Supplementary Materials: Computational Investigation of Nickel-Mediated B–H Activation and Regioselective Cage B–C(sp²) Coupling of *o*-Carborane

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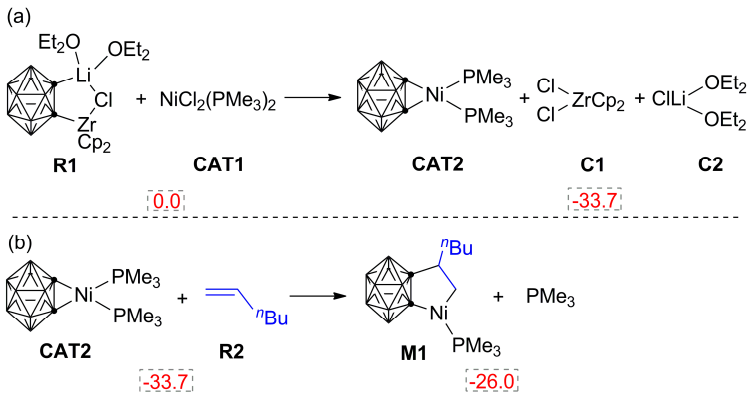

Figure S1. Relativle Gibbs free energies (298 K, kcal·mol^{-1}) corresponding to **M1**'s formation from **R1**+**CAT1**+**R2**.

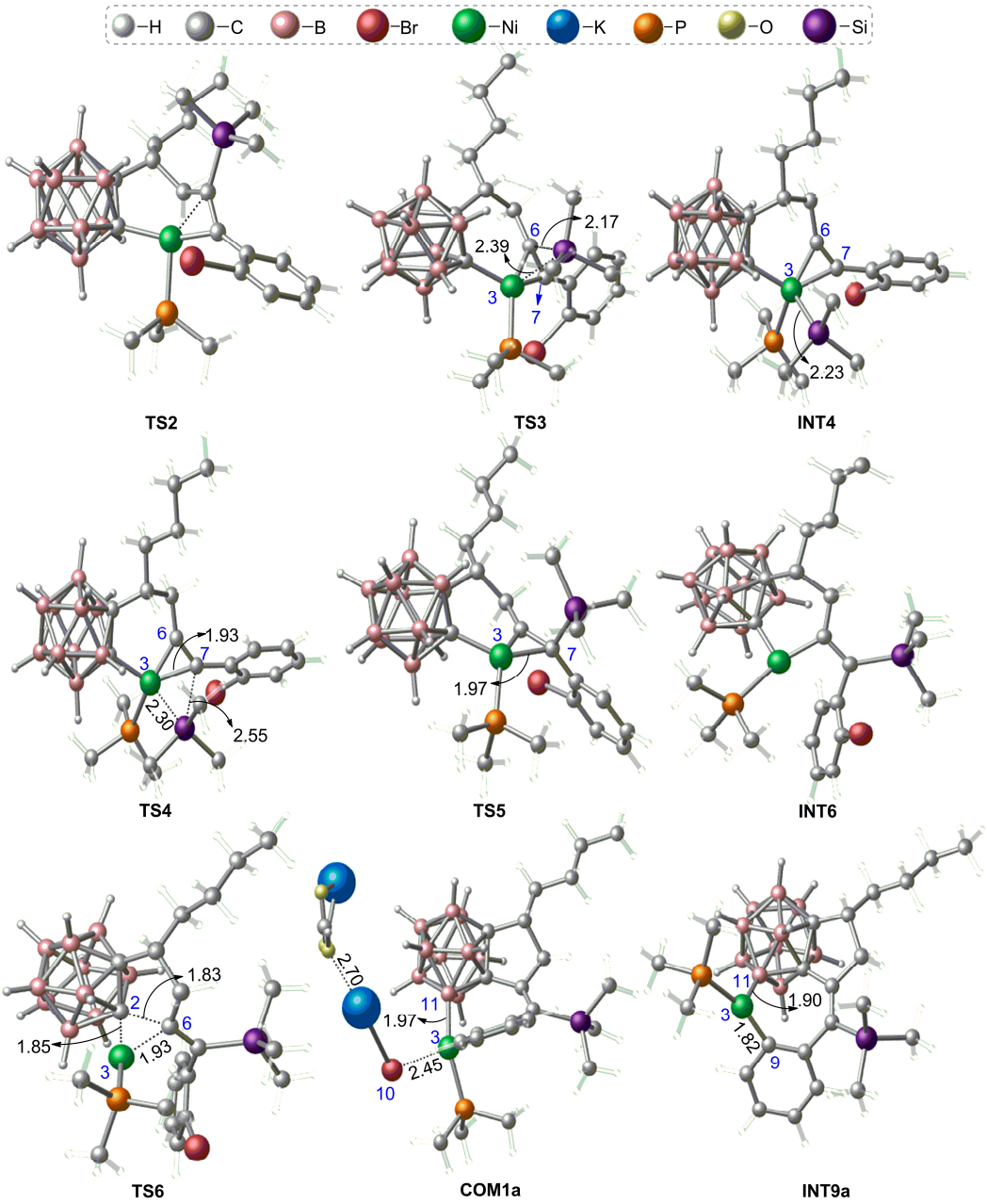

Figure S2. Part optimized structures and key geometrical parameters (bond length in Å) for stationary points involved in the formation of **INT8** from **M1**+**R3**. Noncritical atoms especially hydrogens were made transparent for clarity.

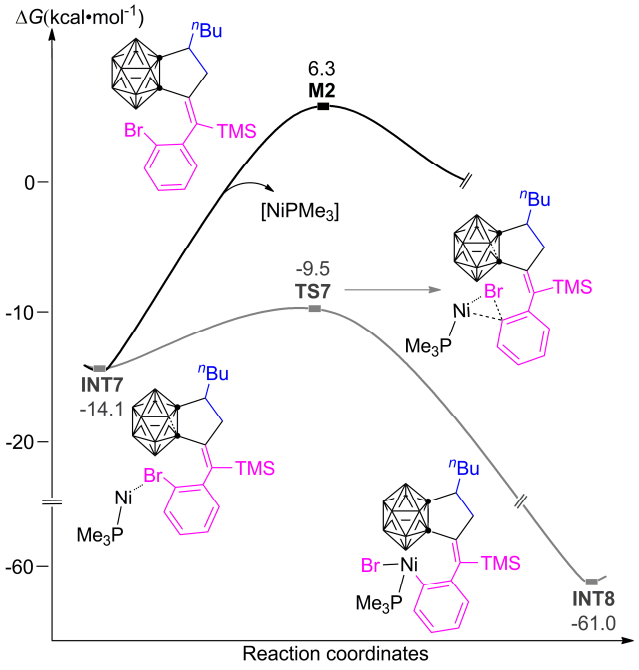

Figure S3. Relative Gibbs free energies (298 K, kcal·mol^{-1}) corresponding to the formation of speculated **M2** from **INT7**, obtained at PCM-LC-ωPBE/DZVP level in toluene solution.

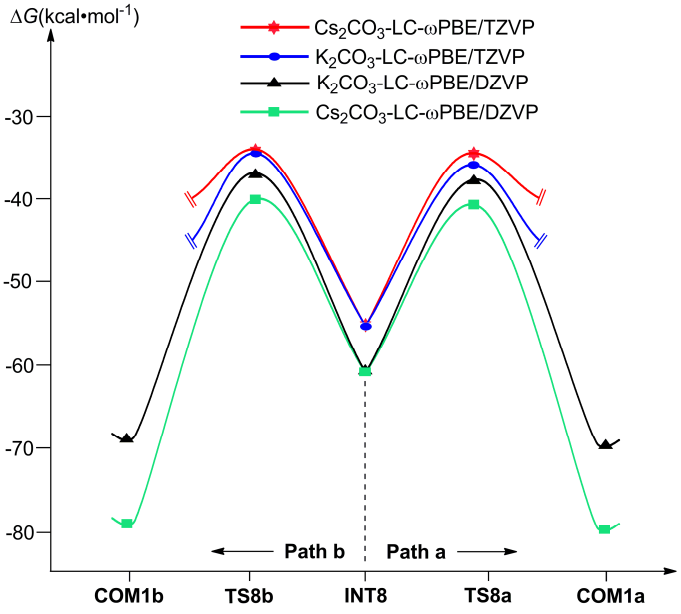

Figure S4. Potential energy surfaces (PESs, in kcal·mol^{-1}) for **COM1a/b**'s formation from **INT8**, obtained at PCM-LC-ωPBE/TZVP (SDD for Cs) and PCM-LC-ωPBE/DZVP (SDD for Cs) levels when employing Cs_2CO_3/K_2CO_3.

Entry	Method/Basis set	Additive	Barriers (kcal·mol^{-1})		$t_{1/2,TS8a}$	$t_{1/2,TS8b}$	dr^{calc}
			TS8a	TS8b	(h)	(h)	(P1a:P1b)

1	LC-ωPBE/DZVP	K_2CO_3	23.1	23.9	3.905×10^{0}	1.508×10^{1}	3.9:1
2	LC-ωPBE/DZVP*	Cs_2CO_3	19.8	20.5	1.484×10^{-2}	4.840×10^{-2}	3.3:1
3	LC-ωPBE/TZVP	K_2CO_3	19.0	20.4	3.844×10^{-3}	4.088×10^{-2}	10.6:1
4	LC-ωPBE/TZVP*	Cs_2CO_3	20.0	20.5	2.081×10^{-2}	4.840×10^{-2}	2.3:1

*: Fuentealba's SDD basis set (Fuentealba, P. etc., *Chem. Phys. Lett*. **1982**, *89*, 418.) is used for Cs atom.

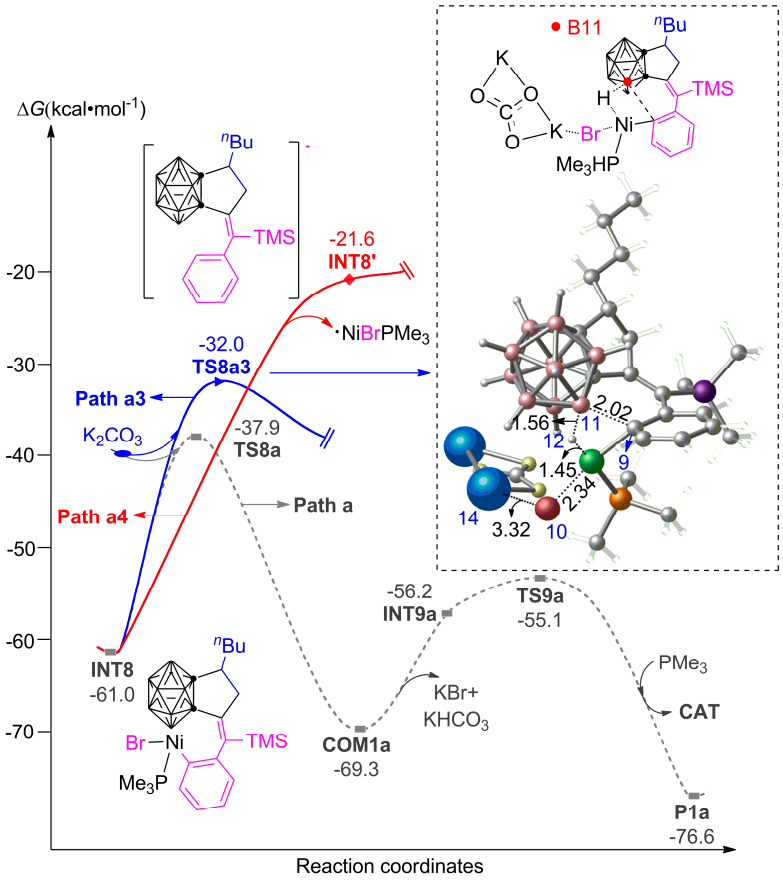

Figure S5. Relative Gibbs free energies (298 K, kcal·mol^{-1}) for **Path a3** and **a4**, obtained at PCM-LC-ωPBE/DZVP level in toluene solution. **Path a** is plotted in grey dotted line for comparison.

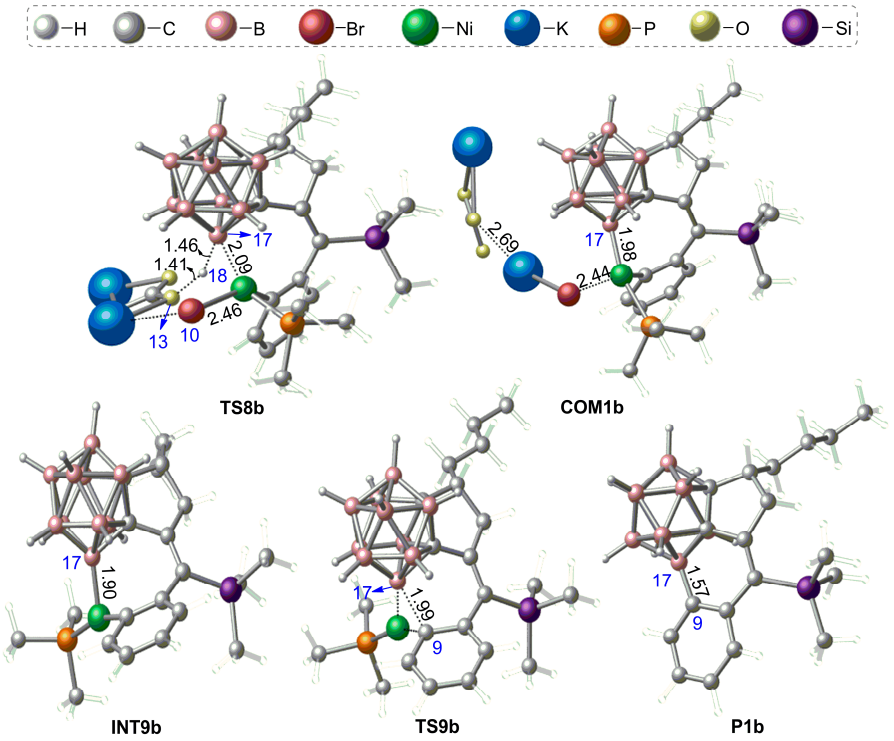

Figure S6. Optimized structures and key geometrical parameters (bond length in Å) for stationary points involved in the B(17)-H activation and cage B-C(sp²) coupling process of intermediate **INT8**. Noncritical atoms especially hydrogens were made transparent for clarity.

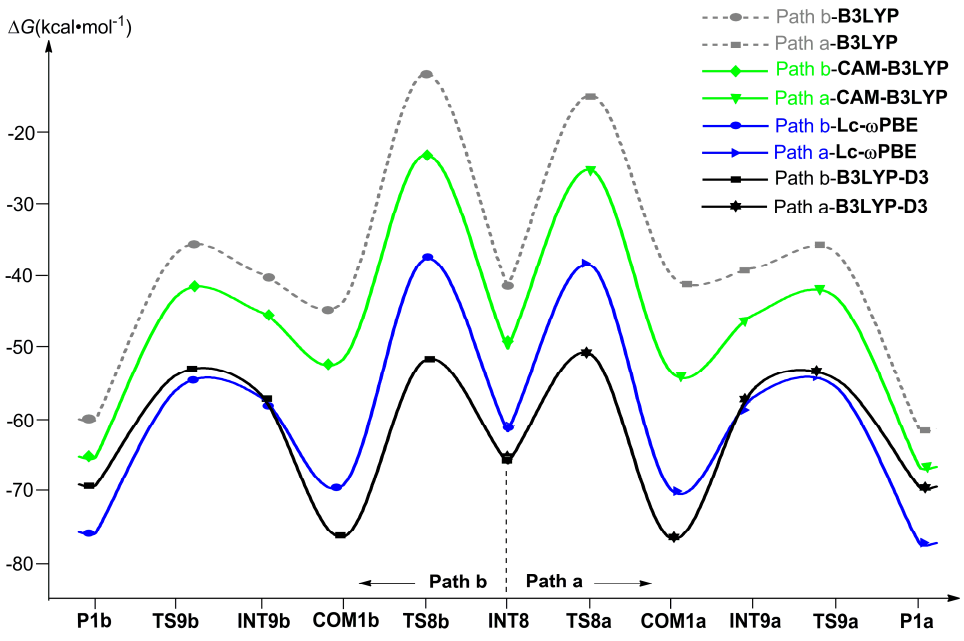

Figure S7. Potential energy surfaces (PESs) for B(11)-H (**Path a**, right) and B(17)-H (**Path b**, left) activation in intermediate **INT8**, obtained at PCM-B3LYP/DZVP (denoted B3LYP), PCM-CAM-B3LYP/DZVP (denoted CAM- B3LYP), PCM-LC-ωPBE/DZVP (denoted LC-ωPBE) and

PCM-B3LYP-D3/DZVP (denoted B3LYP-D3) levels in toluene solution.

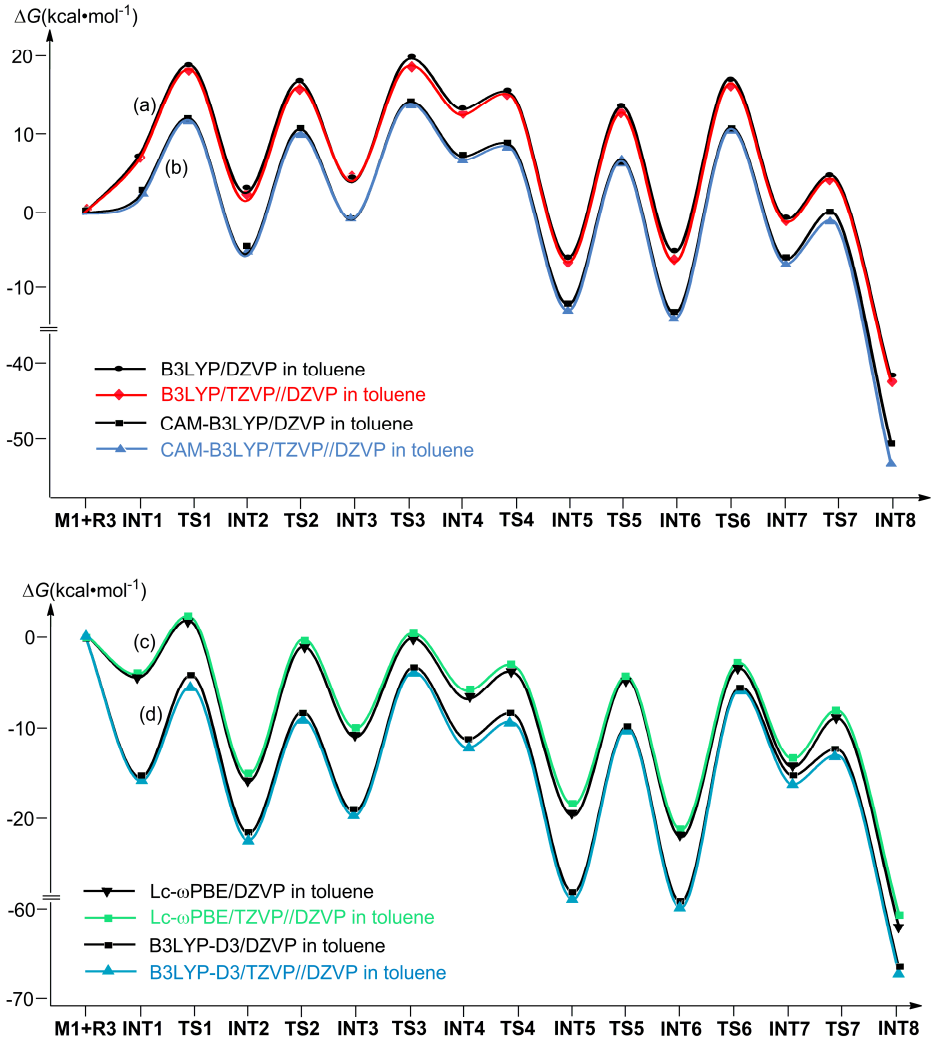

Figure S8. Relative Gibbs free energies (298 K, kcal·mol^{-1}) corresponding to the formation of **INT8** from **M1+R3**, obtained at PCM-METHOD/DZVP and PCM-METHOD/TZVP// DZVP levels in toluene solution (METHOD = B3LYP, CAM-B3LYP, LC-ωPBE and B3LYP-D3 respectively).

