	5	-4.905473	-0.313942 0.847338		5	4.977114	-0.477045 -1.739962
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	5	-5.911837	0.447949 -0.398803		5	5.885183	-0.683983 -0.225361
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	6	0.114934	0.857257 2.855614		6	-0.600388	-1.591732 2.741824
	6	2.333653	0.688932 4.540239		6	-2.845377	-0.820975 4.213051
	1	3.513475	0.609104 2.749333		1	-3.719552	-0.279388 2.324104
	6	-0.059117	0.866873 4.242868		6	-0.609168	-1.738507 4.130680
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	1	-1.062893	0.929366 4.657462		1	0.264077	-2.147775 4.634108
	1	0.916807	0.781671 6.170438		1	-1.737632	-1.460019 5.955519
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	6	4.415747	1.078443 0.325270		6	-4.409807	-1.209431 -0.360597
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Species	Cartesian coordinates				Species	Cartesian coordinates			
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	1	2.619467	-1.713499	-0.458056		1	-2.675663	1.720962	-0.436142
	6	5.881542	-0.740004	-0.328620		6	-5.868545	0.640863	-0.941968
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	1	4.898445	-2.591759	-0.852984		1	-4.923999	2.583317	-1.024010
	1	6.883485	-1.124291	-0.507392		1	-6.853903	1.015115	-1.211558
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	5	2.100889	1.997385	-0.014912		5	-2.967893	-1.874259	0.152252
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	1	-0.623830	3.655016	2.300759		1	-3.536105	0.771783	-2.711468
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	6	-4.901464	-1.462205	-1.395084		6	1.556952	4.255283	-0.201748
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	1	0.313290	-4.131504	2.640128		1	-1.079099	-3.039217	2.393634
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	6	2.105479	-1.172309	-0.195939		6	2.277493	-1.102034	-0.371581
	6	3.152323	-1.319233	0.728881		6	2.971085	-1.398845	0.815036
	6	2.288825	-1.650229	-1.504210		6	2.953382	-1.271816	-1.594782
	6	4.352581	-1.933636	0.356930		6	4.293323	-1.853379	0.782807
1	3.030370	-0.948851	1.744204	1	2.476929	-1.268835	1.774497		
6	3.488427	-2.265413	-1.877964	6	4.271493	-1.736266	-1.630696		
1	1.486484	-1.548808	-2.231465	1	2.440032	-1.063482	-2.531592		
6	4.524917	-2.408739	-0.948306	6	4.949553	-2.025672	-0.440663		
1	5.151761	-2.040460	1.087256	1	4.809758	-2.070419	1.715347		
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	6	-0.955035	-2.231892	-0.231617		6	0.276632	-2.187254	-0.921189
	5	-0.156171	-3.201778	-1.416399		5	1.601838	-2.352008	-2.024161
	5	-1.436663	-3.203305	1.114346		5	0.468969	-3.297257	0.382034
	5	-2.612444	-2.668522	-0.081456		5	-0.713031	-3.572168	-0.906178
	5	-1.816381	-2.671382	-1.656061		5	0.001718	-2.983348	-2.410400
	5	-1.872190	-5.400642	-0.692162		5	1.613472	-5.189243	-1.480971
	5	-0.168639	-4.887062	-0.823608		5	2.617463	-3.714286	-1.467072
	5	-0.976945	-4.890096	0.757335		5	1.899333	-4.315267	0.041571
	5	-1.345981	-4.354283	-2.049979		5	1.446775	-3.962533	-2.779632
	5	-2.894792	-4.026179	-1.212274		5	-0.008566	-4.736353	-2.069961
	5	-2.659514	-4.350366	0.532604		5	0.275320	-4.935762	-0.310988
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	1	-1.320029	-2.779916	2.212276		1	0.206465	-2.952801	1.481961
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	1	-2.183950	-6.537552	-0.849200		1	2.105155	-6.255496	-1.671608
	1	0.797327	-5.551544	-1.005631		1	3.794670	-3.619711	-1.579546
	1	-0.556574	-5.554707	1.645198		1	2.591395	-4.626778	0.952963
	1	-1.275859	-4.726955	-3.176715		1	1.802262	-4.140220	-3.900176
	1	-3.946956	-4.174343	-1.746473		1	-0.700065	-5.479002	-2.690734
	1	-3.527150	-4.719640	1.256467		1	-0.202591	-5.812392	0.334372
	28	0.132634	-0.530086	0.013588		28	0.021429	-0.246394	-0.519716
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 1.607847 0.641921 -0.425736	6	2.745923 -1.694978 0.444885
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1	3.844406 -1.697376 -0.220068	1	3.454924 2.417837 -0.174611
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1	2.113385 -3.456454 0.297539	6	3.741945 1.201698 -1.930405
1	1.374183 -3.772957 1.854215	1	2.946345 1.665263 -2.524838
6	3.960665 -0.645277 -2.105011	1	3.750376 0.139344 -2.201026
1	3.282493 -0.345934 -2.913417	6	-2.466770 1.810795 0.775916
1	4.367701 0.279885 -1.682040	6	-2.655406 2.791465 -0.215447
6	2.118062 1.986100 -0.678681	6	-2.656377 2.165219 2.120796
6	1.637996 2.797326 -1.723206	6	-3.024493 4.092693 0.130303
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6	2.203555 4.049759 -1.971414	6	-3.025629 3.471128 2.465916
1	0.833854 2.438543 -2.358202	1	-2.539050 1.430186 2.909737
6	3.726673 3.734679 -0.119960	6	-3.209906 4.438895 1.474048
1	3.548524 1.862134 0.935360	1	-3.165165 4.835191 -0.651743
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1	4.690654 -2.427267 -3.092994	1	-3.940205 -2.097666 0.846097
6	5.904337 -0.766055 -3.762195	6	-1.607021 -1.653442 3.916193
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1	6.711477 -1.396422 -4.151403	6	-2.616933 -2.622953 3.936513
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1	0.132605 2.481025 1.832539	1	-4.953660 0.337247 0.305874
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1	0.613992 4.876426 2.185378	6	-5.324247 -0.709001 -2.913936
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6	-2.472225 0.032368 2.544416	1	-6.100999 -0.890282 -3.653654
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6	-3.278428 0.013909 3.688745	1	3.115086 -2.280924 1.290091
1	-1.633161 -0.649514 2.475941	1	1.081934 -0.639845 1.326969
6	-4.623989 1.797262 2.760648	6	2.759205 0.078986 2.306285
1	-4.015112 2.551548 0.846664	6	4.100719 -0.168524 2.633169
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1	-3.057237 -0.686247 4.491286	1	4.743195 -0.736366 1.966476
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1	-4.990009 0.877911 4.684078	6	3.767726 1.045724 4.683462
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6	-4.020783 0.615893 -1.444430	1	1.749267 1.791829 4.910660
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1	-0.933119 1.193796 -2.762546	6	0.150249 2.796682 -2.298975
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1	-5.810540 0.295465 -2.599551	1	1.410561 3.789769 0.709567
1	-2.217184 1.050250 -4.856916	6	-0.033338 4.048446 -2.887836
1	-4.671500 0.597722 -4.796050	1	-0.109161 1.892885 -2.846761
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6	3.602266 -1.978880 2.358510	1	-0.435105 4.117906 -3.896562
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1	3.756224 -2.922777 1.844628	1	5.887683 1.373265 -1.701395
6	4.353541 -0.304156 3.913928	1	5.080373 2.896844 -2.036494
1	2.927711 1.300860 4.187334	6	5.430827 1.682663 -3.792905
1	5.488344 -2.076186 3.406199	1	4.671367 2.161438 -4.422217
1	5.079582 0.103344 4.612483	1	6.396856 2.142739 -4.029011
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	5 -1.885721 4.769425 -1.669483	6	1.067462 2.172704 -0.724396
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	5 -3.871454 2.813463 -0.941830	5	1.571709 2.967838 -2.156603
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	5 -2.084886 4.814337 0.113544	5	2.892675 4.901578 -0.455925
	5 -1.590079 3.212504 0.742445	5	2.316695 4.011578 0.974040
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Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -1.922720 5.795072 0.766033		1 1.270193 2.510026 -3.207375
	1 -1.128988 2.970441 1.806337		1 -0.794769 3.709940 -1.427213
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	1 0.085487 -3.805400 -0.201013		1 -4.897391 1.442498 0.396466
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	1 0.883913 -5.418754 -1.899638		1 -5.738761 3.121022 1.986876
	1 0.697467 -2.340562 -4.911598		1 -2.074964 2.844131 4.240534
	1 1.197390 -4.696746 -4.264608		1 -4.345684 3.830243 3.928081
TS4_I_1c	6 -1.887182 -1.577099 -2.114816	TS2_I_2c	6 -1.427048 -2.652530 -1.368679
	6 -0.886295 -1.977610 -0.828919		6 -2.201033 -1.116811 -0.731869
	5 -0.186206 -1.536436 -2.423765		5 -2.859313 -2.680022 -0.449942
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	5 -1.357931 -3.953739 -3.454399		5 -3.385182 -2.936298 -3.289637
	5 -1.318679 -2.181628 -3.623556		5 -2.597664 -3.726378 -1.896200
	5 -2.662187 -2.957064 -2.758587		5 -1.630352 -2.755986 -3.032687
	5 0.183095 -3.063769 -3.239932		5 -4.160454 -2.914465 -1.667251
	5 -0.246583 -4.402483 -2.125481		5 -4.178599 -1.456899 -2.711939
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	1 0.321408 -0.480317 -2.612628		1 -2.829804 -3.132257 -0.640128
	1 -3.257732 -2.571256 -0.266655		1 -0.325759 -0.608796 -2.372301
	1 -0.720445 -4.096367 0.476740		1 -2.953799 0.836239 -2.086131
	1 1.555236 -2.846696 -0.978700		1 -4.633501 -0.829769 -0.184003
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	1 -3.775208 -2.821965 -3.141642		1 -0.729580 -3.218703 -3.648148
	1 1.084224 -3.112854 -4.012079		1 -5.136579 -3.534373 -1.397416
	1 0.351754 -5.428275 -2.095646		1 -5.178530 -1.022528 -3.183874
	1 -2.678143 -5.294389 -1.603290		1 -2.430770 -0.837929 -4.587564
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6	-2.621727 -0.238659 -2.041653	6	-1.425104 1.215913 0.455874
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6	-3.766100 4.637294 -1.500215	1	4.185168 -4.316154 0.549887
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6	-2.254283 -2.919341 3.681377	1	-3.173870 3.133795 -0.451302
1	-3.240238 -2.108305 1.959211	6	-2.236678 5.002828 0.110274
6	-1.045616 -3.082159 4.367076	1	-2.774640 5.108289 1.062011
1	1.071500 -2.645242 4.350376	1	-1.221947 5.383202 0.287418
1	-3.170825 -3.349608 4.079963	6	-2.922799 5.859496 -0.961820
1	-1.013704 -3.636614 5.302512	1	-3.952478 5.526261 -1.137169
6	-2.820032 0.830912 1.459296	1	-2.960449 6.913369 -0.664176
1	-2.657625 1.916399 1.428555	1	-2.388621 5.801249 -1.917299
1	-2.481861 0.498408 2.444514	6	-3.150312 -0.119891 1.812978
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1	-4.704931 0.906370 0.367228	6	-2.950701 -1.149100 2.751017
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6	-5.132132 1.300082 2.450203	1	-4.439868 1.522295 1.250580
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1	-7.052818 1.382401 1.411680	1	-3.668818 -2.128476 4.528377
1	-6.871213 -0.023050 2.470623	1	-5.630282 -0.612514 4.796716
6	2.503973 1.836376 -1.105636	6	3.053773 -0.338162 -0.854318
6	2.599702 1.502425 -2.470055	6	4.321192 -0.348276 -0.249902
6	2.523915 3.191492 -0.739763	6	2.851976 -1.138744 -1.993466
6	2.725130 2.498166 -3.441209	6	5.367647 -1.098572 -0.797622
1	2.591565 0.459164 -2.778306	1	4.505566 0.212153 0.659535
6	2.637638 4.190685 -1.715613	6	3.899680 -1.875893 -2.549173
1	2.456097 3.478102 0.305870	1	1.869984 -1.209233 -2.450514
6	2.739642 3.848624 -3.067259	6	5.166726 -1.852820 -1.957072
1	2.806229 2.220061 -4.489857	1	6.340313 -1.092449 -0.310423
1	2.651222 5.235990 -1.414011	1	3.718516 -2.480947 -3.434804
1	2.830663 4.624947 -3.823748	1	5.983272 -2.430353 -2.384883
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6	1.101044 1.733029 2.295955	6	1.493023 1.791777 -2.845230
6	3.464321 2.271485 3.683747	6	1.341673 4.441563 -1.992677
1	4.473191 1.278855 2.065852	1	1.495119 3.668183 -0.003446
6	1.054671 2.419195 3.513509	6	1.373054 2.822962 -3.781035
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1	0.095458 2.731067 3.921063	1	1.339504 2.580370 -4.840907
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6	3.944018 -0.396224 0.056668	6	2.243246 1.501819 1.301057
6	5.116900 0.213743 -0.419703	6	3.373029 2.343491 1.306275
6	4.012579 -1.717544 0.532099	6	1.544770 1.303618 2.502025
6	6.331141 -0.481835 -0.416026	6	3.796855 2.956073 2.487626
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Species	Cartesian coordinates				Species	Cartesian coordinates			
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	1	5.262733	-3.430352	0.919855		1	1.410971	1.755515	4.605898
	1	7.335379	-2.332732	0.071618		1	3.426040	3.223241	4.600823
INT2_I_2c	6	2.812571	-1.164439	0.465780	TS3_I_2c	6	2.468380	-1.319915	0.599903
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	5	3.578872	-2.232519	-0.676264		5	3.384267	-2.673846	0.031450
	5	1.441034	-1.974112	1.071504		5	1.057099	-1.882770	1.394365
	5	1.403932	-3.658166	0.498282		5	1.111275	-3.655578	1.455826
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	5	3.826677	-3.258926	2.009497		5	3.376618	-2.622822	2.911109
	5	4.272022	-1.900319	0.938479		5	3.899878	-1.737481	1.457519
	5	2.902853	-1.734217	2.064208		5	2.431304	-1.232150	2.315232
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	5	2.907923	-4.444170	1.051777		5	2.564817	-4.118562	2.384501
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	1	2.691203	-4.452552	-1.627027		1	2.586656	-5.102482	-0.113028
	1	4.530304	-3.565384	2.915412		1	3.995768	-2.535520	3.920533
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	1	-1.948669	-5.919646	-2.242948		6	1.947132	3.230187	-0.343132
	1	-4.341320	-5.103808	-2.179855		1	1.404357	3.342881	0.599797
	7	-2.738121	-2.163041	-1.669172		1	2.984735	3.000241	-0.083072
	6	4.015242	1.001857	-0.135050		6	1.900487	4.551762	-1.123730
	6	4.796195	1.553679	0.896271		1	2.433812	4.430846	-2.076320

Species	Cartesian coordinates	Species	Cartesian coordinates
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -3.476970 -5.493358 2.549650		1 -3.213525 -4.947774 3.596133
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -0.300946 6.136751 0.998497		1 -0.352367 3.697457 2.170480
	1 -0.574659 3.157141 1.843424		1 1.746361 3.724086 0.054428
	5 0.171553 3.569899 -1.965017		1 -2.146021 6.331968 -1.658872
	1 0.989878 3.142559 -2.710733		1 -1.740748 3.758311 -3.396538
	5 -1.299968 4.447904 -2.465430		1 -3.830472 3.717655 -1.294889
	1 -1.515624 4.700174 -3.607364		1 0.706379 5.386252 -2.353387
	6 -1.898063 2.879471 -0.249659		1 0.039585 6.302033 0.521809
	6 -0.248689 2.618053 -0.602174		1 -2.798246 5.315073 1.172016
28	0.344955 0.664830 -0.386418		6 -2.034903 1.192504 -1.775881
	6 -0.655983 -0.840564 -0.773412		6 -2.793005 0.202933 -0.863160
	6 -1.883912 -0.564964 -0.279924		6 -2.130929 -0.309614 0.425089
	6 -2.789295 1.777056 0.353868		6 -0.899174 -0.051740 0.915209
	6 -2.112474 0.473228 0.850963	28	0.487712 0.867854 0.061000
15	2.182316 -0.294255 0.232273		6 -3.248291 -0.948136 -1.766876
	6 2.348350 -2.114697 0.427480		6 -2.365323 -1.966208 -2.158283
	6 3.137194 -2.891721 -0.433994	15	2.221059 -0.644262 -0.220489
	6 1.650187 -2.746079 1.473502		6 -4.938444 -1.854814 -3.048721
	6 3.233937 -4.276538 -0.246447		6 -2.811828 -2.958405 -3.031214
	1 3.684712 -2.426993 -1.249164		1 -1.348461 -1.979410 -1.775752
	6 1.757309 -4.124419 1.665677		6 -4.132387 -2.907376 -3.488764
	1 1.029997 -2.161669 2.149519		1 -5.973157 -1.777951 -3.382553
	6 2.550231 -4.894630 0.804225		1 -2.143997 -3.757247 -3.346950
	1 3.848855 -4.867290 -0.921633		1 -4.529924 -3.658426 -4.166695
	1 1.219114 -4.597802 2.483727		1 -1.138838 0.706276 -2.171631
	1 2.631452 -5.969139 0.952078		1 -2.683241 1.389796 -2.635171
	6 3.478340 0.193829 -0.981148		1 -3.722877 0.696016 -0.555684
	6 4.839060 0.251471 -0.632234	7	-4.515823 -0.892227 -2.212504
	6 3.092257 0.510563 -2.294315		6 -3.107826 -1.129526 1.242582
	6 5.795617 0.606615 -1.587096		6 -4.108224 -0.485157 1.991831
	1 5.158979 0.026465 0.381550		6 -3.068301 -2.534027 1.261194
	6 4.051925 0.861423 -3.249402		6 -5.030603 -1.219175 2.745918
	1 2.040786 0.493590 -2.572556		1 -4.161819 0.601456 1.993714
	6 5.404731 0.909685 -2.897530		6 -3.987638 -3.272524 2.015156
	1 6.845426 0.650924 -1.305985		1 -2.312236 -3.056041 0.680116
	1 3.739694 1.106287 -4.261977		6 -4.973437 -2.617789 2.762152
	1 6.151268 1.189585 -3.637450		1 -5.791286 -0.697445 3.323208
	6 2.763566 0.363162 1.854341		1 -3.934952 -4.359490 2.015930
	6 2.369214 1.655067 2.241070		1 -5.689219 -3.189928 3.348474