Table S1. Gibbs free energy barriers (Δ*G*, kcal·mol^{-1}) and transferred rate constants (*k*, L·mol^{-1}·s^{-1} or s^{-1}) for transition states **TS1**-**TS7** and **TS8a**, obtained at PCM-LC-ωPBE/DZVP level under experimental temperature (298 K).

	Δ*G* (kcal·mol^{-1})	***k* (L·mol^{-1}·s^{-1} or s^{-1})**
TS1	5.9	2.925×10^{8}
TS2	14.4	1.708×10^{2}
TS3	10.5	1.238×10^{5}

TS4	2.4	1.079×10^{11}
TS5	14.6	1.218×10^{2}
TS6	17.9	4.630×10^{-1}
TS7	4.6	2.627×10^{9}
TS8a	**23.1**	$\mathbf{7.113\times10^{-5}}$

Table S2. Relative Gibbs free energies (in kcal·mol^{-1}) for stationary points on **Path a** and **b** (from **INT8** to **P1a/b**), obtained at PCM-LC-ωPBE/DZVP (denoted LC-ωPBE), PCM-CAM-B3LYP/ DZVP (denoted CAM-B3LYP), PCM-B3LYP/DZVP (denoted B3LYP) and PCM-B3LYP-D3/ DZVP (denoted B3LYP-D3) levels in toluene solution.

	Relative Gibbs free energies (kcal·mol^{-1})			
	LC-ωPBE	**CAM-B3LYP**	**B3LYP**	**B3LYP-D3**
Path a				
INT8	-61.0	-49.5	-41.0	-65.4
TS8a	-37.9	-24.7	-14.3	-50.2
COM1a	-69.3	-52.9	-39.5	-76.0
INT9a	-56.2	-44.7	-38.3	-55.0
TS9a	-55.1	-42.6	-36.4	-53.9
P1a	-76.6	-66.0	-60.8	-68.8
Path b				
INT8	-61.0	-49.5	-41.0	-65.4
TS8b	-37.1	-22.6	-11.4	-51.1
COM1b	-68.5	-51.0	-43.0	-76.2
INT9b	-56.2	-44.4	-39.1	-55.8
TS9b	-55.1	-42.1	-36.1	-53.1
P1b	-75.1	-64.6	-59.4	-68.5

Table S3. Relative Gibbs free energies (in kcal·mol^{-1}) for stationary points on **Path a** (from **M1+R3** to **INT8**), obtained at PCM-LC-ωPBE/DZVP (denoted LC-ωPBE), PCM-CAM-B3LYP/ DZVP (denoted CAM-B3LYP), PCM-B3LYP/DZVP (denoted B3LYP) and PCM-B3LYP-D3/ DZVP (denoted B3LYP-D3) levels in toluene solution.

	Relative Gibbs free energies (kcal·mol^{-1})			
	LC-ωPBE	**CAM-B3LYP**	**B3LYP**	**B3LYP-D3**
M1+R3	0.0	0.0	0.0	0.0
INT1	-4.7	2.0	7.1	-15.3
TS1	1.2	12.2	19.1	-4.5
INT2	-15.8	-5.1	2.7	-21.2
TS2	-1.4	10.9	17.0	-8.3
INT3	-11.0	-0.7	4.1	-18.9
TS3	-0.5	14.2	19.7	-3.7
INT4	-6.9	7.5	13.4	-11.2
TS4	-4.5	8.5	15.0	-9.1
INT5	-19.4	-11.7	-5.6	-27.5
TS5	-4.8	7.1	13.8	-9.8
INT6	-21.7	-12.8	-4.9	-28.5
TS6	-3.8	11.1	17.4	-6.1
INT7	-14.1	-5.7	-0.3	-15.0
TS7	-9.5	-0.3	4.4	-12.9
INT8	-61.0	-49.5	-41.0	-65.4

Table S4. Optimized Cartesian coordinates for stationary points on **Path a**, located at PCM-LC-ωPBE/DZVP level in toluene solution.

Species	**Cartesian coordinates**	**Species**	**Cartesian coordinates**
M1	5 -1.590946 1.839332 0.557837 5 -1.223717 3.346475 -0.292379 5 1.122015 2.529418 1.138102	**R3**	6 -1.440385 0.511903 -0.002016 6 -0.241744 0.695742 -0.001839 14 -3.263012 0.198038 -0.000234

Species	Cartesian coordinates	Species	Cartesian coordinates
	5 0.460989 3.775535 0.068305		6 -3.579436 -1.373525 -0.961968
	5 1.495422 2.498047 -0.581435		1 -4.647733 -1.607472 -0.985053
	5 0.453792 1.281786 -1.330897		1 -3.234340 -1.282574 -1.994987
	5 -0.562141 3.055165 1.332346		1 -3.060458 -2.223325 -0.511351
	5 -0.156150 1.344065 1.435341		6 -4.104043 1.658420 -0.811481
	1 -2.649986 1.483917 0.963618		1 -5.188599 1.518113 -0.835743
	1 -2.070229 4.157353 -0.496611		1 -3.900196 2.585360 -0.269288
	1 1.991396 2.623294 1.941906		1 -3.761903 1.791613 -1.840983
	1 0.840996 4.901388 0.125225		6 -3.817639 0.015295 1.776363
	1 2.615410 2.587790 -0.959598		1 -3.610191 0.920867 2.352161
	1 0.839117 0.543585 -2.172830		1 -4.893340 -0.175933 1.830260
	1 -0.918960 3.639360 2.304855		1 -3.305221 -0.816099 2.267018
	1 -0.150074 0.634472 2.385625		6 1.170989 0.958182 -0.001132
	5 -1.218564 1.793493 -1.154640		6 2.122089 -0.066244 0.000234
	1 -2.011885 1.407599 -1.949531		6 1.623160 2.281755 -0.001449
	5 0.049967 2.989573 -1.477912		6 3.479821 0.218954 0.001581
	1 0.133636 3.530237 -2.533739		6 2.976925 2.572526 -0.000278
	6 1.029725 1.098494 0.247280		1 0.887937 3.080851 -0.002761
	6 -0.529105 0.673658 -0.078162		6 3.906639 1.539298 0.001366
	6 1.847077 -0.160137 0.496134		1 4.200778 -0.592515 0.002760
	1 1.947991 -0.255383 1.581275		1 3.308479 3.606779 -0.000600
	6 0.979815 -1.313449 -0.018069		1 4.970661 1.758100 0.002420
	1 1.231320 -1.551047 -1.062223		35 1.581087 -1.868861 -0.000196
	1 1.121056 -2.225047 0.587072		
	28 -0.874511 -1.136165 -0.031188		
	15 -3.119145 -1.504837 -0.020044		
	6 -3.922914 -1.362676 1.609585		
	1 -4.983297 -1.620957 1.551417		
	1 -3.825732 -0.342792 1.983822		
	1 -3.435118 -2.030926 2.321928		
	6 -4.193829 -0.520583 -1.108238		
	1 -3.864419 -0.619754 -2.143845		
	1 -4.133526 0.533309 -0.835195		
	1 -5.232713 -0.851908 -1.029905		
	6 -3.521462 -3.219882 -0.507426		
	1 -3.013393 -3.929580 0.149129		
	1 -3.187919 -3.406074 -1.530339		
	1 -4.597071 -3.404732 -0.451275		
	6 3.251127 -0.113870 -0.099736		
	1 3.775112 0.770556 0.279335		
	1 3.181759 0.005928 -1.187065		
	6 4.068881 -1.357099 0.229179		
	1 3.570554 -2.246706 -0.172650		
	1 4.106225 -1.491047 1.317545		
	6 5.490040 -1.290282 -0.317482		
	1 5.453187 -1.149588 -1.403464		
	1 5.992295 -0.404912 0.087772		
	6 6.307263 -2.533325 0.008055		
	1 7.321755 -2.461012 -0.392390		
	1 5.846312 -3.430675 -0.415022		
	1 6.386652 -2.681010 1.089029		
INT1	5 -2.718664 -1.028424 -1.822425	**TS1**	5 1.775409 -3.256389 0.289099
	5 -4.356702 -1.545751 -1.398667		5 2.467707 -3.945979 -1.184628
	5 -4.059019 1.201037 -0.661977		5 4.128685 -1.782115 -0.330693
	5 -5.189503 -0.159700 -0.672566		5 3.930122 -3.021633 -1.573759

Species	Cartesian coordinates	Species	Cartesian coordinates
	5 -4.324172 0.273385 0.804291		5 3.442312 -1.352922 -1.892641
	5 -2.959788 -0.836613 0.981614		5 1.688642 -1.257948 -1.696975
	5 -4.070936 0.088063 -2.033939		5 3.529119 -3.377324 0.123394
	5 -2.529728 0.652267 -1.371592		5 2.784295 -1.926954 0.812727
	1 -2.067523 -1.442635 -2.723110		1 1.160555 -3.858442 1.104392
	1 -4.916900 -2.383527 -2.032341		1 2.342712 -5.102339 -1.436738
	1 -4.324864 2.355470 -0.707864		1 5.142269 -1.296796 0.044376
	1 -6.361637 0.020450 -0.772907		1 4.877066 -3.497631 -2.114615
	1 -4.738723 0.803504 1.782996		1 3.970661 -0.535122 -2.574536
	1 -2.469610 -1.052539 2.038970		1 1.047353 -0.410548 -2.215560
	1 -4.415757 0.442581 -3.116079		1 4.167885 -4.103654 0.815896
	1 -1.768622 1.402878 -1.880770		1 2.855811 -1.527079 1.928678
	5 -2.975437 -1.951736 -0.362481		5 1.084870 -2.835882 -1.259026
	1 -2.502730 -3.026998 -0.201169		1 -0.040395 -3.103200 -1.532355
	5 -4.501883 -1.429945 0.366549		5 2.408695 -2.685391 -2.432854
	1 -5.155464 -2.174733 1.025183		1 2.241206 -2.907833 -3.589216
	6 -2.761250 0.689931 0.297534		6 2.737783 -0.817206 -0.449763
	6 -1.945370 -0.589226 -0.369816		6 1.362337 -1.642635 -0.069447
	6 -1.831945 1.562363 1.119555		6 2.648364 0.655038 -0.071009
	6 -0.489523 0.818835 1.239317		1 2.544912 1.214862 -1.005200
	1 -0.379564 0.407056 2.245668		6 1.393287 0.860204 0.762854
	1 0.340662 1.522328 1.111390		1 1.225784 1.920138 0.948389
	28 -0.059325 -0.620021 0.035968		1 1.494516 0.401839 1.761502
	15 0.554678 -2.255127 -1.540643		28 -0.058804 -0.440320 0.522080
	6 1.383556 -1.155280 1.372024		15 -1.174870 -1.882703 1.758720
	6 1.939229 -0.394689 0.568529		6 -1.443497 0.802764 0.336549
	14 1.021449 -2.332024 2.775496		6 -0.437838 1.268140 -0.314239
	6 2.695126 -2.976705 3.310591		6 -0.146047 -2.324564 3.199984
	1 2.583817 -3.712347 4.112684		1 -0.017501 -1.434872 3.821328
	1 3.225565 -3.463635 2.487842		1 -0.630701 -3.099776 3.799850
	1 3.329181 -2.170693 3.689793		1 0.838837 -2.672929 2.895882
	6 -0.066975 -3.710701 2.150219		6 -1.739525 -3.464778 1.058771
	1 -0.378446 -4.350188 2.982024		1 -2.516393 -3.262097 0.319253
	1 -0.971620 -3.319317 1.678238		1 -0.929161 -3.995662 0.564564
	1 0.450874 -4.346801 1.427642		1 -2.157017 -4.096447 1.847419
	6 0.202573 -1.418459 4.181880		6 -2.687147 -1.348567 2.625649
	1 -0.828480 -1.142046 3.950972		1 -2.974514 -2.109604 3.356612
	1 0.178215 -2.062580 5.066595		1 -2.517648 -0.406244 3.148729
	1 0.747587 -0.509891 4.450103		1 -3.514690 -1.208401 1.930191
	6 0.818708 -1.654184 -3.246551		14 -0.203550 2.676587 -1.535119
	1 1.019931 -2.492383 -3.919274		6 -1.945334 3.209142 -1.963484
	1 -0.052976 -1.109715 -3.609112		1 -2.514832 2.394092 -2.418008
	1 1.673156 -0.976318 -3.269274		1 -2.498928 3.555358 -1.087140
	6 -0.416027 -3.775767 -1.828764		1 -1.915729 4.032376 -2.684390
	1 -0.552690 -4.321414 -0.894074		6 0.669270 2.197495 -3.116950
	1 -1.400267 -3.544692 -2.232206		1 0.652707 3.058702 -3.793650
	1 0.113651 -4.419653 -2.536556		1 1.713895 1.909344 -2.984557
	6 2.191749 -3.001817 -1.208825		1 0.158212 1.375214 -3.623368
	1 2.968620 -2.236465 -1.178125		6 0.684251 4.100292 -0.703500
	1 2.189734 -3.515484 -0.245661		1 0.213665 4.364992 0.247725
	1 2.446113 -3.724245 -1.989211		1 1.738757 3.894388 -0.511535
	6 3.029479 0.343886 -0.032930		1 0.639528 4.984057 -1.347732
	6 4.312615 0.118846 0.484753		6 -2.859074 1.062292 0.563861
	6 2.896617 1.256780 -1.079986		6 -3.861047 0.442856 -0.185078
	6 5.416271 0.779290 -0.023195		6 -3.249327 1.975334 1.547335

Species	Cartesian coordinates			Species	Cartesian coordinates		
	1	4.425034	-0.590569 1.299124		6	-5.203743	0.717464 0.035189
	6	4.000424	1.924307 -1.594125		6	-4.586987	2.254462 1.776572
	6	5.259690	1.685361 -1.066577		1	-2.479579	2.466632 2.136524
	1	6.400534	0.588514 0.394370		6	-5.568365	1.622861 1.021265
	1	3.869439	2.630831 -2.407700		1	-5.960057	0.222645 -0.566404
	1	6.119715	2.209938 -1.472855		1	-4.865128	2.968432 2.546717
	35	1.211658	1.621659 -1.831352		1	-6.619356	1.835758 1.194108
	6	-1.679606	2.993958 0.603813		6	3.912091	1.158557 0.636975
	1	-2.660346	3.390862 0.325699		1	4.772213	0.918061 0.005054
	1	-1.070005	2.997243 -0.304840		1	4.050231	0.600176 1.569250
	6	-1.057818	3.925939 1.638405		6	3.942662	2.654135 0.926362
	1	-1.693826	3.948187 2.532106		1	3.822934	3.209719 -0.011309
	1	-0.086657	3.537125 1.965227		1	3.107367	2.944293 1.573146
	6	-0.875287	5.346242 1.116731		6	5.247403	3.083608 1.588793
	1	-0.235977	5.324552 0.227053		1	6.088329	2.803546 0.945044
	1	-1.843919	5.737997 0.786698		1	5.378791	2.525884 2.522593
	6	-0.273300	6.284634 2.154160		6	5.299392	4.578251 1.875055
	1	0.711216	5.934706 2.478340		1	6.243485	4.860863 2.347558
	1	-0.152286	7.295887 1.756953		1	5.201858	5.160136 0.954007
	1	-0.908923	6.350409 3.041981		1	4.489118	4.880917 2.544726
	1	-2.287051	1.631927 2.113875		35	-3.403500	-0.795275 -1.532808
INT2	5	1.656845	-3.441669 0.249455	**TS2**	5	-2.612264	-2.635601 -0.894566
	5	2.403414	-4.047073 -1.237837		5	-4.163559	-2.942152 -0.106493
	5	3.941346	-1.839799 -0.284256		5	-4.102165	-0.234912 -0.992731
	5	3.820350	-3.039796 -1.571634		5	-5.089311	-1.437180 -0.158680
	5	3.256482	-1.384564 -1.839165		5	-4.192850	-0.224148 0.761739
	5	1.497778	-1.377190 -1.666047		5	-2.717842	-0.979200 1.372671
	5	3.414861	-3.471149 0.107128		5	-4.070338	-1.899896 -1.542092
	5	2.589814	-2.074499 0.832800		5	-2.551770	-0.968605 -1.428308
	1	1.048173	-4.088106 1.038710		1	-1.981308	-3.440375 -1.492978
	1	2.339978	-5.198537 -1.532152		1	-4.664360	-4.022060 -0.138091
	1	4.935089	-1.342893 0.122208		1	-4.502045	0.671581 -1.638833
	1	4.800178	-3.442843 -2.113571		1	-6.277219	-1.394308 -0.225139
	1	3.758076	-0.522567 -2.486210		1	-4.613039	0.726453 1.339653
	1	0.819244	-0.540069 -2.164679		1	-2.167984	-0.568819 2.338699
	1	4.082806	-4.186709 0.783305		1	-4.501234	-2.205682 -2.608605
	1	2.622481	-1.712542 1.964762		1	-1.887661	-0.567483 -2.328847
	5	0.971612	-3.004288 -1.299209		5	-2.695189	-2.643511 0.846015
	1	-0.134843	-3.317522 -1.599496		1	-2.092580	-3.435956 1.497743
	5	2.299794	-2.745034 -2.444031		5	-4.227444	-1.897213 1.327560
	1	2.162510	-2.934159 -3.610359		1	-4.774980	-2.194805 2.341563
	6	2.507395	-0.917115 -0.390487		6	-2.701372	-0.040207 -0.032443
	6	1.167448	-1.854804 -0.063766		6	-1.801182	-1.451586 0.019873
	6	2.458734	0.585470 -0.036033		28	0.173868	-1.350362 0.147747
	1	2.377001	1.098385 -0.995294		6	1.489536	-0.203149 0.181377
	6	1.240950	0.978481 0.818348		6	0.361173	0.480643 0.609168
	1	1.500824	1.879155 1.380018		6	-2.020661	1.339199 0.098698
	1	1.108239	0.251976 1.645175		1	-2.127730	1.604001 1.151605
	28	-0.275102	-0.737182 0.598582		6	-0.531062	1.378446 -0.244391
	15	-1.465012	-2.043023 1.737919		1	-0.199342	2.414229 -0.131581
	6	-1.235375	0.781781 0.521988		1	-0.396079	1.123504 -1.299611
	6	-0.106162	1.400762 0.133074		15	0.909540	-3.240993 -0.747118
	6	-0.570226	-2.583460 3.229380		6	0.200166	-4.830494 -0.196249
	1	-0.370092	-1.717206 3.863637		1	-0.886250	-4.822418 -0.256662
	1	-1.159628	-3.308060 3.797802		1	0.588017	-5.656837 -0.798388

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 0.383232 -3.034334 2.955090		1 0.477483 -4.998804 0.846934
	6 -2.000124 -3.585871 0.941374		6 2.685286 -3.667221 -0.654559
	1 -2.657475 -3.349454 0.103071		1 3.300335 -2.858339 -1.051322
	1 -1.142601 -4.137043 0.558833		1 2.983480 -3.854142 0.378987
	1 -2.542242 -4.211934 1.655346		1 2.885405 -4.572248 -1.235274
	6 -3.022110 -1.421730 2.444143		6 0.691823 -3.236571 -2.560753
	1 -3.469087 -2.179399 3.093542		1 0.981266 -4.197341 -2.995175
	1 -2.837256 -0.517855 3.026748		1 -0.340357 -3.018290 -2.830721
	1 -3.732317 -1.176484 1.653477		1 1.325476 -2.455243 -2.986836
	6 -2.640087 1.182599 0.436894		6 2.923373 -0.005351 0.055271
	6 -3.541575 0.601668 -0.457566		6 3.749790 -0.881515 0.767588
	6 -3.135560 2.141142 1.325835		6 3.530932 1.039420 -0.652364
	6 -4.877587 0.974196 -0.487721		6 5.121581 -0.697025 0.819596
	6 -4.471554 2.510446 1.316895		6 4.906259 1.201637 -0.646275
	1 -2.447891 2.597004 2.033656		6 5.700014 0.342540 0.104001
	6 -5.345096 1.928309 0.405927		1 5.738718 -1.373395 1.403641
	1 -5.549315 0.517531 -1.208184		1 5.356455 2.006552 -1.218851
	1 -4.831107 3.258627 2.017813		1 6.776593 0.487239 0.119291
	1 -6.392476 2.215686 0.385993		14 0.650790 0.950460 2.461559
	14 -0.099208 2.960967 -0.958503		6 -0.729526 1.991701 3.184947
	6 1.172621 2.891312 -2.339410		1 -0.899790 2.912410 2.620716
	1 2.203659 3.014896 -2.001858		1 -1.679996 1.467744 3.296299
	1 1.110972 1.965482 -2.917538		1 -0.406394 2.290989 4.188314
	1 0.967324 3.715712 -3.030655		6 2.190120 2.021972 2.573259
	6 0.289748 4.418300 0.160317		1 3.118610 1.471066 2.407956
	1 -0.453750 4.519201 0.956219		1 2.157419 2.844033 1.851612
	1 1.273619 4.335872 0.629961		1 2.250057 2.468633 3.570982
	1 0.283561 5.349241 -0.415036		6 0.866024 -0.602937 3.483007
	6 -1.750984 3.240185 -1.793055		1 0.997917 -0.349956 4.539909
	1 -1.642896 4.085650 -2.480957		1 -0.007445 -1.255369 3.402232
	1 -2.059181 2.377090 -2.389114		1 1.741666 -1.179545 3.173866
	1 -2.560334 3.482073 -1.101993		1 3.283478 -1.696987 1.310858
	6 3.770631 1.050799 0.609799		35 2.502304 2.229858 -1.681287
	1 4.591071 0.741323 -0.041209		6 -2.765474 2.421264 -0.694782
	1 3.922256 0.530218 1.562451		1 -2.694322 2.211633 -1.768158
	6 3.899359 2.556808 0.820935		1 -3.826406 2.363955 -0.439859
	1 3.624452 3.087288 -0.098580		6 -2.300857 3.849897 -0.420519
	1 3.215095 2.910053 1.600119		1 -2.215054 4.010361 0.661698
	6 5.316859 2.956798 1.218469		1 -1.306138 4.028646 -0.841902
	1 6.013395 2.646706 0.432217		6 -3.260683 4.883238 -1.001379
	1 5.607679 2.405151 2.119280		1 -3.376567 4.703337 -2.075978
	6 5.459364 4.452301 1.466393		1 -4.253225 4.742976 -0.559818
	1 6.483657 4.713929 1.743342		6 -2.796850 6.315031 -0.770471
	1 5.200132 5.027021 0.572533		1 -1.823179 6.495217 -1.235429
	1 4.801948 4.783893 2.275404		1 -3.503294 7.035723 -1.190184
	35 -2.941963 -0.696100 -1.689151		1 -2.698311 6.530202 0.297535
INT3	5 0.219661 -2.844767 -1.221364	**TS3**	5 -1.214482 -2.872762 -1.251588
	5 -0.815627 -4.282692 -1.236801		5 -2.663433 -3.864513 -1.030708
	5 -2.365249 -2.039650 -2.088646		5 -3.469990 -1.242085 -1.811715
	5 -2.427018 -3.776259 -1.763935		5 -4.066867 -2.844296 -1.367120
	5 -3.041471 -2.623467 -0.573070		5 -4.068414 -1.532976 -0.183899
	5 -1.814743 -2.412680 0.677255		5 -2.665472 -1.735080 0.868725
	5 -0.981244 -3.046548 -2.500965		5 -2.586566 -2.665830 -2.340084
	5 -0.733484 -1.467197 -1.737143		5 -1.704571 -1.251541 -1.719122
	1 1.391227 -2.813588 -1.410278		1 -0.150465 -3.260377 -1.604689

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -0.363674 -5.362052 -1.456678		1 -2.639340 -5.036488 -1.238794
	1 -3.024057 -1.430095 -2.862593		1 -3.995129 -0.461569 -2.530801
	1 -3.172213 -4.477957 -2.371676		1 -5.087860 -3.254545 -1.820916
	1 -4.173189 -2.419505 -0.278756		1 -5.000326 -0.937026 0.247829
	1 -2.109965 -2.064526 1.768523		1 -2.658683 -1.277852 1.963498
	1 -0.658306 -3.215177 -3.633734		1 -2.513834 -2.953899 -3.492241
	1 -0.271391 -0.502701 -2.248031		1 -1.027119 -0.498844 -2.339207
	5 -0.455117 -3.433482 0.276332		5 -1.813050 -3.168506 0.361335
	1 0.235370 -3.821039 1.163700		1 -1.182852 -3.754902 1.177517
	5 -2.093157 -4.010203 -0.034591		5 -3.576027 -3.150148 0.313650
	1 -2.587531 -4.872529 0.619791		1 -4.226359 -3.779993 1.085823
	6 -1.968157 -1.302964 -0.602278		6 -2.631813 -0.665387 -0.442893
	6 -0.443376 -1.771515 -0.076571		6 -1.277944 -1.622208 -0.102460
	6 -2.535146 0.091259 -0.230813		6 -2.675669 0.831738 -0.059156
	1 -2.820664 0.010642 0.823755		6 -1.362624 1.600834 -0.206635
	6 -1.547766 1.260592 -0.356397		28 0.455306 -0.796338 0.317498
	1 -2.108093 2.181429 -0.168756		6 -0.148094 0.909076 0.302965
	1 -1.182424 1.325213 -1.385475		6 1.165995 0.941210 0.114399
	28 0.767646 -0.406630 0.604392		14 0.208706 0.395113 2.376818
	15 2.488266 -1.452397 1.518069		1 -2.946553 0.840955 0.998692
	6 0.916456 1.301842 0.205300		1 -1.483193 2.570750 0.281971
	6 -0.391113 1.151589 0.615065		1 -1.179295 1.812420 -1.265829
	6 2.082669 -2.076576 3.185423		15 1.980182 -2.416879 0.396075
	1 1.264084 -2.795731 3.126276		6 1.625810 -4.017458 1.201318
	1 2.948485 -2.563148 3.642987		1 0.850260 -4.547001 0.648026
	1 1.767652 -1.252663 3.828844		1 2.528242 -4.635567 1.219101
	6 3.937893 -0.395937 1.854883		1 1.274805 -3.876205 2.224425
	1 4.366496 -0.051445 0.912496		6 3.495855 -1.926128 1.291721
	1 3.636138 0.482970 2.426361		1 3.913060 -1.017594 0.857002
	1 4.703643 -0.939930 2.415082		1 3.257144 -1.725302 2.338257
	6 3.269778 -2.905201 0.746111		1 4.250171 -2.717233 1.257275
	1 4.083879 -3.275748 1.375401		6 2.625908 -3.021674 -1.207811
	1 2.537780 -3.699761 0.603338		1 3.651158 -3.385664 -1.101283
	1 3.675448 -2.638181 -0.231042		1 2.002532 -3.846621 -1.554702
	6 1.588893 2.245863 -0.663240		1 2.597272 -2.243117 -1.967973
	6 2.596879 1.891134 -1.569310		6 -1.193626 1.448152 3.052164
	6 1.258491 3.604990 -0.554736		1 -1.274436 2.438199 2.597912
	6 3.257968 2.849000 -2.321245		1 -2.165545 0.955926 2.989799
	6 1.929268 4.571202 -1.283409		1 -0.979621 1.599055 4.116250
	1 0.464440 3.890287 0.129685		6 1.785437 1.172310 3.037580
	6 2.932510 4.190179 -2.166728		1 2.692180 0.732146 2.617542
	1 4.023199 2.546805 -3.029343		1 1.838100 2.252048 2.886983
	1 1.664352 5.618688 -1.173311		1 1.802784 0.995220 4.119010
	1 3.460327 4.938140 -2.751772		6 0.082370 -1.278969 3.229921
	14 -0.701104 1.467842 2.473872		1 -0.283883 -1.085479 4.245889
	6 -1.989530 2.832423 2.552300		1 -0.595282 -1.990664 2.760111
	1 -1.693145 3.718365 1.982795		1 1.066283 -1.743400 3.325728
	1 -2.962855 2.504472 2.177239		6 2.100671 2.033305 -0.149942
	1 -2.132747 3.144723 3.591618		6 3.268861 1.925808 -0.909950
	6 0.885129 2.093068 3.254464		6 1.793968 3.301682 0.366431
	1 1.629239 1.298766 3.348258		6 4.103669 3.015456 -1.119023
	1 1.341513 2.905371 2.681784		6 2.622015 4.392573 0.176442
	1 0.682273 2.471495 4.261420		1 0.878271 3.417407 0.939205
	6 -1.319942 0.021965 3.487966		6 3.788187 4.246452 -0.565318
	1 -1.297057 0.302592 4.546809		1 4.998215 2.897680 -1.722448

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -2.349422 -0.251629 3.246978 1 -0.703764 -0.871302 3.366325 6 -3.810912 0.430902 -1.018393 1 -3.534278 0.817965 -2.005731 35 3.023405 0.084567 -1.863531 1 -4.392637 -0.474220 -1.198267 6 -4.717659 1.432130 -0.308352 1 -4.993678 1.033408 0.675798 1 -4.194861 2.377200 -0.123352 6 -5.986624 1.726941 -1.100592 1 -6.524638 0.790247 -1.282406 1 -5.713924 2.118752 -2.086729 6 -6.906131 2.714858 -0.395399 1 -7.808226 2.908276 -0.981404 1 -7.219732 2.333989 0.580841 1 -6.405051 3.673337 -0.231039		1 2.356667 5.356893 0.600050 1 4.449238 5.093297 -0.726588 6 -3.780359 1.595768 -0.801092 1 -4.701804 1.010339 -0.776443 1 -3.509108 1.700823 -1.857044 6 -4.076645 2.973486 -0.213054 1 -3.234334 3.655311 -0.372721 1 -4.209019 2.890017 0.873190 6 -5.326027 3.601110 -0.821843 1 -5.207772 3.658322 -1.909540 1 -6.184021 2.944392 -0.642117 6 -5.619679 4.988141 -0.266553 1 -4.793909 5.677223 -0.466531 1 -6.521898 5.413541 -0.713233 1 -5.769111 4.955817 0.816602 35 3.733941 0.318505 -1.766621
INT4	5 -1.538688 -2.266999 -1.819513 5 -3.103688 -3.089545 -1.826952 5 -3.560465 -0.273114 -1.900946 5 -4.362610 -1.849761 -1.863050 5 -4.206711 -0.895399 -0.386373 5 -2.853329 -1.530472 0.549809 5 -2.864282 -1.621393 -2.794348 5 -1.814318 -0.542514 -1.866020 1 -0.540754 -2.710748 -2.281974 1 -3.222579 -4.165686 -2.321962 1 -3.969044 0.737062 -2.369119 1 -5.423417 -2.002207 -2.380569 1 -5.070236 -0.333425 0.200588 1 -2.810638 -1.364557 1.722731 1 -2.813075 -1.616430 -3.983062 1 -1.038694 0.234375 -2.313698 5 -2.181111 -2.883413 -0.330042 1 -1.620934 -3.749810 0.251143 5 -3.927711 -2.633603 -0.325960 1 -4.662221 -3.349416 0.277220 6 -2.664992 -0.178011 -0.456964 6 -1.451462 -1.335412 -0.380972 6 -2.448838 1.171095 0.256437 1 -2.444267 0.940651 1.324948 6 -1.115147 1.838048 -0.078528 1 -1.022004 2.753176 0.512555 1 -1.103920 2.148033 -1.127954 28 0.381552 -0.830181 0.236007 15 1.898335 -2.253990 -0.340732 6 1.319084 0.823828 0.337946 6 0.073881 1.005991 0.167631 6 1.593256 -4.045800 -0.416191 1 2.340707 -4.536423 -1.045271 1 1.651790 -4.474294 0.586308 1 0.598952 -4.242955 -0.816908 6 3.632720 -2.187171 0.217770 1 3.938293 -1.151912 0.378430 1 3.788105 -2.745093 1.138898	**TS4**	5 -1.960397 -2.825050 -1.089809 5 -3.398870 -3.583672 -0.380466 5 -4.109023 -0.974174 -1.305204 5 -4.732301 -2.425486 -0.504337 5 -4.290765 -1.000336 0.449707 5 -2.682092 -1.271808 1.141675 5 -3.542343 -2.556870 -1.827447 5 -2.383739 -1.216992 -1.646517 1 -1.085647 -3.396769 -1.647709 1 -3.546895 -4.763468 -0.420117 1 -4.713284 -0.208394 -1.976375 1 -5.871151 -2.744095 -0.630440 1 -5.012354 -0.241703 1.008043 1 -2.343202 -0.712390 2.129343 1 -3.798359 -2.978713 -2.909268 1 -1.825807 -0.657308 -2.529454 5 -2.145328 -2.859558 0.647607 1 -1.394183 -3.440901 1.354991 5 -3.849716 -2.605673 1.034897 1 -4.334280 -3.053745 2.023993 6 -2.892845 -0.367514 -0.278423 6 -1.577774 -1.453676 -0.148875 6 -2.647333 1.150022 -0.144929 1 -2.522734 1.336668 0.926362 6 -1.366661 1.607902 -0.846252 1 -1.242472 2.685127 -0.702260 1 -1.457970 1.441332 -1.923723 28 0.299305 -0.796836 0.101932 15 1.546532 -2.652247 -0.126075 6 1.090772 0.953335 -0.067723 6 -0.166798 0.911665 -0.352385 6 0.998768 -4.341367 0.320262 1 0.029712 -4.570788 -0.118071 1 1.733997 -5.065535 -0.043532 1 0.914978 -4.442900 1.403509 6 3.282549 -2.746126 0.453903 1 3.840579 -1.865107 0.138953 1 3.328521 -2.818527 1.542202

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 4.267996 -2.622564 -0.558432		1 3.763623 -3.633657 0.032343
	6 2.130036 -1.745061 -2.080801		6 1.772683 -2.780992 -1.939292
	1 2.660862 -2.523917 -2.635487		1 2.412030 -3.632577 -2.190232
	1 1.182347 -1.538783 -2.574364		1 0.808000 -2.906455 -2.430622
	1 2.725997 -0.830813 -2.095168		1 2.229673 -1.866367 -2.318377
	6 2.638350 1.424718 0.473736		6 2.124725 1.997321 -0.052548
	6 3.273889 2.071071 -0.590208		6 3.387369 1.898461 -0.645242
	6 3.307019 1.393522 1.701397		6 1.813094 3.221799 0.560984
	6 4.534118 2.636519 -0.446843		6 4.308490 2.939340 -0.594092
	6 4.558848 1.965529 1.858130		6 2.720827 4.268285 0.622664
	1 2.817202 0.922542 2.547738		1 0.826294 3.344115 0.996325
	6 5.181407 2.580630 0.778313		6 3.981938 4.123799 0.052896
	1 5.001754 3.127517 -1.294760		1 5.277275 2.822051 -1.069492
	1 5.050205 1.931003 2.826435		1 2.442000 5.197191 1.112444
	1 6.165841 3.026137 0.888504		1 4.705802 4.932751 0.095032
	14 0.418160 -1.700470 2.293162		14 1.171970 -0.276630 2.164136
	6 -0.351095 -0.297647 3.275434		6 0.132870 1.044075 3.006061
	1 0.251854 0.611487 3.231019		1 0.367886 2.055647 2.672733
	1 -1.359434 -0.053447 2.941249		1 -0.936754 0.874696 2.866334
	1 -0.419021 -0.612931 4.323523		1 0.332889 0.999757 4.083320
	6 2.105458 -2.013981 3.068651		6 2.978763 0.145668 2.466374
	1 2.470957 -3.024684 2.868008		1 3.683879 -0.404089 1.842173
	1 2.887176 -1.304369 2.796893		1 3.175552 1.211102 2.330427
	1 1.964025 -1.945232 4.153701		1 3.204039 -0.098993 3.511159
	6 -0.526926 -3.275284 2.649340		6 0.780387 -1.865166 3.101697
	1 -0.346544 -3.493363 3.709533		1 0.876135 -1.637072 4.171013
	1 -1.602800 -3.186708 2.507026		1 -0.240468 -2.210166 2.928227
	1 -0.179756 -4.138451 2.079112		1 1.464317 -2.688601 2.886442
	35 2.418565 2.222918 -2.265722		35 3.892727 0.362441 -1.628339
	6 -3.579719 2.180624 0.009969		6 -3.834472 2.003526 -0.619093
	1 -3.422827 2.672075 -0.956613		1 -4.769412 1.531757 -0.309894
	1 -4.536649 1.662809 -0.064341		1 -3.851294 2.031236 -1.714576
	6 -3.696840 3.234172 1.108364		6 -3.819759 3.430148 -0.068305
	1 -3.869458 2.734814 2.069497		1 -2.931631 3.974181 -0.410278
	1 -2.761638 3.794723 1.216923		1 -3.758310 3.395478 1.026971
	6 -4.829159 4.220681 0.846455		6 -5.060945 4.222198 -0.475298
	1 -4.660243 4.718018 -0.115043		1 -5.135705 4.241312 -1.568794
	1 -5.771082 3.670691 0.744362		1 -5.955725 3.700122 -0.117540
	6 -4.965697 5.266796 1.944476		6 -5.055085 5.650536 0.060538
	1 -5.784037 5.960314 1.734877		1 -4.191820 6.210317 -0.313128
	1 -5.166678 4.798677 2.912408		1 -5.956428 6.192225 -0.239553
	1 -4.049212 5.855403 2.045601		1 -5.009349 5.662398 1.154045
INT5	5 -3.177460 -1.891968 -0.728220	**TS5**	6 -1.057226 1.418044 -0.266709
	5 -4.640978 -1.943625 0.261810		6 0.098508 0.613430 0.158515
	5 -4.256908 0.726150 -0.662740		6 1.406020 0.569836 0.578844
	5 -5.308949 -0.307079 0.308181		14 1.343655 0.677608 2.524187
	5 -4.117027 0.737797 1.089435		5 -1.717583 -2.888333 -1.261038
	5 -2.719773 -0.249635 1.522272		5 -3.212873 -3.716686 -0.799046
	5 -4.568563 -0.920390 -1.188844		5 -3.819070 -0.983033 -1.356430
	5 -2.922828 -0.250737 -1.290835		5 -4.519502 -2.523343 -0.846601
	1 -2.753591 -2.776008 -1.393554		5 -4.145953 -1.275121 0.347761
	1 -5.308141 -2.927801 0.311419		5 -2.615163 -1.694916 1.121552
	1 -4.573974 1.697257 -1.259191		5 -3.230577 -2.478732 -2.071879
	1 -6.472243 -0.073337 0.394888		5 -2.083328 -1.212590 -1.598357
	1 -4.297426 1.739502 1.702586		1 -0.791545 -3.371828 -1.824542