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 3.626524 -0.366706 2.691737 6 2.827913 2.208046 3.440093 1 1.705982 2.234451 1.608236 6 4.083466 0.188708 3.890941 1 3.945281 -1.368572 2.418554 6 3.685366 1.476162 4.268819 1 2.511868 3.208914 3.725298 1 4.750821 -0.386960 4.528456 1 4.040190 1.905077 5.203344 6 -0.288071 -1.830397 -1.859407 1 -0.854570 -1.552181 -2.759511 1 0.764960 -1.703195 -2.131236 6 -0.539052 -3.321768 -1.557076 1 -1.598419 -3.473891 -1.327773 1 0.021638 -3.613365 -0.663370 1 -3.570251 1.528779 -0.367348 1 -3.306934 2.227396 1.202178 1 -1.134389 0.729614 1.277860 6 -2.892026 -0.150089 2.013894 6 -2.223950 -0.979410 2.929893 6 -2.937966 -1.549024 3.983391 1 -1.159243 -1.167652 2.815419 6 -4.883441 -0.434075 3.139716 6 -4.305534 -1.274707 4.093049 1 -2.438454 -2.189397 4.707327 1 -5.944221 -0.189490 3.193059 1 -4.907554 -1.692115 4.896084 7 -4.201781 0.119222 2.123688 6 -0.138792 -4.224578 -2.733018 1 -0.696272 -3.922106 -3.629943 1 0.923697 -4.071591 -2.964689 6 -0.389600 -5.712771 -2.456059 1 -1.450240 -5.905689 -2.255937 1 -0.094672 -6.332118 -3.310677 1 0.180586 -6.053971 -1.584169 6 -3.114707 -1.187797 -0.888974 6 -3.610935 -0.730177 -2.122112 6 -3.789964 -2.243331 -0.249450 6 -4.749452 -1.305434 -2.698265 1 -3.102303 0.080197 -2.637218 6 -4.926643 -2.820182 -0.823806 1 -3.418097 -2.626274 0.697131 6 -5.412910 -2.352803 -2.050737 1 -5.115476 -0.933351 -3.652909 1 -5.430142 -3.638440 -0.313107 1 -6.297194 -2.802046 -2.497544		6 -0.444310 -0.481152 2.303441 6 -0.461271 0.652935 3.347636 6 -0.039785 0.174102 4.744002 6 -0.055059 1.293834 5.793124 1 -1.086099 -1.294768 2.662189 1 0.572211 -0.890832 2.667054 1 0.203613 1.461366 3.020998 1 -1.468804 1.084629 3.394738 1 -0.707483 -0.636073 5.066828 1 0.967061 -0.261249 4.689637 1 0.629132 2.105374 5.518065 1 -1.056835 1.727427 5.896086 1 0.249033 0.921679 6.778034 6 1.953078 -2.388510 -0.740926 6 2.759763 -3.017415 -1.704620 6 0.926031 -3.124476 -0.124055 6 2.542948 -4.357666 -2.042582 1 3.558838 -2.468690 -2.195314 6 0.717006 -4.465974 -0.457296 1 0.287471 -2.654528 0.617499 6 1.523616 -5.085654 -1.419137 1 3.174360 -4.831538 -2.790876 1 -0.078708 -5.024328 0.030861 1 1.357767 -6.128154 -1.681546 6 3.287934 0.072724 -1.541620 6 4.622732 0.450335 -1.325346 6 2.714754 0.281557 -2.810434 6 5.372431 1.019047 -2.362175 1 5.085779 0.301931 -0.353950 6 3.467755 0.838890 -3.845793 1 1.681038 -0.002644 -2.998318 6 4.799238 1.212984 -3.622864 1 6.405356 1.307889 -2.181045 1 3.012952 0.989165 -4.822326 1 5.383701 1.654996 -4.426654 6 3.051147 -0.750209 1.261353 6 3.357125 0.364158 2.117966 6 4.079983 -1.882328 1.562644 6 4.182537 0.353761 3.245748 1 2.751305 1.243805 1.905377 6 4.898111 -1.894707 2.697501 1 4.047247 -2.757818 0.919644 6 4.953608 -0.777488 3.538683 1 4.215937 1.223471 3.897982 1 5.491382 -2.778096 2.923010 1 5.590121 -0.790067 4.420632
TS4_I_3c	6 1.836472 2.460332 -1.397134 6 0.690426 2.347142 -0.170063 5 0.189972 2.286854 -1.886674 5 2.045544 3.380584 0.049563 5 0.410835 3.913804 0.484350 5 -0.746674 3.248633 -0.702601 5 1.046684 5.028661 -2.100357 5 1.292493 3.385681 -2.738535 5 2.434606 4.052013 -1.552464 5 -0.350887 3.923107 -2.304976 5 -0.214576 4.942129 -0.835591 5 1.517722 5.020033 -0.370183 1 -0.133887 1.270359 -2.405930 1 2.885834 3.052340 0.808920 1 0.111419 3.997261 1.623898 1 -1.832804 2.903664 -0.357105 1 1.205311 5.979904 -2.793402 1 1.680215 3.056775 -3.808391 1 3.580026 4.172076 -1.829855 1 -1.190062 4.069689 -3.132328 1 -0.964853 5.832107 -0.599280 1 2.005906 5.950950 0.181470 6 2.761725 1.265906 -1.615263 6 2.248336 -0.060939 -1.003014 6 2.019899 0.115445 0.511026 6 1.013355 0.943771 0.937425 28 -0.622984 0.934007 -0.156463 15 -2.096758 -0.704590 -0.243903 1 2.886321 1.131918 -2.693719 1 3.747569 1.491806 -1.204862 1 1.279383 -0.287366 -1.458069 6 3.177455 -1.197798 -1.406967 6 2.643784 -2.408138 -1.874982 6 3.509662 -3.434513 -2.257978 1 1.566318 -2.540255 -1.939053 6 5.327512 -1.976443 -1.700596 6 4.887071 -3.219197 -2.165983 1 3.116705 -4.380725 -2.623933 1 6.394325 -1.765753 -1.624731 1 5.603942 -3.984461 -2.452647 7 4.503148 -0.985507 -1.332022 6 2.957521 -0.550604 1.469358	TS2_I_4c	6 -1.394874 -3.047116 -0.475742 6 -2.176458 -1.416250 -0.629919 5 -2.962310 -2.753508 0.115687 5 -1.100707 -2.043841 -1.842213 5 -2.624043 -1.246393 -2.280015 5 -3.817259 -1.703358 -1.051601 5 -3.026416 -4.110285 -2.435627 5 -2.516289 -4.272144 -0.732903 5 -1.328524 -3.818310 -1.973803 5 -4.055347 -3.462524 -1.113596 5 -3.821781 -2.531977 -2.628753 5 -2.120933 -2.725763 -3.136585 1 -3.131204 -2.754909 1.284814 1 -0.028705 -1.588257 -2.012039 1 -2.593998 -0.156792 -2.738609 1 -4.646750 -0.956825 -0.672433 1 -3.328911 -5.066494 3.072120 1 -2.403615 -5.255745 -0.082744 1 -0.366251 -4.473912 -2.191541 1 -5.093369 -3.940605 -0.791722 1 -4.705130 -2.333503 -3.397795 1 -1.764293 -2.679315 -4.268104 6 -0.277108 -3.134668 0.552153 6 -0.213040 -1.861431 1.389454 6 -2.395276 0.311211 0.328763 6 -1.646271 1.248298 -0.206181 28 -0.525564 -0.290100 0.140953 15 1.558743 0.361507 -0.528556 1 -1.172663 -1.710477 1.898820 6 0.821883 -1.848795 2.452784 6 0.652868 -1.023212 3.589404 6 1.588616 -1.050731 4.616468 1 -0.220477 -0.379441 3.659130 6 2.790666 -2.685908 3.350476 6 2.693699 -1.904996 4.502775 1 1.460430 -0.422076 5.495367 1 3.632875 -3.366673 3.221290 1 3.451757 -1.967737 5.279029 7 1.891543 -2.671573 2.353416 1 -0.457780 -4.019050 1.178743 1 0.666463 -3.308475 0.032381 6 -3.501446 0.261344 1.350914

Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 3.828946 -2.561048 2.550244		6 -3.168094 1.095060 2.605310
	1 2.250747 -2.560376 1.091581		1 -2.262866 0.692121 3.076614
	6 4.767443 -0.405311 3.105376		1 -2.933571 2.124097 2.309436
	1 3.914798 1.285831 2.084025		6 -4.319025 1.101715 3.621368
	6 4.743774 -1.793793 3.280765		1 -4.556686 0.069319 3.910688
	1 3.798566 -3.641274 2.677839		1 -5.222707 1.501776 3.142618
	1 5.475902 0.203549 3.663441		6 -4.001429 1.923926 4.877356
	1 5.429314 -2.271694 3.977208		1 -3.123923 1.526562 5.401096
	6 0.815210 1.291707 2.410906		1 -3.791923 2.969899 4.624436
	1 1.341302 2.229806 2.629953		1 -4.841091 1.913308 5.580954
	1 1.321483 0.527662 3.007770		6 -1.845469 2.665779 -0.451741
	6 -0.633197 1.413248 2.917750		6 -0.856578 3.629759 -0.164045
	1 -1.187887 2.142442 2.315535		6 -3.075795 3.111067 -0.991180
	1 -1.145518 0.453306 2.791387		6 -1.099470 4.987624 -0.376124
	6 -0.693041 1.831365 4.394789		1 0.099302 3.313118 0.239172
	1 -0.133494 1.105777 5.000687		6 -3.306050 4.467202 -1.225461
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	6 -2.126091 1.944315 4.930908		6 -2.321455 5.414141 -0.912213
	1 -2.656325 0.987930 4.851711		1 -0.328491 5.715775 -0.133593
	1 -2.134758 2.243268 5.985115		1 -4.256532 4.788043 -1.646703
	1 -2.701917 2.689891 4.369631		1 -2.503370 6.472100 -1.087729
	6 -1.873239 -1.774807 -1.737953		6 2.633490 -0.888551 -1.379016
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	6 -1.641769 -3.157494 -1.663744		6 3.027028 -0.747003 -2.721119
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	6 -1.429178 -3.907514 -2.828345		6 3.817481 -1.723278 -3.339697
	1 -1.629353 -3.660322 -0.700932		1 2.728240 0.122852 -3.296189
	6 -1.452366 -3.287548 -4.081171		6 4.229769 -2.853356 -2.627633
	1 -1.710630 -1.415707 -5.134783		1 4.153412 -3.876658 -0.724011
	1 -1.250971 -4.978106 -2.751590		1 4.110564 -1.593605 -4.379345
	1 -1.290356 -3.871111 -4.984741		1 4.844959 -3.610779 -3.108653
	6 -2.154149 -1.915473 1.151461		6 2.621867 1.041265 0.812393
	6 -3.337053 -2.546172 1.572448		6 4.025283 0.972225 0.780632
	6 -0.951223 -2.220443 1.810472		6 1.997995 1.712031 1.877455
	6 -3.313236 -3.467681 2.625312		6 4.786583 1.575383 1.786839
	1 -4.282581 -2.319685 1.087740		1 4.529400 0.451562 -0.029004
	6 -0.925181 -3.148874 2.855867		6 2.759520 2.326376 2.875695
	1 -0.034740 -1.722262 1.508141		1 0.912692 1.748117 1.933287
	6 -2.107793 -3.774434 3.267435		6 4.156379 2.260455 2.832406
	1 -4.237894 -3.944708 2.943254		1 5.872042 1.513492 1.749906
	1 0.015479 -3.373344 3.354076		1 2.261258 2.844703 3.691995
	1 -2.091900 -4.490410 4.086317		1 4.750333 2.732579 3.611966
	6 -3.848918 -0.131330 -0.381935		6 1.516857 1.720413 -1.785903
	6 -4.813431 -0.765652 -1.182689		6 2.464917 2.755978 -1.807761
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	6 -6.128487 -0.288190 -1.222425		6 2.437258 3.724293 -2.818277
	1 -4.544672 -1.632187 -1.781191		1 3.228789 2.819316 -1.038549
	6 -5.544115 1.460747 0.345750		6 0.520445 2.634784 -3.811396
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	6 -6.498129 0.823644 -0.457114		6 1.469455 3.663700 -3.826134
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INT2_1_4c	6 -2.936233 -0.699130 -0.819129	TS3_1_4c	6 2.837998 -0.319854 0.929210
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	5 -1.660092 -1.640864 -1.464237		5 1.688845 -1.485614 1.447281
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	5 -3.615949 -3.432984 -0.416146		5 4.060259 -2.859168 0.661961
	5 -4.065063 -2.123181 -2.950915		5 3.947186 -1.516206 3.213846
	5 -4.413201 -0.945426 -1.661026		5 4.220763 -0.286124 1.959041
	5 -2.864181 -0.874303 -2.525444		5 2.593597 -0.512792 2.623762
	5 -4.857432 -2.650201 -1.429507		5 5.003243 -1.873870 1.808481
	5 -3.576764 -3.656204 -2.186051		5 3.851196 -3.107432 2.417316
	5 -2.328356 -2.542022 -2.842269		5 2.349526 -2.255269 2.903661
	1 -4.594848 -1.423850 0.925473		1 4.811666 -0.693563 -0.575871
	1 -0.535496 -1.265994 -1.382771		1 0.538517 -1.319740 1.242891
	1 -1.196959 -4.131311 -1.070674		1 1.759338 -4.007559 1.015281
	1 -3.819338 -4.242595 0.423545		1 4.507671 -3.610210 -0.136612
	1 -4.644784 -2.066446 -3.985321		1 4.376505 -1.356273 4.309209
	1 -5.174700 -0.042350 -1.699697		1 4.790008 0.740487 2.089537
	1 -2.548060 0.082819 -3.142942		1 2.032385 0.366721 3.181226
	1 -5.994858 -2.981462 -1.362964		1 6.182422 -1.983417 1.884404
	1 -3.794379 -4.719642 -2.666440		1 4.206087 -4.116506 2.932374
	1 -1.649941 -2.797082 -3.781493		1 1.620019 -2.636838 3.758221
	6 -2.646616 0.644532 -0.178383		6 2.402488 0.953392 0.224997
	6 -1.435811 1.289341 -0.307361		6 1.102356 1.293718 -0.008574
	6 -1.772849 -2.180526 1.315917	28	0.124631 -0.222178 -0.393252
	6 -0.322544 -1.637939 1.492616	6	2.248626 -2.012209 -1.308904
28	-0.313511 -0.137711 0.147182	6	0.798924 -1.651742 -1.723595
15	1.765247 0.398228 -0.306479	15	-1.817439 0.321291 0.464344
	6 2.614426 -0.799030 -1.435906		6 -2.456409 -1.092975 1.465878
	6 2.326985 -2.169261 -1.327824		6 -2.265068 -2.391102 0.958761
	6 3.559610 -0.380479 -2.391016		6 -3.166869 -0.926792 2.666780
	6 2.972729 -3.101457 -2.145701		6 -2.772911 -3.499714 1.640414

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 1.602216 -2.514672 -0.600801		1 -1.723093 -2.543114 0.029676
	6 4.203267 -1.313234 -3.210486		6 -3.672635 -2.039768 3.347531
	1 3.797438 0.672787 -2.505000		1 -3.334906 0.064339 3.077106
	6 3.912316 -2.676952 -3.091120		6 -3.476537 -3.327891 2.838360
	1 2.735879 -4.158357 -2.044924		1 -2.615770 -4.496357 1.234427
	1 4.930977 -0.971013 -3.943162		1 -4.221343 -1.896253 4.275808
	1 4.411245 -3.400962 -3.731698		1 -3.869710 -4.191296 3.370591
	6 1.968984 1.978370 -1.240502		6 -3.115555 0.523047 -0.825377
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Species	Cartesian coordinates	Species	Cartesian coordinates
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	5 -0.418512 4.290981 -2.517981		5 0.108337 -4.178383 -2.947403
	5 1.078436 4.729166 -1.639166		5 -1.373655 -4.653816 -2.053482
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	1 -1.624366 1.935991 -2.342417		1 1.267497 -1.779662 -2.786916
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	1 1.296342 2.290722 -2.710285		1 -1.666785 -2.250475 -3.162943
	1 -0.662632 6.699748 -1.494666		1 0.424988 -6.570772 -1.901701
	1 -2.914109 4.510421 -1.601763		1 2.607483 -4.329710 -2.051703
	1 -1.819649 5.290878 1.054654		1 1.548844 -5.109208 0.622618
	1 -0.590823 4.512451 -3.673080		1 0.279624 -4.408589 -4.101089
	1 1.989211 5.278967 -2.171016		1 -2.271532 -5.234296 -2.574731
	1 1.234877 5.803208 0.768647		1 -1.480796 -5.700462 0.369263
	28 -0.200945 0.371250 -0.195025		28 -0.231805 -0.289023 -0.586310
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	6 -0.920154 -1.320181 -0.699375		6 2.231477 -2.263925 0.062328
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	6 0.392579 -3.893514 -3.122087		6 -1.976573 3.956897 2.709722
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	6 -0.812972 -5.040534 -1.365684		6 -2.053339 4.962089 1.741074
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 2.086112 -1.900272 1.210372		6 -1.398178 -0.614776 2.874889
	6 3.360643 -2.414319 1.519280		6 -3.786568 -2.041060 3.138145
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	1 4.488561 -3.921258 2.562530		1 -2.995910 -2.721640 5.030305
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	5 -1.629757 5.541949 -1.142793		5 -1.311593 -2.061313 -2.045130
	5 -2.500226 3.994562 -1.317398		5 0.385141 -2.257758 -2.476926
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	6 -0.690949 -0.846339 -0.810097		15 2.580510 0.209036 0.371089
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	6 -2.633950 1.850219 0.456043		6 -2.363356 -1.924565 0.568101
	6 -1.994537 0.505553 0.899373		6 -4.459594 -0.734002 1.096309
	15 2.067731 -0.368998 0.343838		6 -4.256482 0.047980 2.243761
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 4.844707 -0.157978 -0.197488		7 -5.587371 -1.441083 0.905185
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	1 0.983087 5.776520 -3.128608		1 -3.482886 -4.059588 -4.002067
	1 1.291213 2.827184 -4.138008		1 -2.566493 -4.917366 -1.130154
	1 3.427002 3.943189 -2.419096		1 -0.495946 -3.799686 -3.049951
	1 -1.464692 3.904056 -3.146231		1 -5.190396 -3.359777 -1.517218
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 2.071499 -0.043388 0.199390		6 -1.386891 1.412173 0.092095
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	1 -5.145971 -1.117440 -0.938310		1 3.579334 2.752073 -0.257809
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	5 4.050243 -2.301872 1.036147		5 -3.805839 2.141311 1.238731
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	5 2.452176 -4.675822 1.430542		5 -2.301498 4.546613 1.756890
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 4.184418 -3.765354 3.177593		1 -3.844391 3.363566 3.525481
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	6 1.583756 0.770626 0.104762		6 -1.348808 -0.683630 -0.358831
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Species	Cartesian coordinates				Species	Cartesian coordinates			
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	5	2.285068	3.658488	-0.424952		5	-2.469816	3.497386	-1.205822
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	1	6.179330	3.255814	-0.997380		1	-6.289912	2.494691	-1.057456
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	6	1.597948	1.495841	-2.132768		6	-1.617886	1.241939	-2.593854
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	1	0.944538	-0.721005	-3.655789		6	2.807306	-0.370950	-4.290407
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	6	1.048305	-2.194320	-0.166853		6	-3.069491	-1.394340	0.838345
	6	1.077763	-3.041644	-1.302289		6	-4.022328	-2.265016	0.279953
	6	0.397581	-2.665491	0.997821		6	-2.863809	-1.436002	2.227211
	6	0.498060	-4.306641	-1.262219		6	-4.750383	-3.146506	1.084518
	1	1.573886	-2.700819	-2.207165		1	-4.198945	-2.250419	-0.792759
	6	-0.195566	-3.935230	1.026612		6	-3.590539	-2.316490	3.035717
	1	0.390305	-2.048282	1.892488		1	-2.120878	-0.784179	2.677458
	6	-0.147826	-4.759695	-0.098701		6	-4.539573	-3.174271	2.468353
	1	0.547060	-4.948647	-2.139447		1	-5.483092	-3.810789	0.630543
	1	-0.686353	-4.276640	1.935328		1	-3.410645	-2.334805	4.108774
	1	-0.601170	-5.748076	-0.075162		1	-5.105839	-3.859061	3.096115
	6	3.889763	-1.393955	0.368938		6	-0.838450	-2.317587	-0.708834
	6	4.121329	-1.798605	1.694167		6	-1.271005	-3.233241	-1.686435
	6	4.668622	-1.963273	-0.652184		6	-0.068904	-2.818458	0.357638
	6	5.109587	-2.742457	1.992794		6	-0.925193	-4.587177	-1.617340
	1	3.523427	-1.372693	2.496394		1	-1.911141	-2.906262	-2.502193
	6	5.658615	-2.906727	-0.356456		6	0.267272	-4.171770	0.437482
	1	4.499524	-1.668735	-1.685159		1	0.253881	-2.140938	1.140415
	6	5.884611	-3.298523	0.968170		6	-0.148986	-5.065256	-0.557069
	1	5.272613	-3.044401	3.025375		1	-1.277633	-5.269852	-2.388032
	1	6.250911	-3.337275	-1.161333		1	0.857221	-4.527981	1.279574
	1	6.653877	-4.032265	1.199109		1	0.117148	-6.118462	-0.499967
	6	-2.978661	1.969931	0.800949		6	1.551401	-0.071048	2.438249
	6	-3.106853	2.759645	-0.357278		6	0.507132	0.603810	3.099377
	6	-3.374144	2.504371	2.038945		6	2.196963	-1.126426	3.103074
	6	-3.625035	4.055630	-0.272661		6	0.135870	0.247366	4.397808
	1	-2.808855	2.353620	-1.321672		1	-0.012020	1.421663	2.605638
	6	-3.886825	3.804703	2.118764		6	1.815718	-1.492007	4.400752
	1	-3.289021	1.914608	2.946826		1	3.003906	-1.667650	2.616875
	6	-4.013862	4.584245	0.964404		6	0.788119	-0.805146	5.054093
	1	-3.720711	4.654590	-1.176028		1	-0.665007	0.789733	4.896163
	1	-4.188074	4.204139	3.084834		1	2.328712	-2.311531	4.899766
	1	-4.411908	5.594732	1.028031		1	0.496344	-1.085439	6.063826
	6	-2.142285	-0.323889	2.372117		6	2.430903	2.189757	0.877766
	6	-3.027011	-1.243598	2.956544		6	2.944310	2.731566	2.069469
	6	-1.059390	0.155515	3.134350		6	2.295033	3.028644	-0.242342
	6	-2.837680	-1.669270	4.277280		6	3.324006	4.076303	2.134824
	1	-3.865662	-1.634806	2.387660		1	3.042148	2.110643	2.956293
	6	-0.876848	-0.262272	4.455264		6	2.680374	4.371806	-0.178756
	1	-0.358922	0.865640	2.699621		1	1.874127	2.630306	-1.162166
	6	-1.765582	-1.179492	5.030541		6	3.196931	4.899740	1.009907
	1	-3.531878	-2.383054	4.715680		1	3.717595	4.479525	3.065559
	1	-0.038600	0.123607	5.031287		1	2.566124	5.007311	-1.054473
	1	-1.621430	-1.510510	6.056636		1	3.490315	5.946014	1.062492
	6	-3.673935	-0.724818	-0.077385		6	3.553392	-0.447550	0.363280
	6	-5.022874	-0.355667	0.054196		6	4.779925	-0.034734	0.912854
	6	-3.351358	-1.908852	-0.762005		6	3.535271	-1.566851	-0.486046
	6	-6.031773	-1.162487	-0.482758		6	5.957656	-0.732711	0.627987
	1	-5.291276	0.562325	0.570933		1	4.825693	0.835112	1.562231
	6	-4.360956	-2.719818	-1.289273		6	4.711874	-2.271714	-0.764229
	1	-2.309572	-2.196763	-0.886974		1	2.595853	-1.886492	-0.931465
	6	-5.703452	-2.347648	-1.151966		6	5.926358	-1.855873	-0.208573

Species	Cartesian coordinates			Species	Cartesian coordinates				
	1	-7.072946	-0.865228	-0.377189	1	6.899407	-0.398978	1.058681	
	1	-4.098304	-3.634939	-1.815350	1	4.678773	-3.138547	-1.420748	
	1	-6.489103	-2.974059	-1.568957	1	6.843467	-2.398166	-0.428743	
TS2_I_1e	6	3.354972	0.808764	-0.296848	INT2_I_1e	6	3.093064	-1.091749	0.156007
	6	1.754849	1.263550	0.038971		6	1.415384	-1.480566	0.017718
	5	2.923646	1.174561	1.310512		5	2.497596	-1.732256	-1.307162
	5	2.506573	1.734786	-1.439534		5	2.260947	-1.693464	1.506247
	5	1.555448	2.886406	-0.507147		5	1.138884	-2.916116	0.896247
	5	1.807829	2.531117	1.199902		5	1.290626	-2.941975	-0.863179
	5	4.346804	3.358868	0.081553		5	3.825877	-3.768470	0.251879
	5	4.499460	1.669955	0.628104		5	4.075710	-2.240777	-0.637530
	5	4.240360	2.026277	-1.094580		5	3.924372	-2.226954	1.132308
	5	3.533794	2.817851	1.588586		5	2.949929	-3.456436	-1.282824
	5	2.680100	3.896626	0.443449		5	2.100358	-4.203609	0.108886
	5	3.111911	3.394856	-1.221569		5	2.699269	-3.421841	1.606674
	1	2.844822	0.303216	2.103816		1	2.422066	-1.027315	-2.252732
	1	2.163090	1.215111	-2.447501		1	2.052287	-0.954836	2.408799
	1	0.509282	3.232569	-0.919868		1	0.090065	-3.049282	1.429920
	1	0.925972	2.615255	1.987995		1	0.350410	-3.088390	-1.565762
	1	5.281906	4.093504	0.092136		1	4.698405	-4.572320	0.335540
	1	5.469177	1.084933	0.981120		1	5.062445	-1.841480	-1.160773
	1	5.038478	1.684087	-1.902281		1	4.806600	-1.812784	1.807741
	1	3.876269	3.153593	2.676360		1	3.179671	-4.034021	-2.296124
	1	2.410610	5.022885	0.714415		1	1.719859	-5.330340	0.090702
	1	3.151173	4.145663	-2.142352		1	2.750844	-3.971495	2.659497
	28	0.612585	-0.410414	0.129298		6	3.555544	0.373526	0.207492
	6	3.528706	-0.662354	-0.638928		6	2.449737	1.447161	0.365278
	6	2.181440	-1.345396	-0.847622		28	0.402596	0.208437	-0.346530
	6	1.376295	-2.096182	0.962566		6	1.791529	1.944595	-0.956561
	6	0.083397	-2.098926	0.883187		6	0.449001	1.860991	-1.153249
	15	-1.517538	0.355348	-0.071970		15	-1.681726	-0.191220	0.062491
	6	2.568995	-2.627140	1.704317		6	2.739491	2.607716	-1.965422
	1	3.248975	-3.133838	1.014406		1	2.300454	3.561982	-2.274426
	1	3.128799	-1.790566	2.132449		1	3.683057	2.860736	-1.470892
	1	4.106967	-1.161537	0.139238		1	4.150347	0.585788	-0.682709
	1	4.116699	-0.754074	-1.559086		1	4.240810	0.461818	1.052808
	6	2.194323	-3.599516	2.834716		6	3.050889	1.781798	-3.228498
	1	3.111298	-3.982770	3.294606		1	3.669541	2.370708	-3.914848
	1	1.609463	-3.104521	3.614048		1	3.595799	0.864663	-2.991146
	1	1.623689	-4.454762	2.460420		1	2.138354	1.494836	-3.759763
	6	-1.117310	-2.906634	1.287237		6	-0.358969	2.615936	-2.171556
	1	-0.998253	-3.905786	0.847821		1	-1.335729	2.143139	-2.308216
	1	-2.019971	-2.488531	0.838630		1	0.147339	2.549645	-3.144748
	6	-1.351505	-3.045062	2.804253		6	-0.568164	4.103097	-1.817232
	1	-1.439412	-2.066555	3.282115		1	0.384012	4.635321	-1.731018
	1	-2.286113	-3.590286	2.975222		1	-1.163703	4.596061	-2.593098
	1	-0.546976	-3.597460	3.292658		1	-1.099177	4.208797	-0.868087
	6	-2.539759	-0.646912	-1.244037		6	-2.923804	1.141777	-0.248390
	6	-3.847850	-0.247774	-1.582851		6	-4.007301	0.999275	-1.127970
	6	-1.998949	-1.783360	-1.864459		6	-2.802684	2.326975	0.499229
	6	-4.604801	-0.988019	-2.493176		6	-4.951313	2.026516	-1.259932
	1	-4.274791	0.655739	-1.155481		1	-4.131720	0.089783	-1.707781
	6	-2.755685	-2.519715	-2.784079		6	-3.749954	3.344417	0.375061
	1	-0.982937	-2.093613	-1.641881		1	-1.967443	2.456695	1.184810
	6	-4.061031	-2.129682	-3.095834		6	-4.827769	3.198385	-0.508780
	1	-5.614686	-0.667171	-2.739039		1	-5.785328	1.902422	-1.947223
	1	-2.320527	-3.395413	-3.260716		1	-3.645558	4.252796	0.964361
	1	-4.647798	-2.702125	-3.810931		1	-5.564148	3.992708	-0.608564
	6	-1.886678	2.051396	-0.705987		6	-2.207580	-1.590297	-1.006461
	6	-2.274166	3.105680	0.133391		6	-2.714437	-2.797643	-0.503775
	6	-1.744658	2.294777	-2.084457		6	-2.026204	-1.449665	-2.395496
	6	-2.518271	4.379078	-0.395696		6	-3.054993	-3.837657	-1.377029
	1	-2.393776	2.946311	1.200787		1	-2.836724	-2.943248	0.565008
	6	-1.994119	3.562858	-2.611315		6	-2.377785	-2.483683	-3.265037
	1	-1.440481	1.494222	-2.754959		1	-1.604012	-0.533598	-2.803452
	6	-2.380485	4.612013	-1.767110		6	-2.894377	-3.682523	-2.757014
	1	-2.818642	5.186422	0.268669		1	-3.441674	-4.770617	-0.973042
	1	-1.881497	3.733190	-3.679773		1	-2.236242	-2.358447	-4.336163
	1	-2.572080	5.601446	-2.176423		1	-3.159857	-4.492496	-3.432723
	6	-2.363942	0.318663	1.570290		6	-2.102762	-0.623603	1.802229
	6	-3.689988	-0.097494	1.770509		6	-3.436042	-0.879196	2.175290
	6	-1.616792	0.756416	2.679074		6	-1.106401	-0.626013	2.787412
	6	-4.258969	-0.062891	3.048778		6	-3.755365	-1.156797	3.505765
	1	-4.286444	-0.464470	0.941472		1	-4.230308	-0.853502	1.433076
	6	-2.191540	0.807849	3.952479		6	-1.428512	-0.894506	4.122859
	1	-0.581177	1.059036	2.551274		1	-0.078295	-0.413993	2.515873
	6	-3.516054	0.397557	4.141223		6	-2.751368	-1.165369	4.483686
	1	-5.284867	-0.396934	3.187655		1	-4.788304	-1.358381	3.780695
	1	-1.599976	1.157502	4.795677		1	-0.644234	-0.892039	4.876490
	1	-3.962631	0.427692	5.132600		1	-3.002789	-1.375951	5.520868
	1	1.579402	-0.816763	-1.606036		1	1.681156	1.090722	1.069510
	6	2.314542	-2.746031	-1.380863		6	3.023846	2.683329	1.075048
	8	3.330772	-3.423762	-1.315012		8	4.201317	2.998503	1.088262
	8	1.196426	-3.160384	-2.020196		8	2.053994	3.390655	1.682883
	6	1.250512	-4.492946	-2.579797		6	2.476234	4.602769	2.354017
	1	0.280262	-4.649336	-3.050765		1	2.930534	5.292185	1.638938
	1	2.050609	-4.562320	-3.320097		1	1.567152	5.030438	2.775498
	1	1.416678	-5.230912	-1.791493		1	3.193299	4.367603	3.143587

Species	Cartesian coordinates			Species	Cartesian coordinates				
TS3_I_1e	5	2.232149	-2.964119	0.486345	INT3_I_1e	6	2.421483	1.882517	0.532899
	5	3.696106	-3.643619	-0.281967	6	1.171414	1.802168	-0.540838	
	5	4.460067	-1.299326	1.204737	5	0.864431	2.397993	1.050530	
	5	5.076907	-2.603035	0.161257	5	2.760293	2.231806	-1.112701	
	5	4.770707	-0.982647	-0.514665	5	1.313962	3.061794	-1.692201	
	5	3.193505	-1.018035	-1.353064	5	0.153302	3.183970	-0.359229	
	5	3.785329	-2.932928	1.364520	5	2.511704	4.660599	0.410585	
	5	2.694263	-1.514144	1.390116	5	2.322423	3.287885	1.529726	
	1	1.283638	-3.586663	0.831881	5	3.491572	3.181740	0.197429	
	1	3.802356	-4.812915	-0.473216	5	0.878354	4.163824	0.949896	
	1	5.039597	-0.688076	2.039576	5	1.162313	4.594127	-0.767129	
	1	6.188233	-3.007867	0.288005	5	2.782231	3.990912	-1.228502	
	1	5.559014	-0.158067	-0.838630	1	0.282830	1.706762	1.810560	
	1	2.936742	-0.256445	-2.221494	1	3.395107	1.487190	-1.761815	
	1	3.956384	-3.579577	2.347483	1	0.945580	2.868564	-2.802450	
	1	2.108648	-1.071405	2.320044	1	-1.006708	3.054363	-0.564368	
	5	2.541987	-2.653539	-1.222314	1	3.012971	5.677210	0.768268	
	1	1.799243	-3.039405	-2.064114	1	2.694714	3.191053	2.650841	
	5	4.297775	-2.420723	-1.445693	1	4.644195	3.025626	0.426479	
	1	4.835722	-2.696286	-2.469551	1	0.204161	4.802613	1.690545	
	6	3.333136	-0.434814	0.242376	1	0.686435	5.562846	-1.265026	
	6	1.991604	-1.411683	-0.175165	1	3.466261	4.514329	-2.046790	
	28	0.349905	-0.275169	-0.561942	28	0.302268	0.125635	-0.655837	
	6	0.222936	1.319532	-1.475457	15	-1.956099	-0.226694	0.109222	
	6	1.260523	2.048229	-1.003144	6	3.601521	-0.453230	0.258119	
	6	3.213639	1.076963	0.517715	6	2.836544	0.544312	1.150155	
	6	1.832305	1.782657	0.413209	6	3.918384	-1.911077	-1.797739	
	15	-1.714978	-0.465642	0.029397	6	2.954435	-1.001429	-1.021738	
	6	-2.887536	0.939157	-0.138008	1	4.929904	-1.777058	-1.399360	
	6	-4.110950	0.828837	-0.815856	1	3.970862	-1.587725	-2.843215	
	6	-2.539486	2.166046	0.457897	6	1.744635	-0.652958	-1.511486	
	6	-4.979417	1.925611	-0.887663	1	1.940442	0.061361	1.544621	
	1	-4.395218	-0.103682	-1.294313	1	3.472970	0.773743	2.011409	
	6	-3.414852	3.252287	0.397576	1	4.535881	0.027828	-0.056547	
	1	-1.583477	2.281073	0.962732	6	1.277325	-0.971017	-2.931016	
	6	-4.637884	3.135372	-0.276110	1	0.956447	-0.030734	-3.399291	
	1	-5.922283	1.828989	-1.421211	1	2.122502	-1.324966	-3.532780	
	1	-3.137883	4.193784	0.866519	6	0.132566	-1.997948	-3.055859	
	1	-5.315256	3.984751	-0.329339	1	0.397260	-2.952601	-2.591592	
	6	-2.457090	-1.884916	-0.874139	1	-0.789683	-1.649534	-2.581006	
	6	-3.576531	-2.570176	-0.368656	1	-0.095465	-2.184451	-4.111389	
	6	-1.888585	-2.300215	-2.089335	6	3.576832	-3.412579	-1.757802	
	6	-4.126641	-3.639747	-1.079759	1	3.534249	-3.787539	-0.729994	
	1	-4.017607	-2.277252	0.581042	1	2.608213	-3.615714	-2.223035	
	6	-2.442274	-3.369802	-2.800578	1	4.337274	-3.991681	-2.293972	
	1	-1.003056	-1.800022	-2.475386	6	4.070574	-1.598533	1.164091	
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	1	-4.991885	-4.163686	-0.679902	8	3.037130	-2.264560	1.721262	
	1	-1.990833	-3.684367	-3.738670	6	3.386218	-3.341429	2.622800	
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	6	-1.127803	-2.436465	3.588273	6	-3.262582	-2.745935	-0.330500	
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	6	-2.010065	-1.811948	4.478643	6	-1.057533	-4.203690	0.593468	
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	6	1.857502	3.199324	-1.818645	1	-0.195621	-4.764851	0.947352	
	1	1.614072	4.141792	-1.306545	1	-2.240873	-5.962755	0.174272	
	1	1.338279	3.246399	-2.776825	6	-3.270004	0.397461	-1.014095	
	6	3.371623	3.181338	-2.105145	6	-4.621180	0.479225	-0.632272	
	1	3.968363	3.365627	-1.208830	6	-2.900237	0.800762	-2.308219	
	1	3.688600	2.232467	-2.548670	6	-5.582791	0.942816	-1.534531	
	1	3.608559	3.978121	-2.818999	1	-4.925633	0.190813	0.370959	
	6	-0.506259	1.479068	-2.794604	6	-3.863988	1.259579	-3.212334	
	1	0.251306	1.472004	-3.591479	1	-1.854526	0.770635	-2.608338	
	1	-1.119549	0.591580	-2.979787	6	-5.207073	1.330229	-2.827074	
	6	-1.395815	2.727914	-2.955503	1	-6.624594	1.002913	-1.227505	
	1	-0.834455	3.653018	-2.797946	1	-3.563135	1.570913	-4.210082	
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	1	-2.228707	2.719452	-2.251025	6	-2.517176	0.292895	1.787485	
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	1	3.568463	1.233303	1.538893	6	-2.691890	-0.619845	2.839652	
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	6	1.910942	3.115333	1.168917	1	-2.593171	2.389588	1.233157	
	8	2.933020	3.724035	1.432110	6	-3.069715	-0.170783	4.111303	
	8	0.680298	3.550387	1.514048	1	-2.544897	-1.683569	2.676174	
	6	0.629586	4.815253	2.217832	6	-3.278238	1.191833	4.345082	
	1	1.051099	5.610758	1.599293	1	-3.265178	3.170135	3.469929	
	1	-0.427420	4.997800	2.409377	1	-3.205149	-0.890755	4.915495	
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	5 0.965989 -2.937851 0.287660		5 -4.326826 -0.896568 -0.127145
	5 3.533866 -3.873346 1.209576		5 -5.190481 1.219090 1.640143
	5 3.205218 -2.307819 1.990667		5 -4.551088 1.983152 0.157991
	5 4.292171 -2.384132 0.588455		5 -3.545722 1.909185 1.624067
	5 1.869580 -3.459953 1.733183		5 -5.460262 0.459987 0.032082
	5 2.144864 -4.262256 0.150336		5 -5.051490 -0.541083 1.463439
	5 3.653786 -3.591644 -0.558052		5 -3.827852 0.342085 2.420362
	1 1.004335 -0.961074 2.087689		1 -3.875168 0.840797 -2.084887
	1 3.896218 -1.174974 -1.675214		1 -1.282915 0.657479 1.771886
	1 1.619186 -3.147006 -2.205774		1 -2.806240 -1.970400 1.684005
	1 -0.214428 -3.052090 0.139537		1 -4.558368 -1.847987 -0.783942
	1 4.180693 -4.703045 1.760259		1 -6.060664 1.736628 2.260963
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	1 5.417784 -2.028362 0.688145		1 -3.131786 2.881833 2.159254
	1 1.317855 -3.980410 2.646746		1 -6.516714 0.424222 -0.508015
	1 1.789613 -5.372654 -0.076237		1 -5.817761 -1.310038 1.945171
	1 4.373998 -4.209801 -1.270848		1 -3.708507 0.229572 3.596084
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	8 1.074111 3.502044 0.692488		8 -1.479661 3.700238 -0.516324
	6 0.603059 4.853405 0.532114		6 -1.053887 5.035053 -0.200903
	1 1.387683 5.372673 -0.020141		1 -1.816346 5.434828 0.470034
	1 -0.335459 4.874582 -0.026905		1 -0.081810 5.029137 0.298637
	1 0.450063 5.325927 1.506297		1 -0.987222 5.648641 -1.103800
INT3_I_2e	6 3.092228 0.231686 -0.469465	TS4_I_2e	6 3.346804 -1.164684 -0.272373
	6 3.113069 -0.515504 1.108553		6 3.192217 0.500407 -0.156645
	5 4.454454 -0.718762 0.077084		5 4.702200 -0.184683 -0.677353
	5 2.356454 1.010587 0.882107		5 2.395737 -0.516176 0.995331
	5 3.342310 0.671177 2.319453		5 3.222004 0.956812 1.512357
	5 4.663043 -0.403275 1.821842		5 4.656891 1.157945 0.478399
	5 4.985847 2.098234 0.444481		5 4.984475 -1.292191 1.968748
	5 4.684283 0.828723 -0.764186		5 4.891133 -1.699402 0.233192
	5 3.361251 1.913871 -0.272129		5 3.461473 -1.899944 1.270721