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -1.977565 0.072599 2.389216		1 -3.373065 -4.872299 -1.035992
	1 -5.177226 -1.145301 -2.185651		1 -4.362013 -0.107335 -1.941532
	1 -2.323372 0.036290 -2.273148		1 -5.647948 -2.791832 -1.113054
	5 -3.035960 -1.897528 1.015981		1 -4.905622 -0.591047 0.952050
	1 -2.486200 -2.782935 1.587244		1 -2.351152 -1.304187 2.209104
	5 -4.349325 -0.912660 1.678458		1 -3.401518 -2.720635 -3.224251
	1 -4.802492 -1.125537 2.757293		1 -1.441750 -0.533311 -2.329052
	6 -2.735764 0.681892 0.104916		5 -2.044380 -3.189424 0.426493
	6 -2.081960 -0.859083 0.061947		1 -1.341549 -3.879470 1.090111
	6 -1.805528 1.909365 0.107277		5 -3.774389 -2.963479 0.706553
	1 -1.645372 2.153615 1.162783		1 -4.348768 -3.547573 1.569500
	6 -0.436116 1.602034 -0.503484		6 -2.679391 -0.579904 -0.155763
	1 0.197253 2.488200 -0.420845		6 -1.426195 -1.685441 -0.090024
	1 -0.552947 1.369914 -1.567020		6 -2.407933 0.885624 0.231265
	28 -0.238001 -1.244019 -0.015632		28 0.384296 -1.089720 0.302164
	15 0.046096 -3.349220 -0.853169		6 2.687533 1.037741 -0.030528
	6 1.393654 0.291881 0.751434		1 -2.399141 0.904631 1.322736
	6 0.176880 0.451195 0.200540		1 -0.926463 2.461754 0.027110
	6 -0.930154 -4.773087 -0.265730		1 -1.061541 1.404543 -1.359337
	1 -1.996419 -4.596074 -0.400104		15 1.731829 -2.850142 -0.148135
	1 -0.646623 -5.682031 -0.803278		6 1.233658 -4.599557 -0.005297
	1 -0.747062 -4.925595 0.800018		1 0.303597 -4.792048 -0.536884
	6 1.742363 -4.003453 -0.664553		1 2.016704 -5.247998 -0.408260
	1 2.469440 -3.286635 -1.049453		1 1.079261 -4.850723 1.046043
	1 1.964976 -4.180942 0.389572		6 3.366668 -2.933513 0.661181
	1 1.858871 -4.947176 -1.204497		1 3.912415 -2.003375 0.504316
	6 -0.152440 -3.389938 -2.665394		1 3.253552 -3.098713 1.733969
	1 0.048657 -4.387625 -3.064469		1 3.956039 -3.755063 0.244551
	1 -1.162609 -3.091094 -2.945863		6 2.213340 -2.685758 -1.900988
	1 0.546012 -2.681993 -3.116859		1 2.903319 -3.479193 -2.200763
	6 2.452673 1.301179 0.417082		1 1.330216 -2.721624 -2.539867
	6 3.353956 1.135598 -0.634255		1 2.699691 -1.718696 -2.048325
	6 2.549948 2.482146 1.158325		6 3.876597 0.636896 0.598975
	6 4.322422 2.087118 -0.928787		6 2.854838 1.801217 -1.190675
	6 3.506304 3.444981 0.873638		6 5.133679 0.972694 0.132617
	1 1.846695 2.643607 1.970834		1 3.804087 0.026784 1.493578
	6 4.401961 3.244327 -0.169157		6 4.112523 2.146390 -1.677448
	1 5.006468 1.922246 -1.755614		6 5.258814 1.738773 -1.019288
	1 3.551633 4.353440 1.467895		1 6.015620 0.632544 0.668386
	1 5.158507 3.989039 -0.399439		1 4.184224 2.740238 -2.583406
	14 1.898382 -0.832345 2.205174		1 6.235612 2.014041 -1.405959
	6 2.100838 0.297067 3.691582		6 2.402952 2.147201 3.012810
	1 2.915476 1.014396 3.567863		1 3.476822 1.980732 2.918260
	1 1.184441 0.853203 3.909052		1 2.151508 3.027257 2.414183
	1 2.332976 -0.308424 4.573846		1 2.194840 2.391558 4.059619
	6 3.562941 -1.617629 1.859965		6 1.913142 -0.881537 3.394502
	1 3.541326 -2.316359 1.021830		1 2.948400 -1.155482 3.181526
	1 4.315715 -0.856960 1.634415		1 1.831062 -0.737304 4.477162
	1 3.906435 -2.163814 2.744185		1 1.275902 -1.730409 3.128733
	6 0.634545 -2.125243 2.702015		6 -0.376653 1.057247 3.153205
	1 0.965995 -2.566045 3.649197		1 -0.308206 1.222434 4.233802
	1 -0.354677 -1.694831 2.875124		1 -0.795089 1.968721 2.717619
	1 0.520887 -2.947750 1.992691		1 -1.079149 0.237017 2.998684
	35 3.273228 -0.392725 -1.746253		6 -3.518226 1.842153 -0.222664
	6 -2.442004 3.137551 -0.546765		1 -4.487639 1.365249 -0.064093

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -3.434686 3.288273 -0.113587		1 -3.435150 2.019125 -1.300823
	1 -2.593727 2.951078 -1.615647		6 -3.522644 3.175319 0.521143
	6 -1.640498 4.422715 -0.358894		1 -2.597758 3.733568 0.338954
	1 -1.371703 4.537735 0.698774		1 -3.563859 2.987834 1.601174
	1 -0.698540 4.377883 -0.915260		6 -4.703388 4.053302 0.121316
	6 -2.414781 5.654516 -0.815428		1 -5.636513 3.513835 0.316430
	1 -3.346972 5.728159 -0.244837		1 -4.672836 4.230009 -0.959485
	1 -2.707443 5.528696 -1.863729		6 -4.721546 5.386868 0.855953
	6 -1.617845 6.942590 -0.659589		1 -3.815558 5.964249 0.650000
	1 -2.194439 7.810537 -0.989372		1 -5.578116 5.995417 0.555363
	1 -1.336277 7.108198 0.384400		1 -4.781851 5.240196 1.938197
	1 -0.697321 6.911493 -1.249649		35 1.397877 2.418637 -2.217241
INT6	5 1.604692 -2.587892 1.696739	**TS6**	5 0.403044 -1.981435 2.222488
	5 3.001554 -3.635772 1.372921		5 0.848257 -3.693203 2.159758
	5 3.916578 -0.930433 1.502872		5 3.182813 -2.120175 1.613700
	5 4.435164 -2.601586 1.240582		5 2.584954 -3.775419 1.793685
	5 4.186344 -1.519597 -0.134943		5 2.844955 -3.089601 0.189662
	5 2.617422 -1.883261 -0.846978		5 1.285043 -2.602300 -0.446641
	5 3.177906 -2.233169 2.441902		5 1.969865 -2.484126 2.851471
	5 2.181278 -0.941142 1.792577		5 1.836117 -1.008388 1.887843
	1 0.613060 -2.884087 2.281722		1 -0.495247 -1.518375 2.834463
	1 3.031718 -4.753911 1.778896		1 0.289738 -4.486719 2.846258
	1 4.560570 -0.033464 1.935012		1 4.279971 -1.726494 1.823279
	1 5.529329 -2.952354 1.548842		1 3.293510 -4.635008 2.208007
	1 5.019502 -1.041062 -0.829034		1 3.711750 -3.315969 -0.588703
	1 2.374636 -1.613249 -1.974761		1 1.162150 -2.484163 -1.622463
	1 3.338456 -2.314572 3.617547		1 2.231563 -2.410508 4.008195
	1 1.629777 -0.103164 2.417981		1 2.008458 0.113825 2.210856
	5 1.893887 -3.175600 0.080554		5 0.053342 -2.943127 0.777077
	1 1.110385 -3.899401 -0.433381		1 -1.102695 -3.084036 0.401187
	5 3.629983 -3.192709 -0.227230		5 1.395494 -4.070079 0.505682
	1 4.122623 -3.964452 -0.986690		1 1.236887 -5.124272 -0.020162
	6 2.803266 -0.599122 0.252816		6 2.304979 -1.473616 0.306280
	6 1.463988 -1.540763 0.348952		6 0.730890 -1.360475 0.674495
	6 2.587777 0.800072 -0.342393		6 0.317273 0.192200 -0.198859
	1 2.300444 0.635519 -1.385982		28 -0.707002 -1.418420 -0.492527
	6 1.439289 1.528481 0.347109		15 -1.833002 -1.566843 -2.355364
	1 1.248239 2.455273 -0.201612		6 -0.318650 1.240222 0.382158
	1 1.755790 1.826024 1.350790		6 -1.098250 -2.834771 -3.453392
	28 -0.272630 -0.932166 -0.088301		1 -1.033101 -3.789582 -2.927318
	15 -1.128538 -2.513292 -1.538328		1 -1.691207 -2.971738 -4.362444
	6 -1.063730 1.250136 0.682130		1 -0.086070 -2.541278 -3.739441
	6 0.160309 0.758777 0.426029		6 -1.929493 -0.150997 -3.506123
	6 -0.047637 -3.018009 -2.921007		1 -2.436124 0.690236 -3.033548
	1 0.851730 -3.519571 -2.568808		1 -0.919441 0.173604 -3.765743
	1 -0.587721 -3.691210 -3.592681		1 -2.458569 -0.417611 -4.425229
	1 0.254191 -2.132670 -3.484269		6 -3.563974 -2.151087 -2.289627
	6 -2.557608 -1.899980 -2.498733		1 -3.986840 -2.265246 -3.291538
	1 -3.420009 -1.748737 -1.850333		1 -3.594385 -3.118449 -1.783275
	1 -2.316805 -0.945694 -2.970844		1 -4.179542 -1.455368 -1.718808
	1 -2.829003 -2.618057 -3.277551		6 2.751890 -0.374515 -0.657199
	6 -1.776317 -4.099689 -0.911504		6 1.480664 0.356246 -1.158160
	1 -2.148932 -4.721788 -1.729677		1 1.189772 -0.046242 -2.132834
	1 -0.999984 -4.645540 -0.374742		1 1.717921 1.410875 -1.305980
	1 -2.593898 -3.902346 -0.216007		6 -1.289208 1.067824 1.508719

Species	Cartesian coordinates			Species	Cartesian coordinates		
	6	-2.097251	0.176803	0.871441	6	-2.672980	0.967494	1.368764
	6	-3.341533	0.130525	0.218707	6	-0.806995	1.134101	2.820694
	6	-1.841231	-0.833581	1.812919	6	-3.528406	0.857886	2.458198
	6	-4.289032	-0.832546	0.514231	6	-1.641857	1.039632	3.922293
	6	-2.774218	-1.832787	2.088043	1	0.260127	1.262276	2.972276
	6	-4.003595	-1.821312	1.453987	6	-3.010028	0.881815	3.743121
	1	-5.245163	-0.824636	-0.000905	1	-4.598329	0.770574	2.296028
	1	-2.539295	-2.596503	2.824028	1	-1.220686	1.084225	4.922846
	1	-4.751206	-2.576055	1.681891	1	-3.676442	0.798064	4.596907
	14	-1.449077	3.054923	1.136673	14	-0.065901	3.057950	-0.110805
	6	-3.111606	3.125135	2.001815	6	1.632569	3.702531	0.381507
	1	-3.957362	2.902884	1.348749	1	1.871710	3.449547	1.418599
	1	-3.145213	2.428289	2.844627	1	2.442461	3.329266	-0.249357
	1	-3.266128	4.130164	2.407082	1	1.640800	4.794750	0.302455
	6	-1.393004	4.218010	-0.333486	6	-1.322756	4.105441	0.805107
	1	-0.443549	4.145178	-0.871338	1	-2.352312	3.838527	0.554388
	1	-2.194098	4.022579	-1.048604	1	-1.213357	4.025506	1.889973
	1	-1.494321	5.252760	0.008595	1	-1.181471	5.157232	0.535679
	6	-0.174449	3.644340	2.388042	6	-0.329671	3.326684	-1.951488
	1	-0.545798	4.550790	2.877236	1	-0.192484	4.384992	-2.196078
	1	0.005845	2.902078	3.170905	1	0.352649	2.753298	-2.583462
	1	0.786737	3.896972	1.934965	1	-1.350278	3.053803	-2.232563
	6	3.855774	1.658174	-0.332035	35	-3.478545	1.087824	-0.336671
	1	4.699175	1.062301	-0.687700	1	3.215793	-0.888806	-1.503674
	1	4.094071	1.944924	0.697686	6	3.796034	0.577703	-0.074377
	6	3.756686	2.910765	-1.198569	1	4.536500	0.001747	0.486949
	1	3.000310	3.597286	-0.802852	1	3.322092	1.256589	0.641317
	1	3.425988	2.633403	-2.207154	6	4.526629	1.377090	-1.148317
	6	5.084474	3.654226	-1.293278	1	3.815112	1.945443	-1.759701
	1	5.844642	2.984379	-1.709846	1	5.026533	0.682982	-1.835124
	1	5.425856	3.913813	-0.285079	6	5.558444	2.335801	-0.565720
	6	4.995311	4.915184	-2.142152	1	5.063097	3.025754	0.126442
	1	4.268733	5.620107	-1.727739	1	6.279103	1.768343	0.033390
	1	5.959345	5.427082	-2.198271	6	6.296498	3.128996	-1.635552
	1	4.683372	4.681347	-3.164177	1	5.603252	3.733486	-2.227631
	35	-3.741810	1.372351	-1.145586	1	7.032225	3.805497	-1.193500
	1	-0.921887	-0.783047	2.389556	1	6.827161	2.464741	-2.323684
INT7	5	2.898524	-2.631434	0.827493	**TS7**	5	2.485720	-2.581431	1.226979
	5	3.365138	-3.705518	-0.500153		5	3.013524	-3.857185	0.118771
	5	5.105245	-1.429148	-0.560776		5	4.938716	-1.737877	-0.003426
	5	4.731375	-2.960985	-1.361389		5	4.532141	-3.334818	-0.645166
	5	4.167375	-1.431798	-2.054043		5	4.189205	-1.878844	-1.593261
	5	2.462362	-1.260584	-1.639779		5	2.468027	-1.533429	-1.429349
	5	4.615444	-2.832174	0.409987		5	4.216688	-2.957289	1.065424
	5	3.985083	-1.244676	0.785331		5	3.685955	-1.293571	1.150901
	1	2.397251	-2.913946	1.860452		1	1.840321	-2.682468	2.212742
	1	3.223279	-4.881049	-0.405223		1	2.759910	-4.995922	0.342314
	1	6.142434	-0.859842	-0.504311		1	6.006807	-1.239545	0.114519
	1	5.583810	-3.596011	-1.891868		1	5.383629	-4.094353	-0.975932
	1	4.564404	-0.849648	-3.008418		1	4.746153	-1.461875	-2.554185
	1	1.718175	-0.544643	-2.216799		1	1.866716	-0.852045	-2.186386
	1	5.369835	-3.355795	1.163010		1	4.827334	-3.424536	1.970495
	1	4.179226	-0.540086	1.715367		1	3.826156	-0.482703	2.000634
	5	1.962151	-2.641950	-0.670751		5	1.738195	-2.732117	-0.366500
	1	0.821600	-2.947708	-0.669933		1	0.584784	-2.958665	-0.474037