Species	Cartesian coordinates	Species	Cartesian coordinates
	5 5.675334 0.454487 0.656137		5 5.750200 -0.225995 0.745922
	5 4.973969 1.334484 2.053462		5 4.833898 0.484699 2.116708
	5 3.526193 2.220051 1.473339		5 3.418019 -0.558514 2.439334
	1 4.621008 -1.781193 -0.411787		1 4.967307 -0.075739 -1.823394
	1 1.179572 1.069994 0.911652		1 1.215593 -0.612498 0.933885
	1 2.774527 0.497172 3.344184		1 2.567116 1.887455 1.833478
	1 4.992697 -1.312088 2.505647		1 5.005223 2.229061 0.128724
	1 5.658723 3.037944 0.171367		1 5.622271 -1.958066 2.716367
	1 5.117018 0.815218 -1.859672		1 5.350298 -2.631042 -0.336119
	1 2.825209 2.624133 -1.051606		1 2.962310 -2.966467 1.392775
	1 6.831982 0.214491 0.539821		1 6.924320 -0.113084 0.617033
	1 5.632535 1.712442 2.966427		1 5.366081 1.115420 2.970163
	1 3.138961 3.233729 1.954676		1 2.920957 -0.686842 3.509032
28	0.007062 -1.037321 0.082779	6	2.647206 -1.896911 -1.418217
15	-1.755230 0.451815 -0.050639	6	1.409108 -1.236314 -2.049496
6	0.985414 -0.779745 -1.491608	28	0.074584 -0.390241 -0.760937
6	2.225876 -0.248597 -1.632730	6	2.386519 1.198151 -1.229269
6	2.841866 -0.002521 -3.017693	6	1.286759 0.616249 -1.880407
1	3.430780 0.916113 -3.004686	15	-1.809322 0.114239 0.335086
1	2.037932 0.196331 -3.729288	1	3.386104 -2.061344 -2.206850
6	2.291613 -1.748061 1.526716	1	2.372651 -2.878827 -1.031212
6	1.338011 -2.382303 0.517803	6	2.920519 2.546664 -1.695482
1	1.732920 -1.454719 2.417448	1	4.006114 2.477201 -1.830000
1	3.020256 -2.500404 1.852560	1	2.517213 2.757689 -2.687631
1	1.847183 -2.959640 -0.249803	6	2.613420 3.751513 -0.782029
6	0.193992 -1.331771 -2.673041	1	1.537402 3.860068 -0.617697
1	-0.832430 -0.950523 -2.635873	1	2.982234 4.673506 -1.246217
1	0.602925 -0.992643 -3.630174	1	3.091617 3.658590 0.195693
6	0.122779 -2.872318 -2.710475	6	0.597150 1.209793 -3.043523
1	1.121531 -3.315899 -2.779543	1	-0.027679 0.429542 -3.486160
1	-0.361090 -3.279284 -1.817756	1	1.348676 1.459409 -3.806173
1	-0.452715 -3.199208 -3.583771	6	-0.295367 2.435677 -2.787528
6	3.707982 -1.151094 -3.567665	1	-0.793043 2.728774 -3.718898
1	4.099346 -0.892050 -4.558804	1	0.268774 3.298854 -2.427369
1	4.561513 -1.366929 -2.919011	1	-1.066939 2.213006 -2.046723
1	3.124149 -2.071982 -3.666435	1	1.603821 -1.026026 -3.099260
6	0.232201 -3.155971 1.101092	6	0.141132 -2.077177 -2.103652
8	-0.127673 -4.307229 0.912677	8	-0.646833 -2.072475 -3.055996
8	-0.542059 -2.260347 1.860504	8	0.063935 -3.030057 -1.106551
6	-1.736574 -2.800840 2.477493	6	-1.019548 -3.976544 -1.239834
1	-2.207237 -1.965515 2.992450	1	-0.926811 -4.646579 -0.384317
1	-2.405028 -3.217742 1.721419	1	-1.984412 -3.464883 -1.224201
1	-1.453943 -3.582494 3.185970	1	-0.920866 -4.535467 -2.173755
6	-2.532887 0.629882 1.613333	6	-1.907258 -0.622607 0.202637
6	-3.903206 0.432578 1.846478	6	-1.343879 -1.896454 2.219049
6	-1.695943 0.947355 2.699987	6	-2.519157 0.021660 3.114572
6	-4.426924 0.553528 3.139912	6	-1.408988 -2.522344 3.467415
1	-4.569381 0.182068 1.025802	1	-0.844670 -2.397527 1.392754
6	-2.221298 1.078159 3.987707	6	-2.575940 -0.601137 4.366434
1	-0.630273 1.098450 2.544154	1	-2.948434 1.012892 2.993352
6	-3.589675 0.877477 4.212253	6	-2.025116 -1.875253 4.545238
1	-5.490379 0.395204 3.305298	1	-0.968276 -3.507932 3.600904
1	-1.561665 1.328316 4.815648	1	-3.050367 -0.089210 5.200945
1	-3.998022 0.971122 5.216053	1	-2.068626 -2.357273 5.519449
6	-1.468055 2.189072 -0.591879	6	-2.038225 1.919830 0.640691
6	-0.615052 2.420329 -1.685349	6	-3.209397 2.615534 0.303503
6	-2.089626 3.284907 0.031119	6	-0.967880 2.627167 1.218815
6	-0.399860 3.719176 -2.154705	6	-3.312124 3.991098 0.548403
1	-0.106762 1.589588 -2.164822	1	-4.046338 2.093866 -0.151964
6	-1.866229 4.585096 -0.435169	6	-1.076731 3.995431 1.475106
1	-2.748110 3.132476 0.881697	1	-0.046529 2.108445 1.473293
6	-1.024183 4.805528 -1.530616	6	-2.250058 4.683415 1.137803
1	0.263340 3.882271 -3.001271	1	-4.225457 4.517396 0.279294
1	-2.352279 5.423703 0.058630	1	-0.243469 4.526448 1.930236
1	-0.851032 5.816876 -1.891848	1	-2.332267 5.750896 1.330209
6	-3.123967 -0.145227 -1.130605	6	-3.379249 -0.418304 -0.474290
6	-3.981325 0.719611 -1.830646	6	-4.548074 -0.723419 0.244982
6	-3.316381 -1.533789 -1.243951	6	-3.398511 -0.504792 -1.876619
6	-5.015752 0.204233 -2.619692	6	-5.716350 -1.094960 -0.428283
1	-3.845101 1.795835 -1.767982	1	-4.552608 -0.678487 1.330668
6	-4.355827 -2.048116 -2.023828	6	-4.570431 -0.866573 -2.549310
1	-2.645422 -2.219045 -0.729395	1	-2.490078 -0.313010 -2.441074
6	-5.208172 -1.178639 -2.715052	6	-5.731924 -1.162277 -1.827007
1	-5.670467 0.885016 -3.159327	1	-6.613110 -1.332274 0.140098
1	-4.491855 -3.124580 -2.099896	1	-4.570107 -0.930075 -3.635243
1	-6.012646 -1.576784 -3.329452	1	-6.641272 -1.452223 -2.349060
Pld	6 -1.498364 -0.706273 -0.009943	Ple	6 1.409125 0.415639 0.137646
	6 -2.152723 0.546846 -0.860166	6	1.086582 -0.854106 -0.875282
	5 -2.298893 -1.058621 -1.505146	5	2.370280 0.227810 -1.298742
	5 -2.214270 0.616993 0.859319	5	0.910580 -1.100234 0.821165
	5 -3.590051 1.128849 -0.132619	5	1.620420 -2.346035 -0.221540
	5 -3.638203 0.104299 -1.587698	5	2.513104 -1.529437 -1.529176
	5 -4.042649 -1.594518 0.710298	5	3.766186 -0.834639 0.974927
	5 -2.529399 -2.092192 -0.086535	5	3.123291 0.655104 0.243192
	5 -2.471188 -1.063218 1.366785	5	2.220344 -0.151701 1.548925
	5 -3.926352 -1.583535 -1.078275	5	3.848209 -0.598020 -0.800648
	5 -4.738879 -0.232089 -0.224022	5	3.393682 -2.197269 -0.127362
	5 -3.839546 0.086700 1.293952	5	2.387987 -1.920836 1.331510

Species	Cartesian coordinates	Species	Cartesian coordinates
1	-1.611124 -1.328061 -2.425600	1	2.163505 0.986959 -2.178475
1	-1.489563 1.354806 1.416345	1	-0.171992 -1.153235 1.279145
1	-3.806244 2.289182 -0.221159	1	0.966262 -3.302269 -0.461858
1	-3.887451 0.585125 -2.640785	1	2.452498 -1.947676 -2.635338
1	-4.704385 -2.387090 1.295527	1	4.733194 -0.798025 1.661889
1	-2.029429 -3.160662 -0.080001	1	3.548068 1.747425 0.384167
1	-1.937481 -1.438584 2.351063	1	2.013568 0.400628 2.572359
1	-4.494667 -2.353691 -1.779117	1	4.857919 -0.394692 -1.389046
1	-5.905772 -0.037621 -0.318521	1	4.092303 -3.149468 -0.242440
1	-4.342189 0.501043 2.285490	1	2.356115 -2.656826 2.261129
6	0.791937 0.208772 -0.476604	6	-0.817587 1.395057 -0.446085
6	0.012914 -0.812981 -0.046474	6	0.398743 1.545278 0.125975
6	0.247382 1.537981 -0.989545	6	0.823737 2.857030 0.776462
6	-1.175631 1.453811 -1.594782	1	1.909982 2.951164 0.746535
1	-1.594422 2.460663 1.644634	1	0.441670 3.690714 0.181150
1	-1.092251 1.091716 -2.621976	6	-1.287274 0.100278 -1.093747
1	0.882145 1.815847 -1.837972	6	-0.169080 -0.742711 -1.729846
6	0.421135 2.729168 -0.031231	1	-0.546280 -1.746682 -1.933442
6	0.892831 2.620120 1.282465	1	0.103914 -0.293464 -2.686861
6	0.266977 5.025454 0.161636	1	-1.955844 0.374485 -1.922198
6	1.053259 3.778510 2.047040	6	-1.813015 2.537843 -0.561834
1	1.121239 1.649585 1.709129	1	-2.825145 2.132812 -0.460730
6	0.734468 5.013327 1.479415	6	0.351998 3.025283 2.236169
1	0.004730 5.966552 -0.321515	1	0.772548 2.254829 2.887033
1	1.417161 3.713664 3.070262	1	0.669443 4.000507 2.621365
1	0.841141 5.941579 2.034653	1	-0.738134 2.968671 2.314780
7	0.117262 3.919590 -0.580017	1	-1.695269 3.252732 0.254290
6	0.582058 -2.158734 0.299668	6	-1.702316 3.280422 -1.910226
6	1.017369 -3.008791 -0.730717	1	-2.466112 4.062431 -1.977745
6	0.682813 -2.601929 1.628096	1	-0.721200 3.752433 -2.025610
6	1.541441 -4.272029 -0.440458	1	-1.846988 2.603203 -2.759387
1	0.946481 -2.678486 -1.764307	6	-2.206259 -0.770188 -0.213773
6	1.209607 -3.863962 1.920076	8	-2.480861 -1.927957 -0.479377
1	0.363071 -1.955934 2.441295	8	-2.725283 -0.103732 0.830066
6	1.638496 -4.705160 0.886857	6	-3.655593 -0.843290 1.659316
1	1.874056 -4.916498 -1.251351	1	-3.160360 -1.712959 2.096468
1	1.287331 -4.187842 2.955711	1	-3.964751 -0.145409 2.436728
1	2.046737 -5.687468 1.114189	1	-4.514052 -1.167874 1.067289
6	2.285154 0.080378 -0.533144		
6	3.047971 -0.197514 0.614554		
6	2.961890 0.262883 -1.753487		
6	4.440704 -0.292355 0.545604		
1	2.552380 -0.336073 1.571163		
6	4.353809 0.155355 -1.827443		
1	2.399878 0.466754 -2.662775		
6	5.100726 -0.119210 -0.676175		
1	5.010069 -0.500968 1.448806		
1	4.853171 0.286005 -2.784968		
1	6.184359 -0.196014 -0.730586		

Table S10 The first three vibration frequencies for stationary points on potential energy surfaces from INT1_I and R3 to products P1 and P2, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)
TS2_I_1a	-242i 17 22	INT2_I_1a	11 21 33	TS3_I_1a	-117i 14 18	INT3_I_1a	14 21 28
TS4_I_1a	-295i 12 17	TS2_I_2a	-352i 15 24	INT2_I_2a	18 20 31	TS3_I_2a	-219i 14 21
INT3_I_2a	15 19 26	TS4_I_2a	-194i 12 18	TS2_I_1b	-219i 16 21	INT2_I_1b	8 13 28
TS3_I_1b	-86i 12 16	INT3_I_1b	9 15 19	TS4_I_1b	-290i 10 23	TS2_I_2b	-341i 13 24
INT2_I_2b	9 16 23	TS3_I_2b	-219i 14 17	INT3_I_2b	18 21 24	TS4_I_2b	-189i 10 16
TS2_I_3b	-196i 14 25	INT2_I_3b	12 22 29	TS3_I_3b	-106i 14 21	INT3_I_3b	13 17 20
TS4_I_3b	-288i 12 13	TS2_I_4b	-325i 21 22	INT2_I_4b	17 18 25	TS3_I_4b	-169i 14 21
INT3_I_4b	16 23 29	TS4_I_4b	-206i 14 18	TS2_I_1c	-217i 14 19	INT2_I_1c	9 18 23
TS3_I_1c	-89i 16 18	INT3_I_1c	11 18 23	TS4_I_1c	-289i 10 21	TS2_I_2c	-343i 15 21
INT2_I_2c	9 17 22	TS3_I_2c	-209i 15 18	INT3_I_2c	15 20 23	TS4_I_2c	-190i 11 21
TS2_I_3c	-212i 9 18	INT2_I_3c	13 17 21	TS3_I_3c	-107i 13 20	INT3_I_3c	16 16 21
TS4_I_3c	-278i 10 17	TS2_I_4c	-323i 20 24	INT2_I_4c	13 15 18	TS3_I_4c	-204i 14 21
INT3_I_4c	14 20 26	TS4_I_4c	-227i 16 20	TS2_I_1d	-188i 13 23	INT2_I_1d	13 19 24
TS3_I_1d	-79i 16 19	INT3_I_1d	11 15 22	TS4_I_1d	-275i 10 16	TS2_I_2d	-330i 18 26
INT2_I_2d	15 15 23	TS3_I_2d	-189i 17 18	INT3_I_2d	13 17 18	TS4_I_2d	-206i 13 14
TS2_I_1e	-287i 12 29	INT2_I_1e	16 26 28	TS3_I_1e	-92i 14 19	INT3_I_1e	13 18 20
TS4_I_1e	-295i 11 17	TS2_I_2e	-361i 22 28	INT2_I_2e	23 26 38	TS3_I_2e	-149i 16 25
INT3_I_2e	15 18 28	TS4_I_2e	-258i 10 18	CAT	6 15 16	P1a	32 43 62
P1b	31 35 54	P2b	27 33 54	P1c	24 32 35	P2c	23 31 37
P1d	23 29 49	P1e	39 50 66				

Table S11 The total energies (E : a.u.), zero-point energies (ZPE : kcal·mol⁻¹) and Gibbs free energies [G and $G(\text{sol}, 383\text{K})$: a.u.] for stationary points on potential energy surfaces from **INT1_I** and **R3** to products **P1** and **P2**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	E	ZPE	G	$G(\text{sol}, 383\text{K})$
TS2_I_1a	-3435.67013	437.94438	-3435.04569	-3435.06737
INT2_I_1a	-3435.70198	439.63000	-3435.07548	-3435.09627
TS3_I_1a	-3435.69668	439.09976	-3435.07155	-3435.09375
INT3_I_1a	-3435.70681	439.29400	-3435.08299	-3435.10594
TS4_I_1a	-3435.68980	438.34420	-3435.06620	-3435.08901
TS2_I_2a	-3435.63721	437.28894	-3435.01448	-3435.03587
INT2_I_2a	-3435.67665	438.76677	-3435.05096	-3435.07294
TS3_I_2a	-3435.66148	438.31562	-3435.03629	-3435.05800
INT3_I_2a	-3435.71015	439.61423	-3435.08382	-3435.10564
TS4_I_2a	-3435.69445	439.32801	-3435.06737	-3435.08870
TS2_I_1b	-3588.10129	453.17306	-3587.45477	-3587.47841
INT2_I_1b	-3588.14123	454.49826	-3587.49500	-3587.51928
TS3_I_1b	-3588.13722	454.22256	-3587.49131	-3587.51477
INT3_I_1b	-3588.15167	454.67378	-3587.50638	-3587.52961
TS4_I_1b	-3588.12408	453.25889	-3587.47868	-3587.50231
TS2_I_2b	-3588.06955	452.29083	-3587.42527	-3587.44768
INT2_I_2b	-3588.10921	453.52206	-3587.46416	-3587.48828
TS3_I_2b	-3588.09658	452.93743	-3587.45191	-3587.47484
INT3_I_2b	-3588.14719	454.39867	-3587.49938	-3587.52325
TS4_I_2b	-3588.12858	453.96741	-3587.48171	-3587.50503
TS2_I_3b	-3588.09936	453.09535	-3587.45289	-3587.47657
INT2_I_3b	-3588.13668	454.44009	-3587.49008	-3587.51393
TS3_I_3b	-3588.13461	453.92261	-3587.48936	-3587.51358
INT3_I_3b	-3588.14270	454.04466	-3587.49958	-3587.52441
TS4_I_3b	-3588.12127	453.08523	-3587.47747	-3587.50178
TS2_I_4b	-3588.07492	452.50169	-3587.42988	-3587.45152
INT2_I_4b	-3588.11011	453.84773	-3587.46282	-3587.48604
TS3_I_4b	-3588.10439	453.17310	-3587.45920	-3587.48336
INT3_I_4b	-3588.14772	454.73687	-3587.49946	-3587.52178
TS4_I_4b	-3588.13024	454.09022	-3587.48288	-3587.50602
TS2_I_1c	-3666.73649	488.61648	-3666.03833	-3666.06446
INT2_I_1c	-3666.77531	490.27092	-3666.07660	-3666.10291
TS3_I_1c	-3666.77157	489.98332	-3666.07207	-3666.09726
INT3_I_1c	-3666.78616	490.45316	-3666.08755	-3666.11398
TS4_I_1c	-3666.75837	488.93361	-3666.06075	-3666.08737
TS2_I_2c	-3666.70144	488.18870	-3666.00328	-3666.02890
INT2_I_2c	-3666.73855	489.09253	-3666.04063	-3666.06677
TS3_I_2c	-3666.72871	488.83052	-3666.03063	-3666.05510
INT3_I_2c	-3666.78134	490.03211	-3666.08147	-3666.10836
TS4_I_2c	-3666.76306	489.65094	-3666.06337	-3666.08836
TS2_I_3c	-3666.73406	488.40720	-3666.03682	-3666.06330
INT2_I_3c	-3666.77226	490.18865	-3666.07354	-3666.10050
TS3_I_3c	-3666.76485	489.70444	-3666.06581	-3666.09108
INT3_I_3c	-3666.78602	490.05304	-3666.08861	-3666.11516
TS4_I_3c	-3666.75734	488.82791	-3666.06026	-3666.08544
TS2_I_4c	-3666.70940	488.18984	-3666.01172	-3666.03795
INT2_I_4c	-3666.74133	489.24742	-3666.04324	-3666.06965
TS3_I_4c	-3666.73436	488.88383	-3666.03638	-3666.06126
INT3_I_4c	-3666.78196	490.46665	-3666.08112	-3666.10651
TS4_I_4c	-3666.76581	489.89410	-3666.06537	-3666.09023
TS2_I_1d	-3740.53141	468.18616	-3739.86330	-3739.88817
INT2_I_1d	-3740.57354	469.53023	-3739.90588	-3739.93088
TS3_I_1d	-3740.57064	469.11286	-3739.90338	-3739.92797
INT3_I_1d	-3740.58639	469.66918	-3739.91953	-3739.94574
TS4_I_1d	-3740.55580	468.03057	-3739.89002	-3739.91486
TS2_I_2d	-3740.50498	467.53136	-3739.83836	-3739.86227
INT2_I_2d	-3740.53999	468.15989	-3739.87421	-3739.89885
TS3_I_2d	-3740.53252	467.98058	-3739.86652	-3739.89089
INT3_I_2d	-3740.58457	468.89606	-3739.91984	-3739.94605
TS4_I_2d	-3740.56338	468.82389	-3739.89597	-3739.92003
TS2_I_1e	-3416.47247	422.04100	-3415.87279	-3415.89493
INT2_I_1e	-3416.50588	423.09091	-3415.90632	-3415.92844
TS3_I_1e	-3416.49809	422.90186	-3415.89859	-3415.92107
INT3_I_1e	-3416.50824	422.90225	-3415.91159	-3415.93376
TS4_I_1e	-3416.49141	421.94612	-3415.89449	-3415.91695

TS2_I_2e	-3416.44938	421.03050	-3415.85171	-3415.87422
INT2_I_2e	-3416.48423	422.60998	-3415.88330	-3415.90569
TS3_I_2e	-3416.47589	422.37138	-3415.87524	-3415.89714
INT3_I_2e	-3416.51359	423.28344	-3415.91374	-3415.93730
TS4_I_2e	-3416.49238	422.47236	-3415.89389	-3415.91589
CAT	-3580.76571	343.53280	-3580.29501	-3580.31504
P1a	-891.30878	268.62681	-890.92869	-890.93715
P1b	-1043.74263	283.37284	-1043.34215	-1043.34955
P2b	-1043.73919	283.57393	-1043.33829	-1043.34776
P1c	-1122.37701	319.05118	-1121.92428	-1121.93546
P2c	-1122.37509	319.30511	-1121.92141	-1121.93300
P1d	-1196.17225	298.24402	-1195.75107	-1195.76111
P1e	-872.11122	252.27379	-871.75691	-871.76499

Table S12 The optimized Cartesian coordinates (Å) for stationary points on potential energy surfaces from INT1_III and R2 to products P1, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	Cartesian coordinates				Species	Cartesian coordinates			
TS2_III_1a	6	2.335498	1.938735	-0.089477	INT2_III_1a	6	2.440373	-1.590744	0.069884
	6	0.691836	1.784008	0.307580		6	0.956388	-1.375673	-0.850268
	5	1.900200	1.879016	1.558886		5	2.525269	-1.140178	-1.580595
	5	1.145459	2.733335	-1.045521		5	1.081088	-2.599742	0.351740
	5	-0.080862	3.311815	0.084435		5	0.315267	-2.903416	-1.221301
	5	0.381822	2.763801	1.687809		5	1.215734	-1.973361	-2.422557
	5	2.422132	4.588882	0.760135		5	2.996929	-3.961986	-1.336281
	5	3.173230	2.987529	0.987818		5	3.643297	-2.349751	-0.916425
	5	2.702118	3.527103	-0.637969		5	2.733795	-3.286465	0.282953
	5	1.927383	3.551090	2.133980		5	2.881382	-2.612850	-2.503203
	5	0.696324	4.460215	1.207157		5	1.499677	-3.732401	-2.274387
	5	1.173121	4.430879	-0.517644		5	1.404483	-4.127934	-0.529021
	1	2.176175	0.941875	2.215769		1	2.902672	-0.059144	-1.872221
	1	0.944134	2.323538	-2.136283		1	0.498870	-2.479925	1.373280
	1	-1.210862	3.327538	-0.259226		1	-0.864314	-3.004834	-1.266600
	1	-0.428529	2.406656	2.474919		1	0.683356	-1.417149	-3.325068
	1	3.058840	5.582630	0.909025		1	3.734605	-4.882795	-1.486957
	1	4.298342	2.740052	1.258850		1	4.771494	-2.034776	-0.748226
	1	3.515344	3.673932	-1.484432		1	3.245947	-3.681169	1.269671
	1	2.200293	3.783590	3.267809		1	3.517714	-2.549437	-3.505436
	1	0.085944	5.361743	1.686649		1	1.147837	-4.488352	-3.122578
	1	0.914551	5.297654	-1.289568		1	0.993045	-5.161263	-0.109446
	6	2.796973	0.698309	-0.812349		28	0.082241	0.318086	-0.251082
	6	2.037608	-0.434270	-0.725920		15	-2.060274	0.128829	0.053748
	6	1.730601	-1.506957	0.949981		6	2.815142	-0.602545	1.194072
	6	0.378191	-2.005719	0.830794		6	2.567931	0.737337	1.237930
	28	0.227012	-0.164640	0.124348		6	3.516235	-1.247647	2.393499
	15	-2.017187	-0.304680	0.034585		1	3.349773	-0.630588	3.274434
	6	3.912470	0.861681	-1.831906		1	3.032411	-2.199103	2.620916
	1	3.960235	-0.024595	-2.464001		6	3.077551	1.608066	2.393403
	1	3.687186	1.701323	-2.498689		1	4.074848	1.277326	2.694353
	6	2.065459	-1.494522	-1.826175		1	3.213357	2.626827	2.016184
	1	3.090532	-1.807675	-2.054643		6	2.181031	1.694567	3.649668
	1	1.556397	-2.400535	-1.493753		1	1.257426	2.244060	3.452814
	6	1.366691	-1.027958	-3.117261		1	1.906188	0.707995	4.034410
	1	0.311112	-0.809383	-2.925499		1	2.714245	2.227883	4.444390
	1	1.824121	-0.126065	-3.533764		6	5.033851	-1.475786	2.250537
	1	1.411590	-1.815192	-3.878595		1	5.271947	-2.202177	1.471815
	6	5.307647	1.074378	-1.207725		1	5.553320	-0.542957	2.009096
	1	5.376418	2.017534	-0.662407		1	5.440511	-1.852436	3.195848
	1	5.551466	0.263133	-0.515313		6	1.765997	1.533522	0.210412
	1	6.064174	1.089687	-2.000538		6	0.387088	1.960311	0.655266
	1	1.892800	-0.842298	1.792669		6	-2.966195	1.596884	0.719671
	1	0.189292	-2.863120	0.189139		6	-2.824881	2.813935	0.027761
	1	-0.215509	-2.014940	1.744193		6	-3.813600	1.545712	1.836511
	6	2.957264	-2.375457	0.811168		6	-3.515897	3.953201	0.444377
	6	2.879506	-3.732019	0.459744		1	-2.177621	2.873193	-0.844701
	6	5.230920	-2.541841	1.157576		6	-4.499832	2.692038	2.259159
	6	4.047724	-4.498307	0.441465		1	-3.952677	0.616708	2.381271
	1	1.924458	-4.189647	0.222163		6	-4.353881	3.896915	1.566255
	6	5.255588	-3.893772	0.792206		1	-3.398028	4.885123	-0.104192
	1	6.149113	-2.038272	1.459927		1	-5.151758	2.636244	3.128264
	1	4.009364	-5.550358	0.167452		1	-4.888833	4.785417	1.894327
	1	6.190562	-4.448056	0.797968		6	-2.448456	-1.234496	1.226280
	7	4.120301	-1.797497	1.167193		6	-3.189715	-2.367755	0.859704
	6	-2.607020	-1.846415	-0.816633		6	-1.918571	-1.157202	2.528128
	6	-2.638925	-3.058758	-0.100572		6	-3.413765	-3.395559	1.783879
	6	-2.968195	-1.860595	-2.173489		1	-3.591175	-2.462146	-0.144792
	6	-3.023700	-4.247635	-0.724810		6	-2.152584	-2.177851	3.451852
	1	-2.382695	-3.081220	0.955062		1	-1.321659	-0.297931	2.827143
	6	-3.348377	-3.054056	-2.799820		6	-2.901907	-3.302015	3.081460
	1	-2.973398	-0.943161	-2.753041		1	-3.987415	-4.269771	1.483996
	6	-3.376747	-4.251738	-2.079966		1	-1.742243	-2.099957	4.456203
	1	-3.050551	-5.170485	-0.149325		1	-3.078315	-4.101212	3.797950

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -3.628691 -3.040187 -3.850837 1 -3.677042 -5.177443 -2.565786 6 -2.816669 1.046204 -0.930008 6 -3.980214 1.712434 -0.515392 6 -2.210767 1.427478 -2.140471 6 -4.535031 2.725874 -1.305620 1 -4.454869 1.460991 0.427797 6 -2.774406 2.426573 -2.937218 1 -1.282280 0.958918 -2.456359 6 -3.940289 3.079927 -2.521088 1 -5.432272 3.238953 -0.966429 1 -2.292436 2.706284 -3.871300 1 -4.374407 3.867103 -3.133558 6 -2.888668 -0.378991 1.653053 6 -4.230542 -0.791393 1.758384 6 -2.193578 -0.020696 2.818480 6 -4.863037 -0.829010 3.003164 1 -4.783267 -1.092852 0.871920 6 -2.827188 -0.060271 4.065718 1 -1.154588 0.288635 2.756209 6 -4.163020 -0.461943 4.160098 1 -5.901006 -1.147422 3.069940 1 -2.274558 0.220388 4.959499 1 -4.656372 -0.494658 5.129026		6 -3.002828 -0.205944 -1.491218 6 -4.410185 -0.205395 -1.498379 6 -2.312216 -0.417807 -2.693207 6 -5.109135 -0.433147 -2.685731 1 -4.964763 -0.021297 -0.581300 6 -3.014004 -0.639987 -3.883821 1 -1.227185 -0.407357 -2.702141 6 -4.411933 -0.651376 -3.881919 1 -6.196897 -0.434275 -2.679060 1 -2.465812 -0.802287 -4.809165 1 -4.958070 -0.823689 -4.806817 1 1.607926 0.806860 -0.677250 1 0.042646 2.899023 0.229736 1 0.160898 1.862098 1.714774 6 2.564503 2.596379 -0.575949 6 3.960533 2.515350 -0.681324 6 4.640949 3.478234 -1.429391 1 4.504607 1.714181 -0.190414 6 2.517325 4.468289 -1.918205 6 3.907358 4.483307 -2.063301 1 5.724297 3.437438 -1.519397 1 1.904290 5.226035 -2.405715 1 4.390583 5.253903 -2.658213 7 1.857239 3.552657 -1.194813
TS3_III_1a	5 0.741176 -3.365177 -0.639237 5 1.954912 -4.220117 -1.639286 5 3.288223 -3.147806 0.671064 5 3.534027 -4.069091 -0.821749 5 3.960139 -2.332140 -0.750940 5 2.635827 -1.433381 -1.520074 5 2.042822 -4.292978 0.148343 5 1.561878 -2.690097 0.775881 1 -0.413240 -3.620862 -0.554219 1 1.659963 -5.161999 -2.303447 1 3.930154 -3.278593 1.652003 1 4.388358 -4.895070 -0.878576 1 5.040652 -1.847621 -0.740286 1 2.840382 -0.402364 -2.056442 1 1.814658 -5.273686 0.780896 1 1.039189 -2.461585 1.814019 5 1.408011 -2.573355 -2.065033 1 0.725011 -2.267548 -2.986481 5 3.139977 -2.994642 -2.191054 1 3.693205 -3.035086 -3.242957 6 2.717809 -1.568609 0.190722 6 1.201137 -1.717751 -0.597082 28 -0.081118 -0.135148 -0.299846 6 0.229498 1.702753 -0.033323 6 1.723789 1.460980 -0.254276 6 2.945928 -0.363500 1.122210 6 2.467201 0.903948 0.969474 15 -2.192573 0.073262 0.005720 6 -3.071460 1.563862 -0.628437 6 -3.819541 1.526645 -1.816565 6 -2.942895 2.787228 0.056651 6 -4.428424 2.687274 -2.307957 1 -3.942104 0.595568 -2.361556 6 -3.554920 3.942896 -0.434154 1 -2.378885 2.843690 0.984058 6 -4.298010 3.897569 -1.620096 1 -5.007897 2.639821 -3.227246 1 -3.449956 4.878176 0.111095 1 -4.773637 4.798151 -2.001967 6 -3.000954 -1.350281 -0.834312 6 -4.077575 -2.054110 -0.269990 6 -2.513286 -1.735423 -2.095803 6 -4.665191 -3.115795 -0.965680 1 -4.459234 -1.786019 0.710914 6 -3.108285 -2.790805 -2.792350 1 -1.663897 -1.215674 -2.534111 6 -4.185527 -3.483530 -2.228219 1 -5.496274 -3.656365 -0.518194 1 -2.721373 -3.078317 -3.767225 1 -4.643463 -4.311130 -2.765441 6 -2.667693 -0.034828 1.776073 6 -1.773087 -0.640684 2.674276 6 -3.907862 0.429274 2.249703 6 -2.113683 -0.785331 4.022679 1 -0.810050 -1.000680 2.320936 6 -4.244378 0.286595 3.599148 1 -4.613220 0.904007 1.572481 6 -3.349080 -0.320991 4.487724 1 -1.412271 -1.255748 4.707971 1 -5.205885 0.650118 3.954716 1 -3.612481 -0.429242 5.537549 6 3.750527 -0.694489 2.381987 1 3.495963 0.005311 3.174019 1 3.459433 -1.673666 2.763951	INT3_III_1a	6 -2.808093 -1.511614 0.219536 6 -1.455643 -1.618429 -0.756618 5 -1.670360 -2.769907 0.502533 5 -2.952004 -1.124563 -1.442695 5 -1.863292 -2.221868 -2.300056 5 -1.072388 -3.252405 -1.096189 5 -3.894684 -3.801720 -1.005200 5 -3.414326 -3.122175 0.560016 5 -4.206287 -2.081011 -0.637041 5 -2.312579 -4.234703 -0.281569 5 -2.442694 -3.894669 -2.041907 5 -3.614594 -2.555166 -2.254469 1 -0.993031 -2.693031 1.472312 1 -3.149956 -0.006594 -1.747355 1 -1.264713 -1.810163 -3.237793 1 0.077733 -3.534197 -1.201327 1 -4.794526 -4.576324 -1.065416 1 -3.936423 -3.361819 1.590273 1 -5.247048 -1.564333 -0.412943 1 -2.068179 -5.307030 0.167967 1 -2.284321 -4.737605 -2.864825 1 -4.299238 -2.423902 -3.216864 28 0.143683 -0.672613 -0.399874 15 2.283840 -0.036181 -0.005505 6 -2.865957 -0.407286 1.274598 6 -2.365430 0.855107 1.182389 6 -3.538223 -0.847681 2.581208 1 -3.126650 -0.278388 3.412865 6 -1.539788 1.603334 0.116171 6 -0.687279 0.928927 -0.980472 6 -2.553425 1.816526 2.368639 1 -2.620907 2.836521 1.976262 1 -3.501053 1.645759 2.881799 6 -1.397574 1.778291 3.390351 1 -1.302863 0.794823 3.861934 1 -0.436342 2.012547 2.921639 1 -1.567360 2.516444 4.182271 1 -3.265545 -1.882677 2.792635 6 -5.073854 -0.721755 2.615199 1 -5.393075 0.306985 2.415440 1 -5.554667 -1.367789 1.877554 1 -5.450906 -1.005091 3.604615 1 -0.807931 2.144782 0.724990 1 -1.250051 0.713150 -1.887599 1 0.116111 1.621422 -1.252942 6 -2.346339 2.725501 -0.557240 6 -3.717191 2.620749 -0.839615 6 -4.362121 3.672376 -1.493210 1 -4.270070 1.736404 -0.539149 6 -2.262354 4.821752 -1.525640 6 -3.621257 4.801623 -1.851956 1 -5.425250 3.610622 -1.716770 1 -1.649530 5.687200 -1.778423 1 -4.078117 5.645981 -2.361724 7 -1.633866 3.819395 -0.893580 6 2.648542 1.271738 1.239589 6 3.351524 1.009669 2.425905 6 2.165143 2.573380 1.005272 6 3.569751 2.030091 3.359877 1 3.738324 0.014820 2.627809 6 2.389128 3.590217 1.936300 1 1.627586 2.807687 0.089284 6 3.090226 3.321052 3.118789 1 4.118860 1.812252 4.273311