Species	Cartesian coordinates	Species	Cartesian coordinates
	5 3.088518 -2.845901 -2.031153		5 2.997149 -3.197465 -1.531869
	1 2.745801 -3.380114 -3.034637		1 2.732188 -3.838534 -2.495602
	6 3.690150 -0.513504 -0.720668		6 3.636824 -0.756127 -0.460756
	6 2.435665 -1.182191 0.064235		6 2.244367 -1.221740 0.231948
	6 3.526092 1.001784 -0.669339		6 3.599316 0.759320 -0.623303
	1 3.125841 1.309286 -1.639275		1 3.345559 0.958582 -1.667965
	6 2.459774 1.235615 0.413097		6 2.436878 1.215884 0.274344
	1 1.844452 2.102595 0.173889		1 1.920168 2.069407 -0.165810
	1 2.956444 1.446455 1.365646		1 2.836036 1.542394 1.239399
	6 0.381697 -0.044379 1.081122		6 0.211410 0.185121 0.894603
	6 1.618830 -0.018682 0.575441		6 1.483921 0.054597 0.505292
	6 -0.378900 -1.307902 1.301512		6 -0.687212 -0.981251 1.129646
	6 -0.210780 -2.028060 2.485807		6 -0.769643 -1.560054 2.395460
	6 -1.353182 -1.766962 0.419965		6 -1.544136 -1.485146 0.148541
	6 -0.964763 -3.159681 2.757777		6 -1.645845 -2.602364 2.663693
	1 0.529175 -1.685018 3.204185		1 -0.123614 -1.181612 3.183428
	6 -2.122956 -2.891677 0.671705		6 -2.425695 -2.532181 0.393150
	6 -1.922550 -3.595007 1.850396		6 -2.475519 -3.089946 1.663099
	1 -0.803646 -3.703539 3.684397		1 -1.676063 -3.036851 3.658969
	1 -2.865616 -3.214543 -0.051452		1 -3.053609 -2.910459 -0.407472
	1 -2.518440 -4.479138 2.058058		1 -3.163076 -3.906461 1.863882
	14 -0.509009 1.532113 1.703665		14 -0.563527 1.887725 1.302729
	6 -2.083087 1.007915 2.567244		6 -2.109557 1.591342 2.313175
	1 -2.766363 0.481312 1.892535		1 -1.884233 1.133614 3.280728
	1 -1.889687 0.358956 3.425778		1 -2.605354 2.548111 2.507910
	1 -2.608344 1.895985 2.933476		1 -2.823179 0.945807 1.790882
	6 -0.947336 2.696724 0.300171		6 -0.986679 2.831114 -0.260200
	1 -0.128827 2.885887 -0.398349		1 -1.853650 2.387557 -0.761064
	1 -1.788310 2.300094 -0.277527		1 -1.237231 3.867718 -0.012043
	1 -1.256266 3.662637 0.713038		1 -0.165411 2.852353 -0.981711
	6 0.576593 2.412852 2.960652		6 0.601421 2.910269 2.369492
	1 -0.027732 3.142297 3.509221		1 1.382329 3.422348 1.803215
	1 0.990891 1.716121 3.695088		1 0.017355 3.683126 2.879706
	1 1.408003 2.959106 2.509675		1 1.084128 2.307671 3.144527
	6 4.825132 1.760158 -0.427611		6 4.921694 1.450423 -0.314980
	1 5.546372 1.486368 -1.204699		1 5.703491 1.021865 -0.950725
	1 5.260784 1.447808 0.528216		1 5.211786 1.243132 0.721298
	6 4.631008 3.272351 -0.437450		6 4.862621 2.956658 -0.543653
	1 3.938245 3.567528 0.359228		1 4.106937 3.406754 0.110707
	1 4.160898 3.573570 -1.381535		1 4.538097 3.156961 -1.572055
	6 5.940369 4.032638 -0.262538		6 6.202398 3.640134 -0.296754
	1 6.633407 3.746338 -1.061139		1 6.959408 3.198740 -0.954140
	1 6.413451 3.726712 0.677075		1 6.529890 3.434132 0.728215
	6 5.749901 5.543284 -0.269774		6 6.146302 5.144991 -0.521767
	1 5.087969 5.862085 0.540549		1 5.421710 5.617883 0.147373
	1 6.701953 6.065108 -0.145162		1 7.118105 5.611008 -0.341044
	1 5.306865 5.880629 -1.211139		1 5.851068 5.379745 -1.548408
	28 -3.621287 0.174008 -0.828973		35 -1.439311 -0.814261 -1.649120
	15 -5.465044 1.096271 -0.710960		28 -3.356055 0.080756 -0.787961
	6 -5.526969 2.909773 -0.984682		15 -5.182287 0.972030 -0.453351
	1 -5.130852 3.144822 -1.974763		6 -6.136285 0.536817 1.054980
	1 -6.546586 3.299448 -0.908918		1 -5.552248 0.784500 1.944214
	1 -4.899145 3.413422 -0.246522		1 -7.092715 1.066209 1.102376
	6 -6.752219 0.532903 -1.890374		1 -6.325925 -0.538629 1.070695
	1 -7.691674 1.078277 -1.759207		6 -5.214864 2.804143 -0.338908

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -6.398673 0.675821 -2.913481		1 -6.228392 3.187127 -0.184965
	1 -6.937447 -0.533713 -1.748286		1 -4.584482 3.130687 0.491301
	6 -6.376693 0.964513 0.876411		1 -4.808078 3.235313 -1.256173
	1 -5.777524 1.395702 1.681289		6 -6.458532 0.694153 -1.741930
	1 -7.340265 1.481134 0.836308		1 -7.393821 1.212185 -1.508742
	1 -6.549002 -0.086850 1.115973		1 -6.086668 1.047541 -2.705763
	35 -1.637402 -0.844390 -1.227654		1 -6.658918 -0.375260 -1.834704
INT8	5 -0.687303 3.241917 0.917920	**K_2CO_3**	6 -0.000016 0.833832 0.000000
	5 -0.721785 4.381407 -0.438005		8 -1.124853 1.456760 -0.000301
	5 -3.213066 2.969274 -0.423668		8 1.125018 1.456420 0.000302
	5 -2.283656 4.211295 -1.270044		8 -0.000214 -0.493360 -0.000002
	5 -2.374400 2.565740 -1.920124		19 2.622951 -0.641087 -0.000054
	5 -0.865522 1.749640 -1.509424		19 -2.622925 -0.641100 0.000055
	5 -2.195949 4.090511 0.503930	**PMe_3**	15 -0.000078 -0.000011 -0.593397
	5 -2.232907 2.394317 0.920176		6 0.627572 1.495378 0.273680
	1 -0.099253 3.329814 1.939528		1 0.039039 2.368207 -0.019191
	1 -0.126945 5.408027 -0.378998		1 0.585967 1.396935 1.362657
	1 -4.388977 2.853094 -0.342942		1 1.662985 1.686188 -0.018733
	1 -2.827571 5.116525 -1.814361		6 0.981468 -1.291083 0.273670
	1 -2.981606 2.163441 -2.856319		1 0.917361 -1.205511 1.362654
	1 -0.474525 0.787231 -2.076186		1 0.629019 -2.283298 -0.018348
	1 -2.672582 4.884468 1.247521		1 2.031538 -1.217772 -0.019503
	1 -2.675578 1.853084 1.873367		6 -1.608928 -0.204289 0.273751
	5 0.151120 2.852691 -0.586551		1 -2.070289 -1.150574 -0.018941
	1 1.318251 2.696232 -0.609327		1 -1.503084 -0.190797 1.362756
	5 -0.829278 3.443637 -1.943041		1 -2.292040 0.596745 -0.018996
	1 -0.319208 3.774078 -2.963835	**$KHCO_3$**	6 1.059499 0.041691 -0.000017
	6 -2.274330 1.566952 -0.565746		8 0.479819 1.150616 -0.000044
	6 -0.841944 1.704002 0.194941		8 2.433918 0.080119 0.000052
	6 -2.722995 0.114558 -0.466052		1 2.712815 -0.851140 0.000059
	1 -2.449986 -0.371718 -1.406539		8 0.530572 -1.106169 -0.000049
	6 -1.859526 -0.474088 0.652669		19 -1.927594 -0.020818 0.000019
	1 -1.643627 -1.522380 0.466983	**KBr**	35 0.000000 0.000000 1.084140
	1 -2.396381 -0.402641 1.604572		19 0.000000 0.000000 -1.997101
	6 0.480671 -0.069827 1.538300		
	6 -0.579715 0.327244 0.790678		
	6 1.678437 0.819556 1.663762		
	6 2.007670 1.599511 2.764375		
	6 2.477800 0.736791 0.527659		
	6 3.175120 2.350171 2.722980		
	1 1.350744 1.644727 3.629272		
	6 3.644344 1.497346 0.504654		
	6 3.984369 2.295990 1.594311		
	1 3.447237 2.983919 3.562810		
	1 4.304365 1.518946 -0.351632		
	1 4.893491 2.891392 1.554789		
	14 0.654326 -1.671519 2.578370		
	6 0.727353 -1.120053 4.372255		
	1 1.643537 -0.572127 4.602700		
	1 -0.124218 -0.491638 4.648953		
	1 0.703669 -2.002763 5.019313		
	6 2.276951 -2.479272 2.113614		
	1 2.232612 -2.895658 1.103130		
	1 3.111396 -1.774721 2.160545		
	1 2.493309 -3.301422 2.803825		

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 -0.722951 -2.931183 2.439970		
	1 -0.477299 -3.754459 3.119911		
	1 -1.696895 -2.543621 2.747886		
	1 -0.810439 -3.353919 1.437034		
	6 -4.219589 -0.059229 -0.242384		
	1 -4.761385 0.442716 -1.051045		
	1 -4.513450 0.440204 0.688189		
	6 -4.636829 -1.525000 -0.195858		
	1 -4.131060 -2.033049 0.633245		
	1 -4.303148 -2.028102 -1.111101		
	6 -6.142982 -1.699971 -0.041981		
	1 -6.651591 -1.201554 -0.874580		
	1 -6.475842 -1.189684 0.868780		
	6 -6.563846 -3.162439 0.010165		
	1 -6.096709 -3.677950 0.854197		
	1 -7.646879 -3.261876 0.118163		
	1 -6.270480 -3.689743 -0.901982		
	35 0.144803 -2.289416 -1.287388		
	28 1.451310 -0.499546 -0.431128		
	15 2.856486 -0.862917 -2.012019		
	6 3.529691 -2.551842 -1.960025		
	1 2.719259 -3.278811 -1.970327		
	1 4.189548 -2.721252 -2.814821		
	1 4.104304 -2.680429 -1.040517		
	6 2.070568 -0.692040 -3.645197		
	1 2.781043 -0.953988 -4.433795		
	1 1.193999 -1.333863 -3.711351		
	1 1.757280 0.344479 -3.785779		
	6 4.381156 0.091414 -2.293254		
	1 5.089620 -0.040780 -1.475520		
	1 4.848403 -0.278809 -3.209674		
	1 4.168123 1.152737 -2.425693		
TS8a	5 -0.133336 -0.276873 -2.201712	**CAT**	28 0.000014 -0.002311 -0.001713
	5 0.898319 -1.722781 -2.218827		15 -2.113219 -0.000218 -0.000267
	5 -1.794748 -2.607471 -2.470240		15 2.113219 -0.000217 -0.000264
	5 -0.128893 -3.152798 -2.365572		6 -2.946088 1.630802 0.090809
	5 -1.165087 -3.209097 -0.931325		1 -2.643064 2.245830 -0.758930
	5 -0.733511 -1.832110 0.098959		1 -4.035551 1.531602 0.086749
	5 -0.516629 -1.669291 -3.263470		1 -2.640773 2.148542 1.002324
	5 -1.778417 -0.852007 -2.392934		6 -2.948471 -0.891386 1.367217
	1 0.078280 0.819403 -2.612652		1 -4.037790 -0.834132 1.284159
	1 1.991302 -1.692484 -2.677591		1 -2.647195 -1.940824 1.359682
	1 -2.714171 -3.141094 -2.994565		1 -2.643117 -0.464134 2.324481
	1 0.230011 -4.148597 -2.909917		6 -2.952392 -0.735738 -1.455151
	1 -1.658843 -4.159355 -0.417287		1 -4.041450 -0.688203 -1.363151
	1 -1.011808 -1.797772 1.246578		1 -2.649772 -0.205670 -2.360462
	1 -0.466404 -1.566024 -4.446664		1 -2.651171 -1.779557 -1.563994
	1 -2.645869 -0.178507 -2.825383		6 2.952363 -0.737940 -1.454056
	5 0.550372 -0.865873 -0.684427		1 2.649700 -0.209265 -2.360166
	1 1.674763 -0.652850 0.225990		1 4.041422 -0.690240 -1.362167
	5 0.523365 -2.668017 -0.782912		1 2.651162 -1.781931 -1.561285
	1 1.314381 -3.336394 -0.204926		6 2.946056 1.630951 0.088347
	6 -2.068771 -1.795993 -1.016196		1 2.640715 2.150079 0.999064
	6 -1.143021 -0.481468 -0.828029		1 4.035522 1.531771 0.084460
	6 -3.422183 -1.492129 -0.384459		1 2.643036 2.244674 -0.762337

Species	Cartesian coordinates			Species	Cartesian coordinates		
	1	-3.387206	-1.860247 0.645611		6	2.948492	-0.889315 1.368552
	6	-3.476597	0.044979 -0.351705		1	2.647211	-1.938762 1.362622
	1	-4.146364	0.365379 0.443601		1	4.037810	-0.832193 1.285385
	1	-3.879634	0.424375 -1.293732		1	2.643161	-0.460604 2.325170
	6	-1.754024	1.374032 0.886475	**M2**	5	0.045439	2.546939 -1.367747
	6	-2.046226	0.488928 -0.082357		5	0.139289	4.023847 -0.396764
	6	-0.465439	1.487351 1.628308		5	2.742677	2.825646 -0.425311
	6	-0.616687	1.654970 3.016766		5	1.809681	4.196956 0.188418
	6	0.826845	1.376701 1.109318		5	2.161716	2.815845 1.239426
	6	0.457115	1.755153 3.879330		5	0.706133	1.823888 1.315088
	1	-1.617262	1.675381 3.441639		5	1.497477	3.570118 -1.447598
	6	1.910217	1.497187 1.995751		5	1.654525	1.829355 -1.386821
	6	1.743063	1.691727 3.354767		1	-0.681440	2.305124 -2.268193
	1	0.291567	1.876647 4.946709		1	-0.560410	4.952720 -0.639288
	1	2.919796	1.388786 1.604529		1	3.902880	2.766803 -0.656973
	1	2.611960	1.768847 4.004227		1	2.324355	5.252132 0.370737
	14	-3.165076	2.552156 1.445775		1	2.931373	2.735670 2.138754
	6	-2.493933	4.170610 2.124642		1	0.494869	1.037329 2.172646
	1	-1.729546	4.056350 2.894517		1	1.782139	4.149410 -2.444554
	1	-2.080091	4.797144 1.330945		1	2.016110	1.060714 -2.210036
	1	-3.331244	4.723837 2.564320		5	-0.538355	2.545265 0.300092
	6	-4.281249	1.797764 2.767078		1	-1.669806	2.314393 0.546639
	1	-4.520910	0.745823 2.592639		5	0.548614	3.564786 1.270768
	1	-3.834149	1.865525 3.762340		1	0.152643	4.142343 2.229760
	1	-5.226085	2.349548 2.801485		6	1.983040	1.467195 0.240741
	6	-4.223694	3.070258 -0.026317		6	0.456901	1.296817 -0.288170
	1	-4.676676	4.041974 0.195869		6	2.559859	0.075152 0.476407
	1	-3.623900	3.192783 -0.933110		1	2.512709	-0.108186 1.553278
	1	-5.039126	2.382163 -0.257570		6	1.581756	-0.871475 -0.238695
	6	-4.602396	-2.138887 -1.096359		1	1.500172	-1.819873 0.290758
	1	-4.442069	-3.221547 -1.140684		1	1.964346	-1.090278 -1.241116
	1	-4.641582	-1.786916 -2.133174		6	-0.931712	-0.839546 -0.521209
	6	-5.933557	-1.857256 -0.408454		6	0.229188	-0.194238 -0.372268
	1	-6.134304	-0.779668 -0.408215		6	-2.231042	-0.138261 -0.725272
	1	-5.873303	-2.160092 0.644182		6	-2.606416	0.280662 -2.002311
	6	-7.100668	-2.577835 -1.073127		6	-3.159805	0.028915 0.301480
	1	-6.909366	-3.656556 -1.067266		6	-3.840963	0.868151 -2.237928
	1	-7.154353	-2.282958 -2.126938		1	-1.909156	0.138918 -2.823776
	6	-8.433862	-2.292527 -0.395041		6	-4.397026	0.617010 0.084944
	1	-8.667513	-1.224168 -0.417225		6	-4.737925	1.040591 -1.191983
	1	-9.253354	-2.821694 -0.887965		1	-4.101176	1.192903 -3.241485
	1	-8.418523	-2.605874 0.652828		1	-5.087703	0.744197 0.912820
	28	1.502436	0.993699 -0.571982		1	-5.705853	1.502209 -1.365366
	15	1.586408	3.137763 -0.908445		14	-1.048576	-2.744872 -0.618999
	6	3.124643	3.926482 -0.342651		6	-2.853134	-3.217373 -0.769575
	1	3.124764	4.993473 -0.580792		1	-3.422769	-2.967027 0.128892
	1	3.216439	3.804505 0.738193		1	-3.339483	-2.731265 -1.619212
	1	3.974180	3.441226 -0.824264		1	-2.932554	-4.299101 -0.917798
	6	0.310280	4.200410 -0.165167		6	-0.328487	-3.588998 0.899775
	1	0.359603	4.142359 0.922633		1	0.734209	-3.824489 0.801803
	1	0.438225	5.240268 -0.479219		1	-0.463678	-2.986274 1.801326
	1	-0.675143	3.852838 -0.481796		1	-0.850101	-4.537173 1.062499
	6	1.469179	3.621808 -2.661660		6	-0.156103	-3.324849 -2.165071
	1	0.496454	3.322491 -3.057096		1	-0.273706	-4.406572 -2.282381
	1	1.575303	4.704711 -2.770720		1	-0.567163	-2.851613 -3.061284

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 2.245133 3.115568 -3.235321		1 0.915982 -3.114928 -2.139580
	6 2.777358 -2.203920 1.675702		6 4.007765 -0.081730 0.029149
	19 2.834865 -4.510309 3.599608		1 4.620218 0.670359 0.537343
	8 3.786946 -3.025025 1.616346		1 4.085330 0.124605 -1.044355
	8 1.803814 -2.392295 2.468955		6 4.567356 -1.467520 0.330674
	35 3.415934 0.761047 -2.093858		1 3.986039 -2.231019 -0.199326
	8 2.810574 -1.169283 0.865660		1 4.454147 -1.681766 1.400403
	19 4.583529 -2.027116 -0.808739		6 6.035000 -1.604264 -0.057158
			1 6.621267 -0.848112 0.476281
			1 6.149214 -1.382989 -1.124051
			6 6.596462 -2.988071 0.239886
			1 6.050942 -3.761880 -0.307904
			1 7.649163 -3.060032 -0.044511
			1 6.523433 -3.223146 1.305569
			35 -2.731736 -0.531375 2.054840
COM1a	5 0.071922 -0.691475 -1.958785	**INT9a**	5 -0.216914 -0.789714 2.361309
	5 1.539932 -1.423691 -1.297478		5 -1.081257 -2.309619 2.133827
	5 -0.498752 -3.421615 -1.246017		5 1.733120 -2.812506 1.750351
	5 1.182544 -3.093490 -0.840554		5 0.133474 -3.574271 1.764774
	5 -0.051002 -3.060054 0.424956		5 0.903066 -3.147492 0.233640
	5 -0.399415 -1.362838 0.760516		5 0.142600 -1.654320 -0.325154
	5 0.482640 -2.402039 -2.314598		5 0.514031 -2.299527 2.938752
	5 -1.147570 -1.947077 -1.948755		5 1.506356 -1.109820 2.127584
	1 -0.048958 0.149923 -2.785412		1 -0.486663 0.121739 3.064977
	1 2.620827 -1.127921 -1.694383		1 -2.071007 -2.561376 2.744370
	1 -1.001109 -4.461257 -1.517347		1 2.786970 -3.303158 1.983417
	1 1.994503 -3.970210 -0.882554		1 -0.001025 -4.710090 2.090655
	1 -0.243527 -3.857355 1.284331		1 1.400559 -3.851944 -0.582925
	1 -0.920410 -1.054815 1.776262		1 0.211294 -1.298088 -1.454190
	1 0.766019 -2.750260 -3.415941		1 0.662360 -2.498923 4.100905
	1 -2.081714 -1.942535 -2.669388		1 2.357653 -0.393287 2.532410
	5 0.573988 -0.266836 -0.306947		5 -1.092308 -1.094783 0.814055
	1 5.159452 -1.679653 3.494215		5 -0.833627 -2.854357 0.469593
	5 1.233247 -1.810578 0.394572		1 -1.631516 -3.488198 -0.143966
	1 2.062798 -1.817301 1.254027		6 1.623757 -1.650384 0.521836
	6 -1.375537 -2.323565 -0.314527		6 0.522339 -0.515445 0.874325
	6 -1.043837 -0.779178 -0.667200		6 2.720013 -0.999816 -0.317582
	6 -2.867122 -2.376377 0.028295		1 2.582208 -1.360036 -1.340608
	1 -2.952891 -2.282678 1.115634		6 2.418589 0.513081 -0.267816
	6 -3.451822 -1.091682 -0.610156		1 2.594623 0.977112 -1.238768
	1 -4.366911 -0.816743 -0.089200		1 3.107595 0.989281 0.438343
	1 -3.706166 -1.270199 -1.657232		6 0.294006 1.880897 0.188518
	6 -2.537576 1.027240 0.371201		6 1.007842 0.750053 0.242855
	6 -2.349986 -0.068901 -0.390656		6 -0.964242 2.020197 0.984482
	6 -1.526346 1.582753 1.320205		6 -1.058282 3.142344 1.812789
	6 -2.062324 1.866949 2.589789		6 -1.995250 1.064608 1.003159
	6 -0.134476 1.659937 1.132377		6 -2.142129 3.341498 2.655152
	6 -1.279341 2.183482 3.684267		1 -0.245255 3.865055 1.823679
	1 -3.136257 1.795067 2.742335		6 -3.082386 1.282136 1.867253
	6 0.642000 1.959100 2.273753		6 -3.170429 2.407403 2.675455
	6 0.102818 2.216956 3.521000		1 -2.176101 4.215981 3.299874
	1 -1.737799 2.382617 4.649230		1 -3.872170 0.533840 1.930790
	1 1.726263 2.009766 2.167674		1 -4.024711 2.543518 3.334546
	1 0.753640 2.449103 4.361522		14 0.829903 3.308615 -0.947467
	14 -4.298078 1.776597 0.365988		6 2.528891 3.980195 -0.510317