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 5.280050 -0.656546 2.191237		1 2.013304 4.591416 1.737799
	1 5.779741 -0.847704 3.147800		1 3.262061 4.112874 3.844470
	1 5.626715 -1.406535 1.477400		6 3.157688 -1.542399 0.589563
	1 5.606151 0.325510 1.830987		6 4.423833 -1.934251 0.125010
	6 2.661103 1.958424 2.067357		6 2.493430 -2.351318 1.530940
	1 2.536153 2.949845 1.624650		6 5.017969 -3.107378 0.602713
	1 3.688835 1.938251 2.441449		1 4.948635 -1.332959 -0.612164
	6 1.685156 1.861233 3.261796		6 3.091547 -3.519560 2.011734
	1 1.733061 0.891379 3.764866		1 1.509492 -2.065830 1.900717
	1 1.924686 2.634476 4.000489		6 4.355587 -3.900709 1.546664
	1 0.648448 2.013261 2.950507		1 5.998235 -3.401562 0.234283
	1 1.799827 0.728135 -1.067771		1 2.567198 -4.133409 2.740529
	1 -0.215477 2.324100 -0.813106		1 4.819479 -4.813441 1.913822
	1 -0.043419 2.085589 0.950156		6 3.175701 0.499670 -1.518343
	6 2.456307 2.684733 -0.837685		6 4.320942 1.313433 -1.479182
	6 3.716472 2.514270 -1.435648		6 2.691646 0.054368 -2.760757
	6 4.374294 3.623731 -1.965668		6 4.974279 1.667625 -2.663759
	1 4.172546 1.529162 -1.478217		1 4.704298 1.676152 -0.528666
	6 2.504108 4.948664 -1.269792		6 3.350014 0.404428 -3.943574
	6 3.755409 4.875575 -1.884329		1 1.797052 -0.564514 -2.803937
	1 5.349632 3.513613 -2.435030		6 4.491917 1.212529 -3.896916
	1 1.989205 5.905266 -1.181926		1 5.859120 2.298949 -2.622656
	1 4.226113 5.770719 -2.282665		1 2.966038 0.053753 -4.898861
	7 1.862572 3.886085 -0.754821		1 5.000587 1.491143 -4.817196
TS4_III_1a	6 -2.673123 -1.829868 0.105078	TS2_III_2a	6 -3.437762 -0.352616 -0.129473
	6 -1.441232 -1.436789 -0.926182		6 -2.538171 1.113570 -0.348906
	5 -1.061700 -2.424252 0.504105		5 -4.018071 0.886482 -1.179212
	5 -2.991286 -1.780664 -1.596187		5 -2.570239 0.341037 1.204419
	5 -1.509550 -2.388000 -2.349827		5 -2.729938 2.093972 1.051899
	5 -0.317777 -2.822613 -1.079648		5 -3.670812 2.447283 -0.401267
	5 -2.617982 -4.506257 -0.741316		5 -5.375287 0.970655 1.375371
	5 -2.480750 -3.466942 0.697864		5 -5.106034 -0.020999 -0.083370
	5 -3.657173 -3.072912 -0.580378		5 -4.199191 -0.362135 1.406626
	5 -1.008802 -4.104140 -0.071288		5 -5.280278 1.740197 -0.242222
	5 -1.276013 -4.091445 -1.852022		5 -4.479094 2.497350 1.170940
	5 -2.925850 -3.454787 -2.160091		5 -3.785866 1.193780 2.175302
	1 -0.544226 -1.941874 1.458288		1 -3.983871 0.706511 -2.345788
	1 -3.653013 -0.894048 -2.006567		1 -1.622523 -0.206397 1.637623
	1 -1.138044 -1.881120 -3.355256		1 -1.821806 2.771726 1.388301
	1 0.846593 -2.639694 -1.280685		1 -3.417831 3.376075 -1.088596
	1 -3.080386 -5.596945 -0.655927		1 -6.392591 0.894046 1.983769
	1 -2.843064 -3.734217 1.790023		1 -5.855080 -0.807710 -0.547022
	1 -4.815128 -3.055741 -0.347674		1 -4.282047 -1.411603 1.948992
	1 -0.324343 -4.894301 0.492726		1 -6.211763 2.214445 -0.805181
	1 -0.766926 -4.877044 -2.583175		1 -4.828149 3.535979 1.629323
	1 -3.596077 -3.782477 -3.083742		1 -3.642989 1.274807 3.351445
	6 -3.271088 -0.756553 1.000096		6 -2.842588 -1.601673 -0.718225
	6 -2.896387 0.546379 1.007853		6 -1.490425 -1.724736 -0.746378
	6 -1.908474 1.252111 0.078364		6 -1.243203 1.724083 -1.703813
	6 -1.303059 0.474979 -1.095452		6 0.195084 1.589506 -1.568353
	28 0.223978 -0.749168 -0.454082		28 -0.501671 -0.064601 -0.603492
	15 2.230382 0.042588 0.043149		15 1.446711 -0.676157 0.200934
	6 -4.370335 -1.248685 1.948360		6 -3.829132 -2.641323 -1.247156
	1 -4.304965 -2.328497 2.071379		1 -3.350224 -3.619900 -1.233313
	1 -4.209624 -0.835904 2.948053		1 -4.687227 -2.722477 -0.570804
	6 -3.405093 1.486219 2.102627		6 -0.852851 -3.019803 -1.239146
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	1 -5.951886 0.173544 1.377806		1 -0.533519 -3.928032 0.728804
	1 -6.021578 -1.361729 0.510914		1 -1.975115 -4.523615 -0.086099
	1 -6.532723 -1.281589 2.202406		1 -0.377108 -5.058699 -0.622412
	6 -2.477948 1.507724 3.336516		6 -4.338868 -2.384310 -2.680366
	1 -2.875185 2.189166 4.096775		1 -4.923654 -1.464533 -2.754810
	1 -2.385763 0.513794 3.786976		1 -3.502784 -2.308132 -3.384112
	1 -1.472882 1.855554 3.077067		1 -4.979608 -3.212325 -3.005580
	1 -1.079240 1.600492 0.705456		1 0.665022 1.048113 -2.388342
	1 -0.400070 0.992114 -1.457789		1 -1.628573 2.723968 -1.557379
	1 -1.970479 0.455023 -1.952049		1 -1.697452 1.237216 -2.563149
	6 -2.509462 2.531454 -0.521255		6 1.027854 2.751875 -1.185522
	6 -3.726458 2.511160 -1.223434		6 0.614764 3.753585 -0.282812
	6 -2.249332 4.784780 -0.937805		6 3.009201 3.889547 -1.573288
	6 -4.202420 3.691154 -1.793714		6 1.437294 4.852378 -0.050687
	1 -4.291678 1.586494 -1.310445		1 -0.334873 3.669982 0.233837
	6 -3.447584 4.860539 -1.650911		6 2.667415 4.934892 -0.712374
	1 -1.632307 5.672828 -0.802354		1 3.962125 3.906191 -2.103478
	1 -5.144506 3.700106 -2.337957		1 1.125550 5.632286 0.641199
	1 -3.775992 5.805344 -2.076337		1 3.342158 5.774011 -0.564527
	7 -1.782893 3.653790 -0.381878		7 2.225707 2.829152 -1.813402
	6 2.602098 1.656912 -0.773529		6 1.502829 -2.145346 1.341024
	6 2.305548 1.765705 -2.145753		6 2.189109 -3.323651 1.000964
	6 3.121072 2.775601 -0.103493		6 0.818447 -2.104279 2.570130
	6 2.549181 2.955367 -2.836625		6 2.216497 -4.415626 1.876483
	1 1.889375 0.912650 -2.680009		1 2.701642 -3.410751 0.049300
	6 3.351225 3.972832 -0.793121		6 0.844539 -3.194544 3.442698
	1 3.345694 2.724207 0.958033		1 0.257730 -1.224566 2.865889
	6 3.072229 4.065099 -2.160355		6 1.549751 -4.355217 3.102514
	1 2.322782 3.018306 -3.898829		1 2.756595 -5.315348 1.589953

Species	Cartesian coordinates			Species	Cartesian coordinates		
	1	3.750162	4.832079 -0.258141		1	0.309897 -3.135563	4.388165
	1	3.254517	4.995003 -2.694544		1	1.570959 -5.203777	3.782667
	6	2.589356	0.321404 1.832894		6	2.734717 -1.073312	-1.052295
	6	3.896815	0.384667 2.346427		6	4.069554 -1.352567	-0.697722
	6	1.506809	0.465926 2.715642		6	2.364724 -1.166814	-2.403288
	6	4.113361	0.600900 3.710735		6	5.010236 -1.683659	-1.675481
	1	4.750753	0.258025 1.685536		1	4.378887 -1.335186	0.343676
	6	1.721910	0.686716 4.080428		6	3.304944 -1.506070	-3.382108
	1	0.491810	0.394424 2.332185		1	1.335011 -0.986008	-2.697902
	6	3.026626	0.755245 4.580800		6	4.631679 -1.757347	-3.021844
	1	5.130329	0.645927 4.094541		1	6.037051 -1.891832	-1.383162
	1	0.872974	0.795921 4.751740		1	2.997030 -1.573197	-4.423026
	1	3.196646	0.920419 5.642507		1	5.365187 -2.017623	-3.781718
	6	3.639319	-1.041081 -0.475891		6	2.103243 0.690093	1.269964
	6	4.743543	-0.584765 -1.212804		6	3.385537 1.243780	1.129026
	6	3.588319	-2.395988 -0.099729		6	1.257587 1.208568	2.268726
	6	5.775024	-1.464491 -1.565709		6	3.828531 2.245553	2.000174
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	1	2.739879	-2.770869 0.468924		1	0.233873 0.860465	2.360686
	6	5.719406	-2.807577 -1.180211		6	2.998817 2.715793	3.021159
	1	6.622545	-1.095436 -2.139500		1	4.825126 2.661414	1.869604
	1	4.568890	-4.313735 -0.137530		1	1.032970 2.577811	3.912726
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	5	2.884620	-2.492184 -1.835418		5	-3.309687 -1.151767	2.283748
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	1	1.766785	-3.082635 -4.117787		1	-2.662095 -0.808489	4.779332
	1	-0.082561	-5.002952 -2.585506		1	-0.749242 -3.210747	4.487605
	1	1.005878	-5.241396 0.294765		1	-1.349656 -4.536415	1.761129
	6	2.531538	-0.468414 0.211227	28	0.392442	0.505988	0.317955
	6	1.722402	0.621394 0.350583	15	2.364605	-0.196971	-0.267221
	6	1.025884	1.807116 -1.112784	6	-2.739286	-0.095203	-0.277729
	6	-0.288104	2.200064 -0.638281	6	-2.291930	1.093080	-0.767665
28	-0.186782	0.269234	-0.259673	6	-2.942518	1.746741	-1.989669
15	-2.395228	0.172374	0.154960	1	-4.015149	1.542304	-1.983272
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1	1.618699	2.583498	1.297569	1	-1.342853	1.647425	-3.500963
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1	1.225460	1.809570	3.595034	6	0.150900	1.869468	-0.985383
1	1.008037	1.256709	-2.050828	6	3.361603	0.885085	-1.386575
1	-0.355376	2.919594	0.175268	6	3.529291	2.229259	-1.006694
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6	2.131058	4.067960	-0.731060	1	3.044796	2.606036	-0.108314
6	4.346926	3.083242	-1.975547	6	4.786801	1.289398	-3.316645
6	3.226391	4.915677	-0.914529	1	3.899850	-0.613978	-2.855846
1	1.220816	4.442735	-0.273499	6	4.948376	2.623497	-2.932335
6	4.365508	4.416171	-1.546955	1	4.441107	4.126281	-1.461133
1	5.209317	2.661045	-2.491421	1	5.274181	0.915989	-4.214695
1	3.182803	5.949015	-0.577471	1	5.559753	3.295260	-3.530824
1	5.241448	5.036459	-1.718207	6	2.251685	-1.809788	-1.143372
7	3.307678	2.260775	-1.795635	6	2.775950	-2.999924	-0.617305
6	-2.998592	1.516477	1.285353	6	1.536420	-1.855951	-2.355086
6	-3.224861	2.805575	0.765094	6	2.605897	-4.210359	-1.300286
6	-3.184690	1.308223	2.661567	1	3.313244	-2.995522	0.326243
6	-3.626635	3.852215	1.598103	6	1.375562	-3.062587	-3.039068
1	-3.109431	2.998508	-0.297718	1	1.105689	-0.948426	-2.773081
6	-3.582227	2.359607	3.496794	6	1.910749	-4.245402	-2.512592
1	-3.038089	0.324729	3.095842	1	3.016176	-5.125256	-0.878545
6	-3.803397	3.635084	2.970187	1	0.827556	-3.080377	-3.978552
1	-3.804966	4.837295	1.172270	1	1.780573	-5.186883	-3.041569
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1	-4.116756	4.450218	3.618635	6	4.869802	-0.797334	0.920157
6	-2.938961	-1.370835	1.000192	6	3.099533	-0.153387	2.445159
6	-4.080907	-2.096428	0.627341	6	5.751108	-0.921651	1.996099
6	-2.151002	-1.842566	2.065227	1	5.230694	-0.988060	-0.087815
6	-4.434999	-3.261541	1.317273	6	3.985852	-0.271364	3.522276
1	-4.693326	-1.772361	-0.208206	1	2.072778	0.149378	2.623360

Species	Cartesian coordinates	Species	Cartesian coordinates
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Species	Cartesian coordinates	Species	Cartesian coordinates
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Species	Cartesian coordinates	Species	Cartesian coordinates
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Species	Cartesian coordinates	Species	Cartesian coordinates
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Species	Cartesian coordinates	Species	Cartesian coordinates
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TS4_III_1c	6 -2.140297 -1.780799 -0.707286 6 -0.703693 -1.504100 -1.474561 5 -0.699072 -2.411604 0.070418 5 -2.089686 -1.831483 -2.439756 5 -0.515446 -2.551383 -2.813540 5 0.346878 -2.943816 -1.287925 5 -2.067695 -4.501601 -1.368480 5 -2.189746 -3.374010 0.002923 5 -3.034285 -3.016279 -1.522702 5 -0.621303 -4.125156 -0.383978 5 -0.494060 -4.222996 -2.176620 5 -1.998548 -3.539436 -2.877400 1 -0.372555 -1.888853 1.086996 1 -2.597510 -0.948322 -3.034147 1 0.093078 -2.131291 -3.740491 1 1.533863 -2.825350 -1.240670 1 -2.598106 -5.563388 -1.323236 1 -2.811843 -3.535762 0.991316 1 -4.211182 -2.924315 -1.549905 1 -0.119774 -4.905097 0.358440 1 0.115385 -5.077961 -2.732201 1 -2.469790 -3.899657 -3.906031 6 -2.844383 -0.613412 -0.037479 6 -2.498546 0.691863 -0.152123 6 -1.314376 1.281921 -0.921151 6 -0.431437 0.370378 -1.784530 28 0.813975 -0.823819 -0.647659 15 2.680442 -0.076680 0.276643 6 -3.264862 1.755654 0.630004 1 -3.415621 2.633875 -0.006854 1 -4.260342 1.391926 0.888657 6 -2.561163 2.217388 1.925531	TS2_III_2c	6 2.190883 -1.982875 0.313823 6 0.645415 -2.573000 -0.274532 5 2.102557 -3.265953 -0.837682 5 0.818915 -2.041012 1.368160 5 -0.084567 -3.507775 0.966855 5 0.733060 -4.311204 -0.379414 5 2.566933 -4.281582 1.831138 5 3.264588 -3.276946 0.529047 5 2.454808 -2.508318 1.915037 5 2.368700 -4.757839 0.113227 5 1.000906 -4.912621 1.262393 5 1.039413 -3.500685 2.354286 1 2.435492 -3.046639 -1.950239 1 0.304781 -1.055670 1.757916 1 -1.260160 -3.472976 1.071638 1 0.123175 -4.851311 -1.237875 1 3.268407 -4.879319 2.580285 1 4.408400 -3.099479 0.299505 1 3.025645 -1.761889 2.634846 1 2.921484 -5.683628 -0.383424 1 0.552842 -5.961151 1.594236 1 0.632809 -3.522027 3.469439 6 2.590556 -0.639327 -0.231201 6 1.611316 0.250292 -0.523753 6 -0.419486 -2.128265 -1.847725 6 -1.624359 -1.323185 -1.696127 28 -0.198798 -0.453485 -0.494435 15 -1.288155 1.260251 0.350861 6 1.885092 1.567442 -1.246578 1 2.225648 1.321850 -2.263997 1 0.940346 2.101661 -1.388816 6 2.883557 2.574190 -0.635312

Species	Cartesian coordinates				Species	Cartesian coordinates			
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	1	0.561253	0.833768	-1.903909	1	-0.569717	-3.188809	-2.000424	
	1	-0.812533	0.273269	-2.796729	1	0.342672	-1.750975	-2.528179	
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	6	-2.730718	2.357226	-2.771631	6	-3.170663	-3.274893	-1.114455	
	6	-1.291016	4.647220	-2.430609	6	-5.231617	-1.703321	-1.949838	
	6	-3.017640	3.452382	-3.585636	6	-4.461748	-3.796045	-1.091464	
	1	-3.289664	1.430350	-2.873458	1	-2.342142	-3.893644	-0.791200	
	6	-2.280840	4.629451	-3.415465	6	-5.529423	-2.998319	-1.517669	
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	1	-2.466769	5.510222	-4.024673	1	-6.553029	-3.363401	-1.521199	
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	6	1.331477	0.781559	2.574382	6	-1.852415	2.335211	-2.179201	
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	1	0.456586	0.762286	1.928523	1	-0.995401	1.758236	-2.516009	
	6	2.319051	1.175559	4.752319	6	-3.656182	3.871575	-2.687355	
	1	4.440397	0.785927	4.898229	1	-4.944709	4.378384	-1.026626	
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	1	2.218155	1.470884	5.794439	1	-4.196954	4.487734	-3.402296	
	6	4.082496	-1.284998	0.264359	6	-2.530606	0.673684	1.590797	
	6	5.376733	-0.970824	-0.179437	6	-3.732801	0.106736	1.130402	
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	6	-4.010867	-1.001957	0.835566	6	4.051488	-0.455320	-0.533506	
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	6	-3.827097	-1.268329	2.202256	6	4.977610	-0.172441	0.486118	
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	1	-5.473947	-0.862107	-0.746627	1	3.824359	-0.782941	-2.655707	
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	1	-2.828318	-1.219759	2.629836	1	4.632862	-0.084672	1.513673	
	6	-6.202534	-1.672052	2.482671	6	6.789469	-0.087113	-1.125315	
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	1	-7.047545	-1.929083	3.117693	1	7.843411	0.057096	-1.353173	
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	6	-2.699644	3.741997	3.979313	6	3.956937	4.887062	-0.875375	
	1	-1.716369	4.183755	3.778977	1	4.971587	4.474471	-0.824418	
	1	-3.304573	4.496952	4.493768	1	3.998464	5.797621	-1.484147	
	1	-2.553555	2.905308	4.673038	1	3.666366	5.178556	0.140819	
TS2_III_1d	6	1.674217	2.158100	0.437352	INT2_III_1d	6	1.601942	-1.808545	-0.873946
	6	0.005114	1.959662	0.565104		6	-0.078998	-1.573410	-1.302635
	5	0.979323	2.227478	1.990283		5	1.181446	-1.538297	-2.509176
	5	0.650362	2.803093	-0.781980		5	0.367229	-2.672446	-0.054488
	5	-0.764525	3.423314	0.071009		5	-0.863094	-3.081393	-1.265509
	5	-0.563191	3.046618	1.775746		5	-0.353595	-2.356561	-2.791898
	5	1.550922	4.871195	1.016501		5	1.605211	-4.346012	-2.062320
	5	2.300289	3.332444	1.518311		5	2.410379	-2.751020	-2.066710
	5	2.091771	3.701078	-0.206992		5	1.890126	-3.482912	-0.536717
	5	0.865124	3.943644	2.388485		5	1.179875	-3.124957	-3.299077
	5	-0.221505	4.704286	1.187075		5	-0.101665	-4.106173	-2.517481
	5	0.537893	4.540576	-0.425239		5	0.341231	-4.304037	-0.791912
	1	1.180165	1.362477	2.762770		1	1.482269	-0.522871	-3.031268
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	1	-1.821624	3.355875	-0.451229		1	-2.000370	-3.097895	-0.934409
	1	-1.484595	2.727931	2.449381		1	-1.123838	-1.863475	-3.547640
	1	2.123062	5.902522	1.171003		1	2.221401	-5.330438	-2.318628
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	1	3.030505	3.787587	-0.918728		1	2.672820	-3.776100	0.293522
	1	0.937524	4.293611	3.522611		1	1.471157	-3.219937	-4.447781
	1	-0.931006	5.616669	1.468579		1	-0.730921	-4.920094	-3.114218
	1	0.384074	5.319915	-1.309902		1	0.041348	-5.251872	-0.140395

Species	Cartesian coordinates	Species	Cartesian coordinates
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	6 1.651725 -0.303970 0.028387		15 -2.576052 0.216665 0.349531
	6 0.916490 -1.207612 1.673345		6 2.359796 -0.746476 -0.055516
	6 -0.313456 -1.824317 1.208311		6 2.174155 0.600302 -0.033640
	28 -0.355688 -0.022467 0.419506		6 1.135758 1.387393 -0.843074
	15 -2.520812 -0.255013 -0.107545		6 -0.031321 1.921680 -0.048149
	1 0.768077 -0.453912 2.444194		6 -3.195540 1.809252 1.053902
	1 -0.237640 -2.702020 0.570711		6 -3.255666 2.918512 0.190475
	1 -1.119144 -1.886055 1.938785		6 -3.654765 1.949324 2.371961
	6 2.151404 -1.983333 2.049897		6 -3.761753 4.140551 0.636808
	6 2.214751 -3.377764 1.914885		1 -2.912222 2.828295 -0.837900
	6 4.200538 -1.934222 3.103580		6 -4.154486 3.178783 2.821529
	6 3.336203 -4.055868 2.398282		1 -3.635097 1.106199 3.055968
	1 1.400695 -3.923972 1.450054		6 -4.209220 4.276160 1.957847
	6 4.357399 -3.322600 3.003786		1 -3.803379 4.987420 -0.044598
	1 4.970001 -1.327536 3.580776		1 -4.504501 3.272017 3.847307
	1 3.407024 -5.137093 2.302918		1 -4.598689 5.229533 2.307976
	1 5.249136 -3.803914 3.397078		6 -2.570910 -0.959567 1.763452
	7 3.130621 -1.275547 2.644839		6 -3.370762 -2.111388 1.797009
	6 -2.928069 -1.864461 -0.940091		6 -1.668030 -0.724272 2.817949
	6 -3.071278 -3.028177 -0.159938		6 -3.283605 -3.001680 2.874269
	6 -3.049757 -1.974783 -2.334842		1 -4.060192 -2.327132 0.986366
	6 -3.329264 -4.263137 -0.759086		6 -1.591002 -1.607187 3.896808
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	6 -3.303400 -3.214424 -2.934820		6 -2.399586 -2.750835 3.927655
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	1 -3.445300 -5.146934 -0.135470		1 -2.334766 -3.443188 4.764057
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	1 -3.644630 -5.324878 -2.617354		6 -5.303751 -0.214058 -0.288559
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	1 -4.326261 3.636368 -3.925851		1 -0.460945 2.835522 -0.449813
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	6 -3.196493 0.215423 2.573619		6 2.828575 1.959606 -2.671662
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	6 3.590921 1.091512 -2.237437		6 3.158755 -1.730516 2.140798
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	6 4.786636 1.267060 -2.939913		6 4.166160 -2.253693 2.955824
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	6 5.996679 1.406828 -2.249572		6 5.474938 -2.369750 2.472071
	1 6.935310 1.472779 -0.303527		1 6.781278 -2.031051 0.784109
	1 4.772842 1.294727 -4.027516		1 3.928336 -2.571611 3.968837
	1 6.927021 1.543636 -2.796587		1 6.259397 -2.778471 3.105339
	6 2.045772 -1.441621 -0.862883		6 2.968877 1.465931 0.910745
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	1 -1.018509 -2.675327 -3.115239		1 -3.349233 -3.658942 0.617143
	5 1.419028 -3.680531 -2.881670		1 -4.057316 -2.529805 -2.060867
	1 1.658337 -3.896324 -4.026315		1 -0.921575 -5.510356 0.326587
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	28 -0.803056 -0.242350 -0.527102		28 0.935804 -0.827960 -0.523178
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	6 -4.587536 1.882769 -1.067735		1 -0.126980 0.224770 -2.498806
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	6 4.143567 3.544681 2.213509		6 -4.235249 3.564034 2.271521
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	5 -0.150566 -2.257831 -3.100532		5 -0.388355 3.704470 0.612942
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Species	Cartesian coordinates	Species	Cartesian coordinates
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	5 -2.592390 -3.115596 -1.863807		5 -2.751271 2.540060 1.799548
	5 -0.068053 -4.126038 -0.887490		5 -3.002976 4.496869 -0.302782
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	5 -1.536984 -3.364333 -3.279254		5 -1.465620 3.752586 2.033895
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	6 -5.836987 -2.422909 1.266604		6 -6.046255 -0.601940 -1.609159
	1 -5.176374 -1.685483 -0.643351		1 -4.121030 0.024035 -2.349299
	6 -4.229392 -2.297866 3.067971		6 -6.257054 -0.751140 0.795015
	1 -2.306534 -1.471545 2.557976		1 -4.499991 -0.240758 1.930089
	6 -5.504781 -2.645484 2.607734		6 -6.822327 -0.883918 -0.478915
	1 -6.828195 -2.680667 0.899484		1 -6.474358 -0.704949 -2.604242
	1 -3.960585 -2.462233 4.109330		1 -6.849477 -0.972029 1.680609
	1 -6.233324 -3.081397 3.287899		1 -7.855624 -1.205785 -0.589540
	6 -3.218616 1.306675 0.817870		6 -1.820923 -1.804286 -0.757764
	6 -4.572471 1.546216 0.530385		6 -1.464882 -2.142462 -2.079452
	6 -2.647718 1.954310 1.926697		6 -2.355593 -2.819571 0.059817
	6 -5.336996 2.396393 1.334598		6 -1.668625 -3.431759 -2.577034
	1 -5.030980 1.067750 -0.330731		1 -1.039052 -1.378425 -2.727303
	6 -3.412007 2.797887 2.738931		6 -2.540940 -4.115703 -0.430377
	1 -1.599254 1.794906 2.168650		1 -2.636998 -2.589653 1.083364
	6 -4.761487 3.023753 2.445373		6 -2.206544 -4.428286 -1.753789
	1 -6.383464 2.568989 1.091924		1 -1.396543 -3.661329 -3.605172

Species	Cartesian coordinates				Species	Cartesian coordinates			
	1	-2.951446	3.279725	3.598746		1	-2.958229	-4.881257	0.221090
	1	-5.356593	3.683498	3.072975		1	-2.359695	-5.434991	-2.136615
TS2_III_1e	6	-2.915142	-1.164554	-0.018982	INT2_III_1e	6	2.691028	-1.100009	0.196188
	6	-1.265734	-1.450562	0.274029		6	1.154836	-1.305773	-0.633249
	5	-2.399504	-1.364146	1.595393		5	2.650151	-1.1114295	-1.516473
	5	-2.004466	-2.132997	-1.114275		5	1.480194	-2.133127	0.838790
	5	-0.906648	-3.092862	-0.118773		5	0.689866	-2.935490	-0.534633
	5	-1.141440	-2.597392	1.550448		5	1.416739	-2.280117	-2.004859
	5	-3.612758	-3.780684	0.627458		5	3.474140	-3.692444	-0.562371
	5	-3.933363	-2.073309	1.029045		5	3.935760	-1.967360	-0.638535
	5	-3.689104	-2.559014	-0.662466		5	3.200273	-2.630804	0.832220
	5	-2.811399	-3.024226	2.040014		5	3.143531	-2.735929	-2.035828
	5	-1.889152	-4.115604	0.963165		5	1.920648	-3.890193	-1.413302
	5	-2.426578	-3.813338	-0.717579		5	1.950392	-3.799590	0.376537
	1	-2.403659	-0.452841	2.341365		1	2.880187	-0.121477	-2.115564
	1	-1.759295	-1.684658	-2.180391		1	0.932226	-1.800024	1.831265
	1	0.166358	-3.349428	-0.539483		1	-0.469237	-3.169421	-0.462845
	1	-0.231164	-2.519931	2.304494		1	0.781534	-2.051874	-2.980216
	1	-4.467142	-4.599688	0.743497		1	4.311976	-4.535209	-0.516390
	1	-4.947400	-1.585601	1.395282		1	5.022014	-1.499065	-0.646985
	1	-4.553133	-2.424968	-1.459112		1	3.798731	-2.682069	1.847406
	1	-3.078479	-3.285855	3.168496		1	3.723269	-2.881574	-3.063259
	1	-1.498726	-5.177847	1.328667		1	1.628351	-4.882716	-1.999560
	1	-2.427247	-4.641515	-1.570418		1	1.687122	-4.715900	1.086304
	6	-3.083463	0.208361	-0.617116		28	0.097207	0.382517	-0.455744
	6	-2.046499	1.093032	-0.518443		15	-1.991359	0.052771	0.041482
	6	-1.417620	1.883551	1.206805		6	2.980151	0.192116	0.986948
	6	0.008451	2.075459	1.110112		6	2.559044	1.454288	0.694651
	28	-0.336400	0.331453	0.217533		6	2.968143	2.659697	1.548057
	15	1.875688	-0.062577	0.001329		1	4.015312	2.561644	1.844532
	6	-4.266848	0.438749	-1.541028		1	2.934266	3.553324	0.917027
	1	-4.100500	1.341493	-2.128568		6	2.112817	2.940887	2.804042
	1	-4.350643	-0.384334	-2.258202		1	1.100933	3.262393	2.545102
	6	-1.831251	2.205952	-1.544205		1	2.025639	2.065303	3.453890
	1	-2.733278	2.819883	-1.661242		1	2.571057	3.747074	3.387393
	1	-1.056634	2.891915	-1.199660		6	1.640029	1.831644	-0.460987
	6	-1.393562	1.669358	-2.920082		6	0.223749	2.243959	-0.110940
	1	-0.438889	1.139883	-2.840630		6	-3.031516	1.543255	0.378695
	1	-2.123801	0.977994	-3.349262		6	-3.097060	2.528330	-0.624102
	1	-1.256996	2.499753	-3.621892		6	-3.779092	1.718745	1.552617
	6	-5.607948	0.598578	-0.792308		6	-3.891698	3.663444	-0.454810
	1	-5.901917	-0.317335	-0.275867		1	-2.532660	2.407344	-1.546357
	1	-5.548399	1.403178	-0.052696		6	-4.570052	2.862642	1.724771
	1	-6.398462	0.848532	-1.508744		1	-3.760237	0.967861	2.336618
	1	-1.757111	1.241675	2.013020		6	-4.628759	3.836738	0.724536
	1	0.372266	2.936293	0.557338		1	-3.933969	4.413202	-1.241772
	1	0.599445	1.829801	1.990814		1	-5.142905	2.984573	2.641482
	6	-2.394465	3.047336	1.154526		1	-5.244756	4.723112	0.858972
	6	2.779075	1.359292	-0.778064		6	-2.166870	-0.997371	1.540457
	6	3.123745	2.471764	0.013753		6	-2.808554	-2.244890	1.524504
	6	3.084559	1.390402	-2.148113		6	-1.581570	-0.545402	2.738104
	6	3.757397	3.580888	-0.550907		6	-2.881610	-3.016784	2.690328
	1	2.918872	2.473179	1.080735		1	-3.248651	-2.626850	0.608320
	6	3.714664	2.505687	-2.714065		6	-1.665947	-1.311289	3.902577
	1	2.851173	0.543907	-2.785650		1	-1.058293	0.408329	2.767050
	6	4.052249	3.604862	-1.919740		6	-2.317251	-2.551213	3.881678
	1	4.022977	4.425408	0.081294		1	-3.379120	-3.983662	2.662010
	1	3.945859	2.506560	-3.777015		1	-1.214890	-0.944954	4.822045
	1	4.545813	4.468792	-2.359172		1	-2.376631	-3.152206	4.786354
	6	2.282280	-1.485463	-1.095041		6	-2.941652	-0.762071	-1.305998
	6	3.263478	-2.441061	-0.788583		6	-4.340476	-0.895900	-1.226234
	6	1.559236	-1.614132	-2.294295		6	-2.273788	-1.217543	-2.451847
	6	3.526538	-3.493066	-1.673637		6	-5.051282	-1.493621	-2.269038
	1	3.819126	-2.384231	0.142112		1	-4.879607	-0.528995	-0.356036
	6	1.834338	-2.653881	-3.185160		6	-2.988424	-1.811157	-3.498786
	1	0.762202	-0.913345	-2.529036		1	-1.197167	-1.107836	-2.530362
	6	2.820343	-3.598217	-2.876360		6	-4.376219	-1.953027	-3.408209
	1	4.283900	-4.230968	-1.418346		1	-6.131791	-1.595208	-2.195732
	1	1.266207	-2.735878	-4.108993		1	-2.458300	-2.159218	-4.382447
	1	3.027933	-4.416256	-3.562576		1	-4.932349	-2.413647	-4.221775
	6	2.800773	-0.328550	1.567897		1	1.555688	0.891113	-1.120489
	6	4.204497	-0.240277	1.624788		1	-0.220961	2.953895	-0.805915
	6	2.089055	-0.626493	2.740284		1	0.031904	2.496064	0.929178
	6	4.877823	-0.458741	2.828909		6	2.257010	2.722649	-1.563176
	1	4.775832	0.006699	0.733326		6	3.818712	-0.013648	2.251005
	6	2.764184	-0.843971	3.946560		1	3.612306	0.795296	2.948981
	1	1.005263	-0.688719	2.716289		1	3.485436	-0.918677	2.761507
	6	4.159189	-0.762461	3.992656		6	5.344194	-0.083448	2.040551
	1	5.962918	-0.389309	2.858719		1	5.643792	-0.964725	1.470994
	1	2.198198	-1.073727	4.846462		1	5.711840	0.800440	1.508066
	1	4.685210	-0.929363	4.930035		1	5.848229	-0.125596	3.012661
	8	-3.554525	2.962829	1.519336		8	1.607340	3.284879	-2.424870
	8	-1.818277	4.199845	0.765947		8	3.594646	2.762988	-1.481888
	6	-2.680611	5.362360	0.746832		6	4.270487	3.546748	-2.497989
	1	-2.049479	6.183652	0.408673		1	5.331578	3.459092	-2.267966
	1	-3.512871	5.205792	0.056543		1	4.054408	3.141947	-3.488780
	1	-3.068371	5.560646	1.748385		1	3.947660	4.588706	-2.445823