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 -4.218013 3.629305 0.655128		1 2.578539 4.273076 0.542479
	1 -3.639958 3.917502 1.535272		1 3.336431 3.267958 -0.693774
	1 -3.793821 4.141884 -0.212614		1 2.738805 4.872573 -1.108276
	1 -5.236525 4.010733 0.784117		6 -0.396326 4.726468 -0.894399
	6 -5.463485 1.031623 1.652039		1 -1.430121 4.373863 -0.935981
	1 -5.328103 -0.043689 1.794193		1 -0.298048 5.352952 -0.005294
	1 -5.347768 1.504047 2.631156		1 -0.229751 5.368976 -1.765360
	1 -6.499975 1.193455 1.339251		6 0.801566 2.668239 -2.716190
	6 -5.073616 1.583693 -1.337663		1 1.097305 3.460895 -3.410690
	1 -5.905461 2.290009 -1.428552		1 1.457329 1.813544 -2.895573
	1 -4.354601 1.823104 -2.126244		1 -0.214209 2.361147 -2.982771
	1 -5.473256 0.588828 -1.543258		6 4.135563 -1.359483 0.118370
	6 -3.558548 -3.659838 -0.410751		1 4.238400 -2.449572 0.124770
	1 -3.038671 -4.514083 0.036647		1 4.300970 -1.023556 1.148029
	1 -3.466431 -3.772915 -1.496578		6 5.199704 -0.765140 -0.797479
	6 -5.029743 -3.705563 -0.013023		1 5.124057 0.328528 -0.802097
	1 -5.575307 -2.891420 -0.503520		1 5.014954 -1.090266 -1.828768
	1 -5.122950 -3.533252 1.066355		6 6.613801 -1.162709 -0.390845
	6 -5.693111 -5.030704 -0.369491		1 6.695547 -2.255181 -0.389831
	1 -5.157945 -5.847620 0.127150		1 6.796876 -0.841737 0.640489
	1 -5.590781 -5.207953 -1.445842		6 7.678515 -0.572387 -1.305429
	6 -7.165217 -5.076186 0.017232		1 7.642419 0.520834 -1.299466
	1 -7.731556 -4.291181 -0.492107		1 8.682208 -0.872845 -0.994416
	1 -7.617518 -6.035707 -0.246023		1 7.538181 -0.902433 -2.338781
	1 -7.294854 -4.931794 1.093693		28 -2.434881 -0.218417 -0.206886
	28 0.864785 1.684138 -0.404122		15 -3.406143 -1.468704 -1.756861
	15 0.684996 3.910538 -0.574395		6 -4.525683 -0.466336 -2.802187
	6 2.196922 4.847145 -0.154091		1 -3.959635 0.315070 -3.313716
	1 2.053981 5.922910 -0.290309		1 -5.030745 -1.081146 -3.551875
	1 2.459354 4.660112 0.890245		1 -5.282130 0.018636 -2.181388
	1 3.018435 4.505488 -0.785125		6 -2.381067 -2.308113 -3.009761
	6 -0.551792 4.779695 0.446810		1 -3.000508 -2.837563 -3.738976
	1 -0.382639 4.560346 1.503394		1 -1.767848 -1.571985 -3.533328
	1 -0.511810 5.861588 0.290648		1 -1.713109 -3.022182 -2.526576
	1 -1.550176 4.421377 0.196020		6 -4.520503 -2.795097 -1.184373
	6 0.289535 4.534710 -2.243991		1 -5.290941 -2.368801 -0.538753
	1 -0.681363 4.144623 -2.557383		1 -5.002472 -3.302674 -2.024241
	1 0.257640 5.627636 -2.269539		1 -3.959598 -3.525118 -0.599625
	1 1.042328 4.174768 -2.946621		
	6 5.316232 -2.392841 1.738044		
	19 4.794249 -4.640879 -0.196003		
	8 5.323720 -2.087106 0.518733		
	8 5.386172 -3.528418 2.254690		
	35 2.677562 1.806564 -2.042682		
	8 5.183961 -1.312035 2.592780		
	19 3.967291 0.245197 0.430081		
TS9a	5 0.097090 -0.747272 -2.463438	**P1a**	5 0.847103 -2.149392 -1.418715
	5 0.969994 -2.264176 -2.255308		5 1.256105 -3.499104 -0.358052
	5 -1.831063 -2.760480 -1.765584		5 -1.598171 -3.100247 -0.268843
	5 -0.232979 -3.525876 -1.834200		5 -0.263211 -4.103520 0.350604
	5 -0.944302 -3.088876 -0.277878		5 -0.958525 -2.819137 1.350533
	5 -0.157510 -1.598261 0.246006		5 0.142760 -1.467574 1.283025
	5 -0.654619 -2.258916 -3.001557		5 -0.240158 -3.541818 -1.333634
	5 -1.614948 -1.062704 -2.161922		5 -0.895045 -1.920032 -1.367023
	1 0.338851 0.164113 -3.178205		1 2.178321 -4.209439 -0.598205

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 1.937524 -2.518087 -2.899797		1 -2.734430 -3.403768 -0.412870
	1 -2.893222 -3.251554 -1.956204		1 -0.440164 -5.246431 0.622372
	1 -0.113214 -4.662897 -2.161349		1 -1.669352 -2.908820 2.295846
	1 -1.411254 -3.789638 0.559545		1 0.173267 -0.582433 2.066294
	1 -0.198482 -1.235735 1.374381		1 -0.393069 -4.257058 -2.269037
	1 -0.845927 -2.463757 -4.156361		1 -1.500037 -1.340128 -2.201159
	1 -2.476418 -0.344087 -2.540133		5 1.488346 -1.822533 0.204444
	5 1.029878 -1.033706 -0.947148		5 0.817054 -3.066569 1.309468
	5 0.786599 -2.804064 -0.580721		1 1.409405 -3.442025 2.268330
	1 1.607332 -3.436834 0.003606		6 -1.226816 -1.534602 0.262811
	6 -1.674418 -1.590354 -0.548495		6 0.153790 -1.030626 -0.366445
	6 -0.583138 -0.470693 -0.947757		6 -2.104725 -0.287623 0.419541
	6 -2.735861 -0.911085 0.316144		1 -2.098716 -0.029340 1.482478
	1 -2.563428 -1.247941 1.341957		6 -1.359797 0.823495 -0.366091
	6 -2.424028 0.600183 0.222870		1 -1.547494 1.798127 0.079493
	1 -2.586799 1.092217 1.180291		1 -1.748939 0.859232 -1.389930
	1 -3.110971 1.062786 -0.495201		6 1.233173 1.180888 -0.279318
	6 -0.218899 1.874484 -0.221841		6 0.110974 0.451094 -0.409168
	6 -1.012693 0.798717 -0.294428		6 2.568371 0.501533 -0.167011
	6 1.051312 1.898496 -1.011726		6 3.729211 1.242586 -0.408364
	6 1.300068 3.034592 -1.785559		6 2.723381 -0.857971 0.198306
	6 1.950923 0.813917 -1.083050		6 4.996744 0.708401 -0.233723
	6 2.403274 3.125133 -2.622039		1 3.646977 2.260918 -0.764802
	1 0.593463 3.861512 -1.762165		6 4.003646 -1.372683 0.395748
	6 3.053368 0.917699 -1.950574		6 5.139681 -0.601433 0.201370
	6 3.292798 2.060481 -2.699512		1 5.871689 1.320229 -0.437402
	1 2.556751 4.017979 -3.222621		1 4.110755 -2.416390 0.682823
	1 3.723779 0.067146 -2.059426		1 6.126994 -1.028101 0.357706
	1 4.156106 2.111858 -3.358571		14 0.972850 3.052311 0.037280
	14 -0.640105 3.384194 0.854059		6 2.498381 4.139526 0.165520
	6 0.936767 4.329191 1.223189		1 3.222018 3.790746 0.905772
	1 1.694736 3.666799 1.651827		1 3.017815 4.291853 -0.783898
	1 1.380277 4.804414 0.346657		1 2.151370 5.125222 0.495074
	1 0.729821 5.113489 1.958239		6 0.154623 3.210165 1.724711
	6 -1.333141 2.851050 2.523923		1 -0.737025 2.597334 1.869248
	1 -2.421448 2.753469 2.534144		1 0.870755 2.922565 2.500504
	1 -0.901570 1.906229 2.866618		1 -0.124978 4.251549 1.912702
	1 -1.079465 3.610655 3.270004		6 -0.055654 3.800254 -1.344607
	6 -1.892018 4.494906 0.003843		1 -0.226870 4.862101 -1.142196
	1 -2.153937 5.340566 0.647083		1 0.490428 3.735485 -2.290487
	1 -1.514137 4.901926 -0.937823		1 -1.030119 3.334762 -1.499668
	1 -2.815644 3.953548 -0.220600		6 -3.551314 -0.488025 -0.014279
	6 -4.168632 -1.268913 -0.060494		1 -3.975375 -1.325375 0.549909
	1 -4.279962 -2.357980 -0.036357		1 -3.583018 -0.775745 -1.070806
	1 -4.367774 -0.957108 -1.091756		6 -4.411663 0.750801 0.208630
	6 -5.195338 -0.642654 0.876609		1 -4.024671 1.588145 -0.383445
	1 -5.112524 0.450075 0.848517		1 -4.343894 1.058473 1.259330
	1 -4.975589 -0.941098 1.909074		6 -5.874068 0.521456 -0.154582
	6 -6.625625 -1.040781 0.531875		1 -6.267770 -0.309716 0.440577
	1 -6.714505 -2.132198 0.564581		1 -5.941329 0.206524 -1.201723
	1 -6.843433 -0.747404 -0.500939		6 -6.735926 1.757700 0.062811
	6 -7.653019 -0.417109 1.466780		1 -6.385947 2.595637 -0.546907
	1 -7.610138 0.675222 1.428576		1 -7.778872 1.567418 -0.202274
	1 -8.669144 -0.718677 1.200439		1 -6.711879 2.076600 1.108765
	1 -7.477830 -0.719009 2.503401		1 1.440894 -1.740477 -2.358525

Species	Cartesian coordinates			Species	Cartesian coordinates
	28	2.360031	-0.350241 0.255363		
	15	3.295008	-1.468689 1.891708		
	6	4.486380	-2.765006 1.406731		
	1	5.277709	-2.324700 0.796841		
	1	4.936374	-3.245613 2.279825		
	1	3.981007	-3.521493 0.804204		
	6	4.306466	-0.430717 3.008941		
	1	3.679733	0.331050 3.477265		
	1	4.780130	-1.027814 3.792803		
	1	5.084687	0.080351 2.438284		
	6	2.222376	-2.352523 3.074748		
	1	2.809195	-2.866124 3.841592		
	1	1.548421	-1.643635 3.559875		
	1	1.614151	-3.086105 2.542953		

Table S5. Vibrational frequencies for stationary points on **Path a**, obtained at PCM-LC-ωPBE/ DZVP level in toluene solution.

Species	Frequencies (cm^{-1})
M1	30 46 49 55 68 80 104 114 123 151 167 179 188 194 210 227 231 246 252 256 259 263 312 345 379 434 478 507 529 557 568 591 596 605 612 613 641 656 682 689 708 713 726 729 740 747 755 759 760 768 772 775 778 780 781 788 792 801 806 814 841 856 873 879 884 888 897 925 932 938 940 953 953 956 959 960 961 966 966 968 971 976 982 983 985 987 992 1002 1013 1038 1065 1073 1075 1083 1108 1116 1123 1161 1194 1204 1258 1277 1294 1330 1347 1360 1362 1362 1374 1383 1412 1440 1458 1466 1477 1483 1485 1493 1497 1505 1506 1511 1520 1523 1530 2702 2705 2709 2714 2718 2726 2730 2741 2745 2758 3028 3086 3092 3095 3101 3101 3105 3106 3107 3134 3139 3156 3167 3190 3195 3213 3216 3217 3221 3232 3237
R3	10 38 49 105 113 143 163 164 172 176 202 207 245 294 303 370 380 422 475 581 587 607 660 695 700 722 723 757 789 790 791 850 883 883 898 912 1000 1034 1077 1093 1167 1180 1267 1302 1322 1326 1326 1333 1476 1481 1481 1488 1489 1494 1498 1545 1683 1715 2345 3096 3097 3097 3200 3200 3201 3207 3207 3208 3250 3261 3270 3275
INT1	13 23 33 36 42 49 51 60 63 71 88 98 101 110 116 126 135 138 142 150 158 161 169 176 183 191 197 199 209 213 215 223 230 239 245 251 258 259 276 286 294 314 337 345 355 367 374 426 459 462 474 480 511 530 554 566 573 582 589 599 603 615 616 617 644 656 662 680 697 698 705 710 721 722 726 727 737 741 752 754 756 764 766 769 770 771 777 781 785 786 789 791 793 797 802 811 817 840 849 855 869 877 882 883 884 890 894 900 912 923 933 942 944 953 956 961 962 963 966 969 972 972 973 977 978 982 991 993 999 1000 1004 1014 1033 1036 1072 1077 1077 1086 1094 1107 1109 1120 1130 1167 1169 1182 1208 1228 1253 1261 1283 1291 1298 1326 1327 1328 1329 1336 1346 1359 1360 1360 1372 1382 1417 1441 1458 1470 1476 1477 1479 1481 1482 1485 1488 1491 1492 1494 1498 1501 1506 1507 1511 1521 1523 1530 1545 1684 1712 2166 2697 2699 2705 2712 2725 2734 2739 2742 2748 2757 3087 3092 3094 3095 3096 3099 3104 3105 3108 3109

	3112 3118 3139 3158 3181 3185 3190 3193 3195 3197 3198 3202 3208 3211 3214 3216 3216 3228 3240 3250 3251 3261 3270 3275
TS1	-177 20 24 28 39 49 55 57 59 67 78 95 100 110 124 131 134 153 156 160 166 168 177 182 185 188 199 204 208 212 217 219 235 244 250 253 257 266 276 282 289 313 321 350 374 381 387 429 433 475 480 512 532 552 557 570 590 599 603 607 615 617 623 635 650 655 680 692 697 698 712 714 717 726 729 742 746 748 754 759 762 767 768 769 777 780 782 784 786 789 792 794 796 803 812 816 820 837 864 872 876 876 877 881 885 889 905 909 924 932 935 942 947 953 958 962 963 964 968 970 971 975 977 981 984 986 988 995 996 999 1000 1018 1030 1033 1067 1075 1076 1080 1090 1094 1104 1115 1131 1164 1170 1179 1192 1237 1256 1260 1286 1292 1297 1318 1325 1329 1331 1339 1351 1360 1360 1361 1382 1387 1411 1441 1457 1475 1476 1479 1480 1481 1487 1489 1490 1491 1492 1497 1498 1502 1506 1508 1512 1521 1523 1530 1538 1682 1711 1906 2700 2702 2707 2711 2716 2721 2723 2741 2751 2773 3046 3090 3094 3094 3096 3097 3101 3105 3106 3107 3112 3141 3144 3161 3177 3191 3193 3193 3195 3197 3206 3207 3207 3214 3216 3217 3218 3239 3244 3252 3254 3259 3264 3273
INT2	21 25 38 46 48 50 52 57 64 69 84 96 104 121 129 135 148 152 156 159 170 175 179 183 189 198 207 210 214 215 227 231 239 245 251 259 262 273 282 287 295 309 333 357 369 397 418 437 456 468 504 512 520 561 576 583 591 599 605 615 617 621 624 645 669 678 693 697 699 710 714 717 717 725 727 741 744 751 760 765 766 770 774 774 779 781 784 786 789 791 793 798 804 810 812 831 845 861 872 876 879 881 883 887 893 905 910 915 932 941 948 952 954 959 963 964 965 966 969 971 974 979 981 985 988 990 995 996 998 1001 1020 1030 1031 1055 1074 1078 1080 1088 1099 1104 1117 1138 1157 1163 1171 1178 1206 1245 1256 1284 1296 1302 1311 1322 1324 1328 1338 1342 1358 1359 1363 1366 1379 1405 1411 1441 1456 1473 1480 1480 1481 1483 1484 1489 1491 1492 1494 1497 1501 1503 1505 1510 1519 1523 1527 1530 1532 1680 1684 1721 2699 2700 2706 2709 2710 2715 2717 2724 2735 2762 2967 3090 3092 3093 3094 3095 3102 3104 3105 3108 3110 3143 3154 3163 3179 3189 3190 3191 3192 3193 3197 3200 3212 3212 3215 3218 3219 3234 3238 3241 3250 3253 3263 3272
TS2	-28 19 27 40 44 52 58 65 70 76 78 98 106 112 121 133 138 141 151 156 165 175 178 180 194 199 201 205 213 220 230 240 245 246 253 256 266 277 282 284 290 294 339 360 370 391 417 441 453 492 512 517 529 565 575 593 600 604 614 618 621 628 640 644 668 687 695 699 703 708 711 714 719 726 732 742 747 750 762 762 765 768 771 775 777 783 785 790 791 794 795 800 809 813 820 832 842 862 870 874 875 879 880 883 891 903 917 924 927 939 944 950 955 961 963 964 966 967 970 971 974 979 982 985 992 997 1000 1004 1009 1012 1021 1023 1039 1041 1077 1081 1084 1088 1101 1105 1117 1136 1156 1164 1173 1182 1240 1243 1252 1278 1291 1302 1320 1320 1327 1327 1337 1346 1359 1360 1364 1373 1381 1406 1422 1441 1456 1477 1477 1479 1484 1485 1486 1489 1490 1491 1494 1497 1502 1502 1506 1507 1510 1510 1520 1523 1530 1574 1678 1705 2693 2695 2699 2703 2709 2714 2718 2745 2749 2764 3088 3091 3092 3093 3094 3100 3101 3104 3106 3107 3114 3143 3161 3173 3182 3186 3188 3190 3191 3194 3195 3205 3206 3207 3208 3208 3220 3228 3243 3251 3252 3263 3272 3277