Species	Cartesian coordinates			Species	Cartesian coordinates		
TS3_III_1e	5	-1.176231	3.120395 -0.213075	INT3_III_1e	6	3.007311 -0.978947 -0.296733	
	5	-2.451982	3.980322 -1.127289		6	1.671816 -1.418692 0.598564	
	5	-3.717498	2.413544 0.924074		5	2.014042 -2.265188 -0.859380	
	5	-4.025859	3.525753 -0.419792		5	3.100244 -0.917940 1.414385	
	5	-4.245892	1.763506 -0.638231		5	2.126868 -2.272820 2.002280	
	5	-2.801855	1.149624 -1.471490		5	1.458061 -3.116779 0.594447	
	5	-2.601436	3.759198 0.644372		5	4.322923 -3.342898 0.475559	
	5	-1.953622	2.140509 1.040473		5	3.784571 -2.415551 -0.936114	
	1	-0.063483	3.487276 -0.033730		5	4.452861 -1.560270 0.466880	
	1	-2.250609	5.042482 -1.623451		5	2.801275 -3.783237 -0.364137	
	1	-4.397641	2.312848 1.882590		5	2.881739 -3.791339 1.431959	
	1	-4.969693	4.249172 -0.390107		5	3.903693 -2.409001 1.940523	
	1	-5.260041	1.164188 -0.754342		1	1.338325 -2.061338 -1.811788	
	1	-2.868035	0.191112 -2.157984		1	3.177304 0.134932 1.931327	
	1	-2.509906	4.646987 1.429934		1	1.478770 -2.122226 2.984310	
	1	-1.438663	1.809050 2.054490		1	0.342362 -3.527731 0.609202	
	5	-1.701934	2.493955 -1.775246		1	5.299218 -4.017472 0.406027	
	1	-0.959737	2.416598 -2.698182		1	4.334740 -2.384893 -1.979164	
	5	-3.466435	2.731825 -1.918143		1	5.433975 -0.905411 0.379046	
	1	-3.988748	2.877057 -2.976359		1	2.675187 -4.762620 -1.024631	
	6	-2.950945	1.005831 0.233739		1	2.807881 -4.794208 2.065459	
	6	-1.437614	1.448359 -0.448329		1	4.564091 -2.405949 2.928288	
	28	0.016484	0.000680 -0.334163		28	-0.019170 -0.607490 0.373981	
	6	-0.080485	-1.877042 -0.276439		15	-2.206186 -0.116784 -0.002655	
	6	-1.570011	-1.763478 -0.606318		6	2.955187 0.317079 -1.102652	
	6	-3.087051	-0.355714 0.938022		6	2.324343 1.473713 -0.767318	
	6	-2.487972	-1.529121 0.594779		6	3.684136 0.232226 -2.449036	
	15	2.131220	0.021574 0.026732		1	3.223237 0.920992 -3.155462	
	6	3.204640	-1.245881 -0.769720		6	1.399502 1.881379 0.394902	
	6	3.979338	-0.949480 -1.902827		6	0.609468 0.915301 1.308231	
	6	3.207489	-2.561259 -0.267164		6	2.439721 2.688373 -1.702249	
	6	4.742342	-1.947504 -2.520227		1	2.414917 3.598845 -1.091982	
	1	4.002885	0.058198 -2.306383		1	3.405994 2.715527 -2.207290	
	6	3.972983	-3.553788 -0.883210		6	1.306950 2.789614 -2.744930	
	1	2.626864	-2.815835 0.615913		1	1.308362 1.934343 -3.428206	
	6	4.741071	-3.250814 -2.014259		1	0.320479 2.830784 -2.271608	
	1	5.339956	-1.700462 -3.394808		1	1.423364 3.699595 -3.343947	
	1	3.968136	-4.563489 -0.478871		1	3.521019 -0.756820 -2.880324	
	1	5.335839	-4.024734 -2.494183		6	5.199018 0.513030 -2.408752	
	6	2.756156	1.639922 -0.581736		1	5.410065 1.497669 -1.977853	
	6	3.692918	2.407433 0.129700		1	5.738109 -0.229865 -1.817228	
	6	2.266237	2.116910 -1.810726		1	5.609279 0.493875 -3.424919	
	6	4.143008	3.625305 -0.390572		1	0.623835 2.472354 -0.102388	
	1	4.071172	2.067613 1.089455		1	1.179804 0.579231 2.173104	
	6	2.724399	3.329865 -2.331532		1	-0.270260 1.449589 1.681267	
	1	1.521653	1.545246 -2.360866		6	2.055805 2.912561 1.327913	
	6	3.663743	4.086771 -1.621951		6	-2.640214 1.439099 -0.889064	
	1	4.866340	4.213687 0.169512		6	-3.152074 1.441516 -2.196200	
	1	2.337691	3.687484 -3.282974		6	-2.393792 2.669769 -0.250346	
	1	4.014122	5.035579 -2.022190		6	-3.414467 2.650696 -2.851763	
	6	2.548460	-0.062894 1.811638		1	-3.356767 0.506070 -2.708995	
	6	1.562078	0.282166 2.750796		6	-2.660148 3.874285 -0.905742	
	6	3.831349	-0.422463 2.261948		1	-2.013018 2.698205 0.768194	
	6	1.853690	0.272441 4.118310		6	-3.169039 3.868670 -2.210695	
	1	0.566153	0.560294 2.415106		1	-3.814796 2.635914 -3.863108	
	6	4.119082	-0.434022 3.629929		1	-2.469094 4.815872 -0.395878	
	1	4.607577	-0.696272 1.551952		1	-3.374775 4.806930 -2.720986	
	6	3.131936	-0.086678 4.560128		6	-2.886491 -1.480996 -1.032947	
	1	1.081721	0.541272 4.835704		6	-4.133916 -2.079958 -0.792445	
	1	5.114275	-0.714458 3.967509		6	-2.090677 -1.958226 -2.091389	
	1	3.357841	-0.098495 5.624094		6	-4.580321 -3.128441 -1.603908	
	6	-3.971750	-0.329304 2.187293		1	-4.758601 -1.738770 0.028271	
	1	-3.668507	-1.124867 2.864453		6	-2.541449 -3.001660 -2.905030	
	1	-3.797507	0.594099 2.741028		1	-1.118441 -1.509719 -2.290925	
	6	-5.481993	-0.481438 1.917011		6	-3.787849 -3.589971 -2.661407	
	1	-6.027100	-0.521016 2.866901		1	-5.547362 -3.585775 -1.406841	
	1	-5.882561	0.351301 1.335789		1	-1.916452 -3.358280 -3.720552	
	1	-5.693647	-1.405036 1.367245		1	-4.137246 -4.407065 -3.288583	
	6	-2.696492	-2.799070 1.431554		6	-3.219097 -0.082512 1.527143	
	1	-2.512014	-3.672993 0.797623		6	-4.458832 0.575712 1.604001	
	1	-3.744774	-2.883473 1.728491		6	-2.733149 -0.766647 2.654793	
	6	-1.804382	-2.946135 2.685161		6	-5.201416 0.542258 2.788159	
	1	-1.880826	-2.083574 3.353116		1	-4.846721 1.118162 0.745262	
	1	-2.103751	-3.836129 3.249677		6	-3.480251 -0.803823 3.836279	
	1	-0.749798	-3.065019 2.423810		1	-1.768437 -1.269282 2.610674	
	1	-1.682165	-0.917109 -1.305042		6	-4.715003 -0.148562 3.904901	
	1	0.484199	-2.392491 -1.054634		1	-6.159005 1.055776 2.837914	
	1	0.145753	-2.293156 0.705571		1	-3.093891 -1.336183 4.702442	
	6	-2.055202	-2.919207 -1.505531		1	-5.293689 -0.171258 4.825692	
	8	-1.347740	-3.779882 -1.997527		8	1.428944 3.793252 1.898944	
	8	-3.378721	-2.824157 -1.731726		8	3.378575 2.726777 1.491331	
	6	-3.949740	-3.826817 -2.607282		6	4.039828 3.627177 2.410935	
	1	-5.011284	-3.588069 -2.663452		1	3.611357 3.529899 3.411065	
	1	-3.489234	-3.771326 -3.596114		1	5.086058 3.322451 2.410492	
	1	-3.800607	-4.824404 -2.188057		1	3.939431 4.660081 2.069466	
TS4_III_1e	6	2.917755	1.342221 0.201676	TS2_III_2e	6	-3.188853 -0.912257 0.042983	
	1	1.638944	1.235748 -0.837700		6	-2.626605 0.644060 -0.432267	
	5	1.388215	2.044773 0.729372		5	-4.045988 0.001589 -1.140700	

Species	Cartesian coordinates			Species	Cartesian coordinates		
	5	3.209633	1.502166 -1.500482		5	-2.453368	0.137100 1.216676
	5	1.791498	2.366126 -2.115702		5	-2.979089	1.777833 0.819543
	5	0.672129	2.741481 -0.761422		5	-4.011550	1.700242 -0.613685
	5	3.147654	4.101857 -0.257866		5	-5.321429	0.194903 1.449857
	5	2.917332	2.887901 1.024835		5	-4.887879	-0.931470 0.135975
	5	4.024596	2.557775 -0.331433		5	-3.891119	-0.848252 1.606055
	5	1.513835	3.784296 0.396528		5	-5.432502	0.712152 -0.264300
	5	1.752808	3.996433 -1.376185		5	-4.771578	1.823742 0.977097
	5	3.318523	3.237130 -1.819408		5	-3.795395	0.859735 2.118430
	1	0.835562	1.487217 1.620189		1	-4.001215	-0.344598 -2.268947
	1	3.759851	0.613792 -2.047506		1	-1.400651	-0.139010 1.667869
	1	1.350043	2.050684 -3.169789		1	-2.222544	2.669171 0.983366
	1	-0.508769	2.709782 -0.953128		1	-3.977750	2.545267 -1.440394
	1	3.728668	5.113083 -0.034090		1	-6.283920	0.005838 2.119784
	1	3.324090	2.950641 2.132304		1	-5.463113	-1.918378 -0.164809
	1	5.176404	2.384822 -0.136776		1	-3.737171	-1.798766 2.295416
	1	0.928431	4.554264 1.085686		1	-6.457023	0.894741 -0.835746
	1	1.323437	4.928026 -1.974712		1	-5.322103	2.825625 1.299474
	1	4.008008	3.620694 -2.706359		1	-3.645146	1.144869 3.261406
	6	3.410775	0.095992 0.917977		6	-2.351820	-2.080336 -0.395407
	6	2.883380	-1.142977 0.772388		6	-1.008827	-1.912699 -0.493679
	6	1.775339	-1.576704 -0.184402		6	-1.517901	1.295894 -1.953719
	6	1.285149	-0.598270 -1.256070		6	-0.104627	1.564783 -1.807031
	28	-0.093996	0.686305 -0.425541		28	-0.412979	-0.075304 -0.619600
	15	-2.157902	0.024587 0.032262		15	1.671579	-0.190299 0.104602
	6	4.597134	0.321885 1.861216		6	-3.098050	-3.376100 -0.706227
	1	4.666740	1.374676 2.130355		1	-2.417277	-4.216986 -0.579685
	1	4.425527	-0.204472 2.804336		1	-3.898687	-3.530076 0.025519
	6	3.320291	-2.289342 1.684284		6	-0.110922	-3.100339 -0.821609
	1	3.299100	-3.235889 1.134371		1	-0.506593	-3.637198 -1.695727
	1	4.352544	-2.170414 2.010534		1	0.879716	-2.754342 -1.129813
	6	5.954545	-0.115825 1.270559		6	0.072192	-4.102685 0.339516
	1	5.969557	-1.180399 1.019374		1	0.407686	-3.599723 1.247813
	1	6.189405	0.439961 0.359202		1	-0.856832	-4.625616 0.581587
	1	6.755433	0.071909 1.994590		1	0.821039	-4.858198 0.075604
	6	2.416183	-2.434758 2.926813		6	-3.690755	-3.456546 -2.128263
	1	2.760344	-3.267071 3.550049		1	-4.462646	-2.702878 -2.299949
	1	2.431245	-1.525429 3.536810		1	-2.910927	-3.316988 -2.884868
	1	1.376759	-2.639269 2.650556		1	-4.145558	-4.440806 -2.289731
	1	0.913272	-1.882186 0.418511		1	0.548195	1.102530 -2.542359
	1	0.330148	-0.947682 -1.680044		1	-2.157161	2.166180 -1.947235
	1	1.970722	-0.553976 -2.096496		1	-1.804792	0.569554 -2.710972
	6	2.171058	-2.856417 -0.939296		6	0.364264	2.921866 -1.485031
	6	-2.660312	-1.485859 -0.904317		6	2.096069	-1.405252 1.441405
	6	-2.399298	-1.504236 -2.288138		6	2.948865	-2.499282 1.219622
	6	-3.239158	-2.618418 -0.310696		6	1.532394	-1.241278 2.720312
	6	-2.731947	-2.618590 -3.062447		6	3.251328	-3.389977 2.256067
	1	-1.942707	-0.638635 -2.766391		1	3.378791	-2.677127 0.239675
	6	-3.558946	-3.740982 -1.084968		6	1.829261	-2.134744 3.751794
	1	-3.440890	-2.636165 0.756526		1	0.862226	-0.413501 2.929620
	6	-3.311133	-3.743490 -2.461209		6	2.696145	-3.210997 3.525631
	1	-2.531304	-2.611671 -4.131631		1	3.916881	-4.228220 2.062225
	1	-4.002502	-4.612692 -0.608575		1	1.383480	-1.987193 4.732939
	1	-3.561667	-4.615854 -3.060712		1	2.930710	-3.904194 4.330340
	6	-2.520692	-0.374035 1.798409		6	2.915464	-0.528123 -1.209954
	6	-3.822351	-0.354241 2.329663		6	4.300774	-0.556970 -0.953247
	6	-1.449138	-0.706175 2.643372		6	2.468094	-0.823846 -2.508587
	6	-4.045025	-0.671375 3.673179		6	5.208401	-0.834767 -1.977903
	1	-4.666351	-0.084583 1.699729		1	4.681496	-0.390760 0.050347
	6	-1.670876	-1.028934 3.986541		6	3.376662	-1.108474 -3.533169
	1	-0.435468	-0.701764 2.249776		1	1.403711	-0.853106 -2.724054
	6	-2.970519	-1.012215 4.504340		6	4.749851	-1.105001 -3.272864
	1	-5.057280	-0.649860 4.071160		1	6.274011	-0.847926 -1.760382
	1	-0.830023	-1.283518 4.627994		1	3.007849	-1.335264 -4.530816
	1	-3.145222	-1.256056 5.549988		1	5.458407	-1.322884 -4.068804
	6	-3.477435	1.255803 -0.378184		6	2.096524	1.420492 0.918132
	6	-4.621312	0.948753 -1.131760		6	3.329712	2.075212 0.774144
	6	-3.313730	2.567940 0.102761		6	1.126613	1.992862 1.761139
	6	-5.581003	1.933431 -1.399414		6	3.600746	3.247181 1.488466
	1	-4.773295	-0.056897 -1.513646		1	4.082491	1.701984 0.090410
	6	-4.276950	3.546606 -0.153886		6	1.400842	3.158638 2.481098
	1	-2.433968	2.827333 0.687915		1	0.142960	1.542771 1.852605
	6	-5.413381	3.232972 -0.910860		6	2.644513	3.786544 2.354176
	1	-6.460541	1.679997 -1.987509		1	4.560981	3.741135 1.357659
	1	-4.136608	4.554692 0.230233		1	0.636367	3.579159 3.130673
	1	-6.160133	3.996281 -1.118319		1	2.859359	4.695774 2.911244
	8	3.322776	-2.703279 -1.623284		8	1.474456	3.353452 -1.784962
	8	1.504121	-3.877593 -0.961088		8	-0.563612	3.679806 -0.844285
	6	3.747669	-3.833141 -2.422052		6	-0.168918	5.028314 -0.523303
	1	2.994027	-4.067638 -3.177246		1	0.063485	5.587153 -1.433759
	1	4.679110	-3.520113 -2.892912		1	-1.027719	5.469625 -0.016426
	1	3.912326	-4.705892 -1.786019		1	0.702835	5.024394 0.134522

Table S13 The first three vibration frequencies for stationary points on potential energy surfaces from **INT1_III** and **R2** to products **P1**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)	Species	Frequencies (cm ⁻¹)
TS2_III_1a	-302i 19 22	INT2_III_1a	11 21 23	TS3_III_1a	-117i 11 23	INT3_III_1a	10 15 20
TS4_III_1a	-404i 7 15	TS2_III_2a	-316i 18 20	TS2_III_1b	-309i 18 22	INT2_III_1b	10 19 25
TS3_III_1b	-133i 7 17	INT3_III_1b	10 13 19	TS4_III_1b	-410i 9 13	TS2_III_2b	-334i 14 20
TS2_III_1c	-307i 17 18	INT2_III_1c	11 15 20	TS3_III_1c	-132i 6 15	INT3_III_1c	9 16 19
TS4_III_1c	-408i 8 13	TS2_III_2c	-332i 13 17	TS2_III_1d	-309i 19 19	INT2_III_1d	7 22 23
TS3_III_1d	-118i 8 17	INT3_III_1d	10 15 19	TS4_III_1d	-411i 8 12	TS2_III_2d	-332i 16 25
TS2_III_1e	-307i 21 23	INT2_III_1e	9 21 26	TS3_III_1e	-128i 10 2	INT3_III_1e	7 19 22
TS4_III_1e	-406i 6 16	TS2_III_2e	-306i 21 26				

Table S14 The total energies (E : a.u.), zero-point energies (ZPE : kcal·mol⁻¹) and Gibbs free energies [G and $G(\text{sol}, 383\text{K})$: a.u.] for stationary points on potential energy surfaces from **INT1_III** and **R2** to products **P1**, located at IDSCRF-B3LYP/DZVP level in THF solvent.

Species	E	ZPE	G	$G(\text{sol}, 383\text{K})$
TS2_III_1a	-3435.66262	438.02598	-3435.03760	-3435.05871
INT2_III_1a	-3435.69339	439.12738	-3435.06805	-3435.08968
TS3_III_1a	-3435.68660	439.12546	-3435.06166	-3435.08436
INT3_III_1a	-3435.70261	439.90946	-3435.07776	-3435.10029
TS4_III_1a	-3435.66907	437.79543	-3435.04784	-3435.07060
TS2_III_2a	-3435.63248	438.18234	-3435.00700	-3435.02942
TS2_III_1b	-3588.09505	452.76014	-3587.44964	-3587.47114
INT2_III_1b	-3588.12841	453.59516	-3587.48308	-3587.50542
TS3_III_1b	-3588.12160	453.46564	-3587.47745	-3587.50033
INT3_III_1b	-3588.13826	454.31484	-3587.49379	-3587.51768
TS4_III_1b	-3588.10372	452.43320	-3587.46246	-3587.48724
TS2_III_2b	-3588.06980	452.61760	-3587.42509	-3587.44890
TS2_III_1c	-3666.72934	488.45895	-3666.03134	-3666.05674
INT2_III_1c	-3666.76270	489.26683	-3666.06518	-3666.09144
TS3_III_1c	-3666.75581	489.09656	-3666.05973	-3666.08605
INT3_III_1c	-3666.77237	490.08238	-3666.07466	-3666.10138
TS4_III_1c	-3666.73794	488.12557	-3666.04418	-3666.07149
TS2_III_2c	-3666.70367	488.34417	-3666.00643	-3666.03222
TS2_III_1d	-3740.52779	467.67059	-3739.86068	-3739.88527
INT2_III_1d	-3740.55842	468.37033	-3739.89261	-3739.91865
TS3_III_1d	-3740.55378	468.20173	-3739.88894	-3739.91512
INT3_III_1d	-3740.56948	468.93941	-3739.90439	-3739.93049
TS4_III_1d	-3740.53463	467.14858	-3739.87259	-3739.89888
TS2_III_2d	-3740.51406	467.66653	-3739.84685	-3739.87098
TS2_III_1e	-3416.46174	421.75028	-3415.86254	-3415.88425
INT2_III_1e	-3416.49377	422.69035	-3415.89484	-3415.91768
TS3_III_1e	-3416.48831	422.63566	-3415.88995	-3415.91217
INT3_III_1e	-3416.50401	423.59093	-3415.90527	-3415.92825
TS4_III_1e	-3416.47035	421.49217	-3415.87524	-3415.89921
TS2_III_2e	-3416.44155	422.08502	-3415.84073	-3415.86289