INT3	23 26 34 46 51 55 61 67 72 77 81 92 96 119 125 131 141 146 157 164 170 173 181 183 194 198 199 209 219 224 228 233 236 242 245 253 261 265 274 279 297 322 327 363 377 392 405 431 455 498 507 517 542 567 570 585 595 604 606 616 617 625 642 647 671 685 693 694 701 712 713 717 719 727 738 743 748 752 760 762 769 771 772 774 777 778 778 789 789 793 795 798 802 810 813 830 843 852 870 871 873 876 882 886 892 904 914 925 931 942 945 946 957 960 961 964 965 966 969 973 978 980 981 983 987 997 997 998 1003 1010 1023 1037 1038 1067 1074 1079 1083 1089 1102 1114 1118 1128 1164 1166 1167 1182 1231 1242 1256 1275 1292 1299 1319 1323 1324 1325 1334 1346 1358 1359 1359 1365 1379 1406 1413 1440 1456 1474 1475 1477 1481 1483 1486 1488 1489 1490 1492 1496 1499 1504 1507 1510 1512 1517 1521 1523 1530 1599 1676 1704 2695 2697 2701 2706 2713 2726 2729 2739 2751 2769 3087 3090 3093 3094 3095 3102 3102 3104 3106 3109 3115 3123 3141 3161 3176 3190 3191 3192 3193 3196 3198 3199 3207 3210 3214 3215 3217 3227 3233 3241 3249 3258 3267 3274
TS3	-95 14 19 31 39 49 54 63 68 76 87 93 101 110 119 123 138 150 157 160 165 176 179 186 191 198 206 219 225 230 231 240 242 246 250 253 259 276 283 285 295 302 315 348 358 372 401 418 441 466 492 507 515 555 570 584 592 598 605 616 617 625 635 643 653 674 689 701 704 707 712 713 717 718 728 743 747 750 762 763 764 769 771 772 774 778 780 784 789 794 795 803 805 809 821 826 840 857 862 868 872 874 877 880 883 887 915 917 928 936 943 952 956 958 964 965 966 967 970 970 973 978 978 981 989 995 997 1000 1007 1008 1019 1037 1039 1062 1074 1081 1086 1092 1100 1112 1117 1135 1155 1169 1171 1183 1240 1249 1271 1278 1300 1304 1317 1321 1326 1329 1336 1351 1358 1359 1364 1372 1380 1409 1421 1440 1456 1474 1476 1479 1482 1485 1487 1488 1490 1493 1495 1497 1500 1502 1507 1511 1511 1521 1523 1530 1538 1680 1708 1773 2696 2698 2704 2712 2723 2724 2730 2737 2745 2757 3086 3088 3093 3094 3095 3102 3103 3105 3110 3113 3114 3141 3161 3161 3180 3189 3190 3191 3193 3193 3196 3209 3213 3221 3221 3222 3236 3239 3240 3247 3249 3256 3266 3274
INT4	16 19 33 35 42 47 54 61 70 84 87 90 105 123 124 138 139 148 156 158 169 172 180 183 190 206 217 223 228 230 238 242 243 247 252 259 265 273 285 298 299 323 334 358 367 382 392 421 446 460 497 506 521 543 567 576 579 591 602 609 615 618 625 643 652 658 682 692 693 701 703 706 712 721 728 735 749 752 762 764 764 768 770 772 774 779 781 783 786 788 790 797 805 810 816 825 827 834 850 862 868 873 875 881 883 884 911 921 927 936 945 951 958 960 964 966 968 970 972 973 978 980 982 986 992 996 998 999 1004 1008 1018 1031 1033 1046 1074 1079 1083 1086 1100 1106 1114 1129 1154 1164 1167 1179 1233 1250 1271 1280 1295 1298 1312 1316 1322 1328 1334 1349 1358 1359 1361 1370 1381 1411 1416 1440 1457 1469 1472 1477 1480 1481 1481 1484 1487 1491 1491 1492 1500 1506 1508 1511 1518 1521 1523 1530 1542 1680 1713 2045 2696 2699 2704 2713 2731 2733 2737 2741 2748 2759 3090 3090 3091 3093 3093 3101 3106 3108 3111 3113 3117 3142 3150 3161 3182 3183 3191 3195 3196 3196 3202 3213 3216 3218 3227 3234 3238 3244 3248 3251 3255 3259 3269 3274
TS4	-21 28 34 45 53 57 69 72 76 87 92 101 110 118 125 128 133 142 150 152 157 166 176 181 187 195 206 217 220 231 234 242 245 254 258 262 270 273 286 290 297 299 324 335 361 375 380 409 452 468 500 502 510 548 564 570 587 592 601 609 614 616 624 639 643 665 681 695 696 700 701 703

	710 711 722 738 742 748 755 759 763 765 765 771 772 776 778 780 788 790 791 796 798 809 814 818 833 835 850 858 866 870 874 878 880 885 913 918 929 935 937 942 953 957 958 961 962 965 967 970 974 978 980 982 985 992 997 999 1002 1003 1012 1033 1033 1048 1069 1075 1081 1082 1095 1104 1110 1132 1151 1162 1165 1177 1232 1245 1266 1273 1289 1296 1313 1318 1323 1327 1333 1348 1355 1359 1360 1368 1380 1411 1413 1440 1454 1472 1473 1479 1480 1484 1485 1487 1488 1489 1490 1496 1501 1503 1506 1511 1515 1521 1524 1530 1539 1672 1703 1927 2702 2705 2710 2718 2732 2740 2745 2749 2754 2762 3084 3086 3088 3094 3095 3097 3105 3107 3108 3109 3116 3132 3137 3156 3180 3185 3187 3190 3191 3194 3195 3210 3214 3219 3225 3229 3231 3243 3244 3247 3255 3259 3268 3274
INT5	12 21 29 42 43 55 60 65 67 71 76 81 95 106 118 127 137 141 144 148 156 165 169 175 186 190 198 203 209 212 227 233 240 243 244 248 254 261 270 276 286 291 316 334 350 373 400 439 465 476 508 515 532 562 569 580 591 598 603 611 616 617 647 650 678 681 695 699 704 710 714 715 717 728 738 745 750 751 762 767 769 772 774 775 778 779 782 786 790 792 797 803 807 810 818 832 848 857 868 870 875 877 879 883 886 904 915 920 935 941 946 953 956 960 962 962 964 965 968 970 974 977 983 984 990 993 999 1000 1001 1010 1021 1034 1036 1067 1075 1078 1086 1092 1103 1117 1119 1146 1163 1169 1179 1181 1239 1246 1257 1277 1295 1304 1315 1320 1323 1326 1334 1345 1358 1361 1362 1369 1382 1407 1413 1441 1458 1473 1475 1478 1480 1484 1485 1489 1490 1492 1492 1495 1497 1501 1505 1509 1510 1520 1523 1530 1536 1675 1683 1711 2700 2703 2708 2712 2718 2723 2736 2739 2751 2765 3088 3091 3093 3094 3097 3101 3101 3104 3106 3106 3113 3123 3144 3161 3180 3187 3188 3190 3191 3193 3196 3206 3210 3211 3212 3213 3218 3228 3234 3243 3244 3254 3263 3272
TS5	-12 22 33 36 46 49 53 57 69 80 90 104 107 121 123 126 128 143 153 163 166 176 184 188 195 196 202 213 221 228 232 237 242 245 247 256 260 263 273 280 282 297 341 354 366 396 400 452 472 476 506 508 521 563 574 588 597 602 609 616 618 627 641 650 655 685 693 702 708 711 712 715 721 725 735 745 746 752 762 768 768 770 772 776 779 780 781 785 790 792 796 797 800 812 817 820 832 848 855 863 875 876 878 880 882 883 914 916 923 935 943 944 957 958 963 964 966 967 969 975 978 981 983 984 989 991 998 999 1003 1005 1017 1033 1038 1051 1074 1079 1084 1087 1100 1109 1115 1133 1139 1168 1168 1185 1221 1248 1256 1269 1298 1300 1318 1327 1328 1329 1338 1346 1357 1359 1360 1371 1381 1398 1414 1441 1452 1458 1473 1475 1479 1481 1485 1486 1487 1490 1493 1494 1499 1504 1505 1511 1511 1520 1523 1530 1539 1626 1679 1714 2697 2699 2704 2711 2720 2724 2728 2735 2744 2753 3089 3089 3093 3094 3096 3101 3102 3106 3106 3111 3134 3143 3161 3168 3186 3188 3191 3193 3193 3197 3202 3208 3210 3210 3212 3220 3221 3230 3240 3246 3249 3259 3267 3274
INT6	19 25 33 42 44 52 56 60 66 80 83 89 100 107 113 119 133 135 140 144 151 156 168 176 183 188 189 195 208 217 229 233 239 242 246 250 253 264 274 286 291 312 319 338 352 389 423 443 459 469 506 523 528 552 567 587 592 601 609 613 615 621 640 644 653 679 694 699 700 707 711 714 716 727 729 738 752 753 761 766 766 768 771 775 778 782 784 785 786 793 795 799 802 809 818 836 846 852 871 874 876 877 880 880 892 912 914 923 935 940 942 946 954 957 960 964 965 967

	968 970 978 981 981 985 991 994 995 998 1001 1007 1025 1026 1041 1069 1076 1080 1082 1097 1104 1118 1125 1152 1160 1172 1182 1196 1236 1251 1265 1275 1299 1304 1319 1320 1324 1325 1334 1347 1358 1360 1361 1368 1382 1412 1415 1441 1458 1475 1477 1480 1482 1484 1484 1486 1486 1490 1493 1497 1498 1503 1507 1508 1511 1521 1523 1524 1530 1668 1678 1700 2701 2703 2707 2711 2720 2737 2743 2749 2758 2766 3089 3092 3093 3095 3097 3101 3105 3106 3107 3114 3115 3127 3142 3161 3178 3189 3190 3191 3192 3192 3196 3207 3211 3213 3215 3216 3216 3235 3241 3246 3249 3255 3263 3270
TS6	-260 12 25 39 44 49 57 59 69 73 76 80 86 99 114 124 131 143 148 152 156 167 173 176 177 188 190 200 206 213 214 228 232 236 247 251 260 264 270 277 287 309 320 338 346 368 383 425 462 470 490 505 531 536 546 567 581 594 599 604 610 613 632 640 654 671 689 699 705 709 709 711 712 721 724 736 740 746 754 759 761 762 767 769 770 773 776 779 780 786 787 790 795 801 807 809 837 872 872 873 876 877 878 886 891 903 915 918 929 933 936 938 945 947 952 957 958 960 963 965 965 973 975 976 978 983 986 993 997 1010 1019 1030 1032 1059 1068 1074 1082 1093 1100 1105 1113 1142 1152 1163 1172 1178 1229 1245 1261 1284 1286 1293 1314 1321 1325 1325 1334 1342 1348 1356 1356 1367 1377 1377 1418 1442 1459 1476 1477 1478 1480 1485 1487 1488 1490 1491 1493 1496 1499 1501 1509 1512 1514 1522 1523 1531 1538 1641 1681 1714 2449 2712 2714 2717 2722 2726 2738 2754 2776 2786 3085 3091 3093 3093 3094 3096 3101 3102 3104 3119 3120 3136 3139 3159 3186 3188 3192 3192 3193 3196 3197 3205 3206 3207 3208 3209 3209 3219 3233 3237 3245 3257 3266 3272
INT7	12 15 17 20 32 41 50 53 54 55 65 68 70 87 94 108 125 133 140 159 167 170 174 179 181 183 190 191 200 205 217 218 229 245 249 254 261 262 270 275 279 301 318 341 376 404 444 458 466 485 500 504 530 538 560 587 596 601 610 613 618 624 643 656 669 683 689 705 705 713 716 717 720 733 740 742 751 751 753 756 759 760 768 769 775 779 780 782 783 791 792 801 801 803 804 863 866 868 869 875 878 878 883 899 906 920 929 932 939 942 948 950 953 957 960 960 964 965 967 969 970 970 973 977 979 982 986 991 996 1013 1028 1032 1055 1065 1074 1077 1085 1092 1112 1126 1139 1157 1162 1178 1181 1232 1247 1267 1274 1292 1296 1309 1321 1327 1330 1334 1337 1348 1351 1351 1352 1363 1371 1387 1421 1444 1463 1471 1476 1478 1481 1485 1486 1486 1491 1492 1494 1494 1496 1504 1508 1509 1511 1521 1523 1530 1540 1683 1715 1781 2720 2721 2727 2733 2741 2755 2766 2768 2774 2787 3081 3084 3088 3093 3094 3094 3095 3095 3100 3103 3122 3139 3141 3159 3172 3179 3182 3191 3192 3196 3198 3200 3203 3204 3204 3207 3213 3218 3219 3221 3242 3253 3263 3272
M2	19 35 41 45 50 54 64 68 81 86 118 126 143 147 158 167 171 185 192 202 207 226 242 248 251 268 278 301 323 348 378 443 456 468 485 500 504 532 539 561 588 596 601 610 613 618 624 643 656 670 684 693 704 713 716 719 722 733 740 744 753 756 758 760 767 771 775 779 781 783 783 787 790 802 804 804 864 868 873 876 878 884 899 909 919 929 932 938 942 949 950 953 957 960 960 964 965 967 970 973 976 979 982 991 999 1013 1028 1033 1055 1073 1074 1077 1085 1094 1113 1126 1139 1157 1164 1178 1181 1232 1247 1267 1275 1292 1297 1309 1320 1326 1328 1334 1336 1348 1353 1363 1387 1421 1444 1463 1479 1481 1483 1488 1493 1496 1497 1504 1508 1511 1521 1523 1530 1541 1685 1714 1782 2719 2720 2726 2733 2740 2754 2766 2770 2775 2789 3088 3093 3094 3094 3096 3100 3103 3119 3139 3141 3159 3172 3192 3193 3194 3195 3198 3204 3208 3208

	3218 3242 3253 3263 3272
TS7	-78 20 21 26 31 44 45 55 57 63 65 71 74 92 96 126 128 134 148 158 169 172 173 175 183 186 192 197 199 205 218 218 233 246 248 249 259 262 266 271 275 294 318 340 375 405 441 445 461 486 500 503 530 539 560 588 596 601 610 612 618 625 643 654 668 682 685 705 707 713 714 718 719 733 738 740 747 751 753 756 759 760 762 768 775 778 780 782 783 791 793 800 801 803 804 863 866 867 869 875 877 880 883 900 901 920 929 931 940 941 948 950 952 957 960 960 964 965 967 968 969 970 973 976 979 983 986 991 993 1013 1028 1031 1053 1056 1074 1077 1085 1091 1112 1127 1138 1156 1158 1178 1181 1233 1246 1266 1273 1291 1297 1308 1320 1326 1327 1333 1335 1348 1349 1350 1353 1363 1369 1387 1421 1444 1463 1470 1477 1478 1481 1483 1486 1486 1488 1490 1493 1496 1497 1506 1508 1510 1511 1521 1523 1530 1534 1677 1707 1778 2720 2721 2727 2733 2741 2755 2765 2769 2774 2791 3078 3078 3088 3092 3092 3093 3094 3094 3100 3103 3124 3139 3141 3159 3172 3178 3179 3189 3192 3192 3194 3198 3201 3202 3203 3204 3207 3216 3217 3220 3241 3252 3263 3272
INT8	13 18 38 41 44 46 58 63 70 72 81 93 111 121 131 137 144 154 158 173 176 180 183 188 192 203 204 211 214 217 230 234 247 249 259 263 276 283 286 297 314 320 353 361 381 396 438 451 455 480 497 506 525 536 559 587 596 601 611 612 619 622 638 653 674 683 685 706 710 713 717 719 721 734 739 745 752 756 758 760 766 769 770 775 780 781 782 784 785 790 790 802 807 808 821 860 865 876 879 884 885 887 888 898 909 913 928 931 938 940 947 950 953 957 957 960 963 965 967 969 974 977 980 984 985 988 991 995 1001 1011 1030 1031 1055 1064 1074 1077 1084 1088 1112 1128 1135 1154 1158 1180 1182 1233 1239 1267 1273 1288 1295 1304 1322 1323 1328 1333 1334 1349 1356 1356 1359 1366 1380 1390 1423 1444 1463 1472 1473 1481 1482 1487 1488 1490 1492 1493 1498 1499 1505 1506 1509 1511 1513 1521 1523 1523 1530 1684 1691 1710 2718 2719 2724 2732 2741 2756 2762 2771 2779 2810 3089 3091 3092 3093 3094 3097 3101 3107 3108 3108 3119 3141 3144 3157 3170 3189 3189 3191 3193 3197 3204 3209 3213 3215 3216 3218 3234 3242 3243 3248 3251 3253 3259 3311
K_2CO_3	16 57 99 210 239 248 692 699 881 1071 1420 1559
$KHCO_3$	60 149 195 569 581 682 847 1033 1247 1434 1757 3783
CAT	4 42 47 114 116 180 181 182 193 194 214 215 218 219 257 257 263 263 264 365 382 697 709 755 755 755 755 803 803 864 864 871 871 972 972 972 972 975 1001 1352 1352 1352 1352 1372 1373 1478 1478 1486 1486 1486 1487 1494 1494 1495 1495 1507 1508 3095 3095 3096 3096 3096 3096 3205 3205 3205 3205 3205 3205 3221 3221 3221 3221 3221 3221
PMe_3	174 210 210 255 255 298 697 755 755 806 861 861 978 978 998 1359 1359 1381 1484 1490 1490 1499 1499 1511 3090 3091 3091 3196 3198 3198 3209 3210 3210
KBr	20 20 155
TS8a	-1262 19 24 27 37 42 45 46 57 59 65 67 68 75 82 85 89 95 104 109 111 113 124 128 133 144 147 160 168 172 176 178 182 189 194 197 206 207 211 217 218 229 235 244 248 251 255 260 267 272 280 283 286 295 308 338 360 377 381 433 483 485 489 498 510 525 538 563 589 599 604 611 618 629 631 644 659 668 683 689 696 706 708 711 713 717 720 727 740 742 748 758 759 762 765 767

	775 779 780 784 785 789 793 797 800 803 806 818 820 838 851 858 867 874 875 879 880 887 893 901 906 920 927 931 934 938 942 946 954 956 961 965 966 970 973 980 980 983 990 991 992 999 1002 1017 1019 1028 1050 1067 1072 1075 1080 1091 1103 1110 1118 1128 1150 1151 1161 1181 1182 1221 1225 1258 1266 1283 1292 1296 1325 1329 1331 1338 1342 1349 1350 1351 1355 1361 1370 1375 1385 1420 1444 1457 1463 1469 1473 1480 1484 1486 1486 1487 1490 1494 1494 1497 1500 1506 1510 1511 1520 1523 1523 1530 1541 1595 1672 1701 1739 2700 2707 2715 2724 2731 2739 2748 2782 2785 3087 3092 3093 3093 3095 3099 3100 3102 3103 3104 3130 3139 3143 3157 3170 3188 3191 3192 3192 3196 3202 3208 3209 3211 3214 3221 3222 3229 3231 3233 3237 3241 3242 3255
COM1a	17 18 22 25 33 39 42 50 57 58 60 64 67 70 75 77 83 85 88 101 104 112 117 119 128 132 143 147 148 163 173 178 182 183 185 191 196 201 207 207 211 217 223 228 242 242 251 263 264 270 278 284 286 313 343 348 360 379 424 469 484 491 502 514 535 542 560 560 582 584 599 601 613 616 623 630 645 659 666 685 686 697 709 710 711 712 718 724 740 742 753 754 756 758 762 767 768 773 776 784 785 793 796 798 800 804 808 811 818 835 845 854 862 868 870 874 877 881 888 896 909 919 931 932 936 939 945 950 953 958 960 964 968 972 977 979 980 981 987 988 991 995 1001 1013 1018 1020 1028 1053 1070 1074 1078 1083 1098 1110 1119 1124 1149 1156 1179 1180 1214 1221 1236 1253 1259 1284 1288 1292 1317 1326 1330 1337 1340 1344 1347 1349 1353 1357 1370 1378 1417 1430 1443 1462 1463 1476 1480 1484 1485 1486 1488 1492 1494 1495 1496 1501 1506 1509 1511 1520 1523 1523 1526 1530 1657 1692 1714 1780 2649 2663 2704 2712 2723 2739 2742 2768 2788 3088 3092 3092 3093 3093 3096 3098 3098 3102 3102 3128 3140 3147 3157 3170 3185 3188 3190 3192 3192 3196 3200 3201 3206 3208 3210 3214 3227 3228 3228 3230 3237 3238 3255 3761
INT9a	21 26 31 42 45 54 59 62 66 83 88 103 121 121 130 134 137 147 161 164 177 179 180 183 193 205 210 215 221 228 240 247 250 258 259 273 274 280 293 319 336 369 380 428 444 473 486 501 506 530 542 560 586 594 604 608 622 626 635 642 653 669 690 694 701 708 709 715 716 729 731 739 753 757 760 762 765 768 770 774 775 779 780 782 789 792 797 804 806 811 822 844 869 871 872 874 876 877 880 888 903 905 921 930 935 938 942 951 952 955 960 963 964 966 968 970 972 978 979 982 984 989 991 999 1012 1024 1025 1051 1069 1075 1080 1084 1098 1112 1123 1129 1152 1158 1176 1179 1229 1244 1261 1271 1288 1294 1310 1325 1326 1329 1337 1342 1348 1352 1358 1359 1361 1379 1383 1420 1443 1462 1474 1477 1478 1479 1482 1485 1486 1490 1492 1493 1497 1497 1502 1507 1508 1511 1521 1523 1527 1530 1667 1692 1761 2701 2705 2712 2721 2727 2739 2746 2757 2767 3087 3093 3093 3093 3095 3099 3101 3102 3104 3104 3112 3138 3140 3159 3172 3190 3192 3192 3193 3197 3199 3202 3206 3207 3210 3210 3212 3213 3219 3225 3231 3231 3238 3254
TS9a	-84 23 26 27 37 44 51 55 61 70 79 96 115 125 133 137 144 151 156 162 166 173 185 189 193 198 213 216 222 227 234 247 252 255 258 261 272 291 295 319 345 368 381 423 438 462 482 497 507 528 542 558 583 594 602 608 619 624 632 640 653 662 687 694 702 708 711 715 717 724 729 739 750 755 756 762 764 767 768 770 772 778 778 783 788 793 795 802 805 809 810 845 863 868 872

	874 876 878 879 887 905 906 920 929 932 935 940 950 952 953 957 961 963 966 967 970 972 976 978 980 983 989 990 997 1013 1023 1024 1050 1066 1072 1074 1082 1095 1112 1122 1128 1153 1160 1177 1179 1228 1244 1258 1269 1288 1295 1308 1324 1326 1329 1337 1344 1350 1353 1356 1357 1360 1377 1382 1419 1443 1462 1475 1477 1478 1481 1482 1485 1486 1488 1491 1494 1496 1503 1503 1507 1508 1511 1521 1521 1523 1530 1662 1693 1760 2699 2704 2712 2722 2727 2739 2746 2756 2765 3087 3091 3092 3093 3095 3099 3100 3100 3101 3103 3109 3138 3140 3159 3172 3190 3192 3192 3193 3197 3199 3201 3209 3210 3211 3214 3218 3220 3223 3226 3226 3227 3241 3256
P1a	25 39 45 59 65 78 95 108 113 132 143 158 177 182 193 202 224 227 241 250 262 270 297 304 312 334 364 378 421 444 479 484 511 515 536 549 574 588 595 607 612 621 623 630 643 656 666 692 703 709 710 715 718 723 737 740 751 754 762 764 768 773 776 783 788 791 797 799 801 812 818 860 862 871 878 882 891 891 905 918 922 924 931 936 939 941 951 954 958 958 961 966 967 970 972 976 978 992 1002 1005 1020 1031 1034 1052 1069 1074 1080 1100 1111 1118 1124 1153 1166 1179 1183 1225 1244 1254 1267 1288 1293 1308 1320 1328 1331 1333 1341 1344 1351 1358 1367 1380 1419 1444 1462 1478 1483 1484 1491 1499 1502 1504 1507 1511 1515 1521 1523 1530 1541 1670 1722 1734 2716 2719 2725 2732 2742 2753 2755 2771 2775 3088 3090 3094 3095 3097 3101 3104 3115 3136 3140 3159 3172 3185 3191 3192 3192 3198 3210 3211 3216 3229 3230 3243 3258 3307

Table S6. 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 on **Path a**, obtained at PCM- LC-ωPBE/DZVP level in toluene solution.

Species	***E***	***ZPE***	***G***	***G*(sol, 298K)**
M1	-2535.18478	282.08848	-2534.78759	-2534.77666
R3	-3289.37813	129.49652	-3289.21731	-3289.20677
INT1	-5824.58830	413.64738	-5824.00123	-5823.99088
TS1	-5824.58163	413.95763	-5823.99196	-5823.98158
INT2	-5824.60933	414.88563	-5824.01847	-5824.00853
TS2	-5824.58868	415.13490	-5823.99578	-5823.98567
INT3	-5824.60300	415.09457	-5824.01139	-5824.00092
TS3	-5824.58655	415.12266	-5823.99481	-5823.98428

INT4	-5824.59582	415.50706	-5824.00462	-5823.99446
TS4	-5824.59489	414.75009	-5824.00144	-5823.99066
INT5	-5824.61365	414.83406	-5824.02471	-5824.01438
TS5	-5824.59452	414.98108	-5824.00172	-5823.99111
INT6	-5824.61799	414.99493	-5824.02815	-5824.01794
TS6	-5824.58808	413.36166	-5823.99991	-5823.98943
INT7	-5824.60152	415.14955	-5824.01582	-5824.00591
TS7	-5824.59830	414.97247	-5824.00908	-5823.99863
INT8	-5824.68399	416.69770	-5824.09040	-5824.08058
K_2CO_3	-1463.26077	10.28918	-1463.27965	-1463.26473
$KHCO_3$	-864.10178	17.64647	-864.10395	-864.08966
CAT	-2429.65574	146.89430	-2429.46735	-2429.45712
PMe_3	-460.88869	72.44058	-460.80244	-460.79282
KBr	-3173.13103	0.22234	-3173.15560	-3173.13921
TS8a	-7287.91447	424.75457	-7287.31920	-7287.30861
COM1a	-7287.96402	427.50835	-7287.36834	-7287.35858
INT9a	-3250.70026	408.20851	-3250.11823	-3250.10879
TS9a	-3250.69944	407.82174	-3250.11738	-3250.10702
P1a	-1281.96745	335.62978	-1281.48778	-1281.47713

Table S7. Optimized Cartesian coordinates for stationary points on **Path a1**, **a2**, **a3** and **b**, located at PCM-LC-ωPBE/DZVP level in toluene solution.

Species	Cartesian coordinates	Species	Cartesian coordinates
TS8a1	5 0.280580 -1.839332 -1.002310 5 0.821875 -3.120072 0.100024 5 -1.997894 -3.404935 -0.202419 5 -0.578602 -4.057821 0.614517 5 -1.673032 -2.971949 1.482990 5 -0.923467 -1.380169 1.528055 5 -0.445039 -3.479385 -1.060022 5 -1.448484 -2.069027 -1.208599	**TS8a3**	5 0.327588 0.952061 -0.993884 5 0.808135 0.755173 -2.690310 5 -1.672284 2.150920 -2.687364 5 -0.428341 1.460855 -3.728120 5 -1.935170 0.575621 -3.451969 5 -1.603254 -0.690506 -2.274569 5 0.032065 2.248773 -2.204429 5 -1.177125 1.858709 -1.021559

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 0.835008 -1.321833 -1.916146		1 0.986019 1.095051 -0.015867
	1 1.903740 -3.591829 0.003000		1 1.952548 0.721383 -3.008262
	1 -2.998463 -3.964823 -0.499057		1 -2.397035 3.059849 -2.914442
	1 -0.499397 -5.207679 0.901224		1 -0.173315 1.926775 -4.791026
	1 -2.457877 -3.239197 2.331396		1 -2.842828 0.416680 -4.199141
	1 -1.259306 -0.560029 2.310388		1 -2.318650 -1.623869 -2.153976
	1 -0.284728 -4.177922 -2.006479		1 0.605057 3.286650 -2.126574
	1 -2.039362 -1.675143 -2.151352		1 -1.552835 2.500002 -0.105993
	5 0.669272 -1.389355 0.678682		5 0.124556 -0.654436 -1.746733
	5 0.091190 -2.788551 1.680250		5 -0.383921 -0.305792 -3.457696
	1 0.614802 -3.033405 2.718537		1 -0.126513 -1.078578 -4.323155
	6 -2.105795 -1.813210 0.331630		6 -2.278411 0.845420 -1.818274
	6 -0.835138 -0.918425 -0.092207		6 -1.174661 0.148956 -0.876634
	6 -3.321292 -0.885508 0.286302		6 -3.608357 0.749285 -1.065313
	1 -3.487105 -0.520757 1.304719		1 -4.129647 -0.135806 -1.442899
	6 -2.866354 0.305861 -0.588572		6 -3.204146 0.486181 0.405771
	1 -3.431536 1.194477 -0.316167		1 -4.001333 -0.050876 0.916998
	1 -3.063620 0.096621 -1.643097		1 -3.046429 1.432216 0.929872
	6 -0.805634 1.591041 0.159249		6 -1.764137 -1.550233 0.883424
	6 -1.391334 0.459752 -0.273573		6 -1.949918 -0.355090 0.298014
	6 0.329512 1.534568 1.115887		6 -0.965618 -2.601707 0.207268
	6 0.350646 2.564400 2.066263		6 -1.451539 -3.905408 0.380697
	6 1.225283 0.454785 1.297157		6 0.060341 -2.401672 -0.743377
	6 1.197880 2.566361 3.161523		6 -0.971482 -4.991025 -0.330912
	1 -0.352497 3.384953 1.975170		1 -2.266866 -4.077382 1.074801
	6 2.021699 0.440289 2.456978		6 0.480326 -3.506139 -1.508363
	6 2.043178 1.487715 3.363707		6 0.007568 -4.789702 -1.291117
	1 1.166767 3.391265 3.868225		1 -1.386322 -5.980002 -0.155775
	1 2.656823 -0.419217 2.658036		1 1.211693 -3.361362 -2.300079
	1 2.695705 1.442958 4.231334		1 0.383515 -5.615898 -1.888307
	14 -1.674912 3.249305 -0.268231		14 -2.701619 -1.920192 2.513212
	6 -2.982515 3.681268 1.013506		6 -4.396196 -2.681655 2.219847
	1 -2.548519 3.990547 1.967707		1 -4.934311 -2.741146 3.171035
	1 -3.587956 4.516401 0.647628		1 -5.008186 -2.084716 1.538189
	1 -3.663237 2.852411 1.224363		1 -4.349484 -3.693612 1.810307
	6 -2.471553 3.132329 -1.968919		6 -2.911950 -0.328651 3.489248
	1 -1.859480 2.551991 -2.665550		1 -2.028322 0.312915 3.430388
	1 -3.474968 2.702985 -1.970729		1 -3.776531 0.264800 3.185131
	1 -2.556207 4.143002 -2.380964		1 -3.055220 -0.581517 4.544639
	6 -0.482291 4.695761 -0.420690		6 -1.672773 -3.052953 3.601353
	1 -1.077419 5.615523 -0.412873		1 -2.185945 -3.171067 4.561356
	1 0.266202 4.788085 0.367665		1 -1.504659 -4.052304 3.196614
	1 0.041881 4.668903 -1.379050		1 -0.695216 -2.612509 3.813782
	6 -4.594833 -1.561410 -0.203925		6 -4.509097 1.963275 -1.249934
	1 -4.804159 -2.427011 0.433453		1 -4.694288 2.108530 -2.319610
	1 -4.437021 -1.950162 -1.215974		1 -3.989419 2.861079 -0.897674
	6 -5.800742 -0.628508 -0.193218		6 -5.843044 1.823781 -0.524974
	1 -5.628205 0.215681 -0.870827		1 -5.674942 1.730861 0.554056
	1 -5.923851 -0.200487 0.809215		1 -6.337317 0.897330 -0.842224
	6 -7.089180 -1.333782 -0.600370		6 -6.774116 3.003229 -0.780349
	1 -7.271677 -2.172921 0.079699		1 -6.952115 3.096340 -1.857273
	1 -6.962881 -1.770088 -1.597298		1 -6.277071 3.929265 -0.471080
	6 -8.295233 -0.404426 -0.599063		6 -8.105122 2.871133 -0.052772
	1 -8.155145 0.425980 -1.297093		1 -7.959188 2.807823 1.029386
	1 -9.205569 -0.933493 -0.891552		1 -8.753785 3.728137 -0.250437

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -8.463595 0.022344 0.393828		1 -8.639528 1.970388 -0.368038
	28 2.378357 -0.502735 0.113735		28 1.694300 -1.405639 -0.727802
	15 2.986337 1.087431 -1.325558		15 2.177543 -1.593309 1.457717
	6 4.527546 1.892517 -0.788848		6 2.015805 -3.323927 2.009199
	1 5.299337 1.134321 -0.652474		1 2.705867 -3.947492 1.435912
	1 4.864109 2.632304 -1.519777		1 2.253625 -3.421658 3.072037
	1 4.361231 2.388608 0.169789		1 1.003827 -3.691702 1.834174
	6 3.369161 0.462661 -2.991009		6 3.865932 -1.170019 1.971082
	1 3.786185 1.253264 -3.620222		1 3.990045 -0.089505 1.864860
	1 4.082469 -0.358196 -2.913379		1 4.010081 -1.437579 3.021866
	1 2.458704 0.082283 -3.458393		1 4.598650 -1.692053 1.355204
	6 1.919430 2.515256 -1.684451		6 1.197356 -0.611006 2.625044
	1 1.740889 3.072558 -0.764718		1 0.132339 -0.698740 2.413492
	1 2.387634 3.181144 -2.414858		1 1.392237 -0.925030 3.655051
	1 0.957783 2.178742 -2.076794		1 1.509126 0.435453 2.503759
	1 2.196410 -1.599672 1.035719		1 1.468250 -1.331174 -2.158619
	35 4.331463 -1.698898 -0.299493		35 3.900395 -1.236192 -1.497871
			6 2.659442 3.196834 1.716702
			8 2.896735 1.932518 1.637846
			8 1.963861 3.697331 2.677200
			8 3.141284 3.996803 0.783885
			19 2.296909 6.167489 1.976534
			19 3.879207 2.002901 -0.790814
TS8a2	**5** -0.452047 -0.522162 -1.722585	**COM1b**	5 0.466361 0.416640 -2.197078
	28 0.566621 -1.949531 -0.730947		5 1.907998 1.066715 -1.406388
	1 0.507335 -1.769826 -2.146056		5 0.198677 3.275554 -1.999499
	35 2.672971 -2.640091 -1.480949		5 1.735412 2.821227 -1.270900
	6 -1.332122 -2.134754 -0.908998		5 0.336088 3.153198 -0.243683
	5 0.471742 0.704968 -0.823018		5 -0.307374 1.593416 0.274134
	5 0.838743 0.466262 -2.544697		5 1.172640 1.980575 -2.723639
	5 -0.685401 2.863131 -2.327978		5 -0.541050 1.792181 -2.579753
	5 0.104057 1.772245 -3.467680		1 0.348677 -0.531207 -2.899156
	5 -1.646675 1.686114 -3.234408		1 2.981475 0.578348 -1.559709
	5 -1.982129 0.307213 -2.198228		1 -0.120792 4.304687 -2.498965
	5 0.852327 2.095124 -1.887994		1 2.660789 3.577531 -1.297584
	5 -0.424088 2.209715 -0.712730		1 0.149912 4.103332 0.443011
	1 1.095737 0.410609 0.145712		1 -0.995958 1.513867 1.229264
	1 1.836438 -0.072053 -2.893874		1 1.664199 2.101219 -3.800141
	1 -0.888244 4.023413 -2.447267		1 -1.348390 1.789396 -3.439632
	1 0.569700 2.168059 -4.486027		5 0.643162 0.220224 -0.438704
	1 -2.504577 2.051144 -3.967383		1 4.864332 1.880055 3.622382
	1 -3.053100 -0.190369 -2.153242		5 1.410529 1.770892 0.131246
	1 1.845892 2.724810 -1.725853		1 2.095092 1.821067 1.108807
	1 -0.472807 2.857008 0.271687		6 -0.958648 2.463607 -1.080745
	5 -0.699834 0.174737 -3.372483		6 -0.806226 0.855179 -1.140625
	1 -0.826095 -0.537107 -4.315224		6 -2.459499 2.773619 -1.089433
	6 -1.857378 1.920873 -1.572755		6 -3.120179 1.452011 -1.577455
	6 -1.236046 0.693986 -0.739367		1 -4.135308 1.394859 -1.187200
	6 -3.090204 2.389650 -0.795372		1 -3.185322 1.428524 -2.665796
	1 -3.960179 1.903983 -1.248207		6 -2.688482 -0.537604 -0.103153
	6 -2.895756 1.810834 0.627146		6 -2.229972 0.370448 -0.987822
	1 -3.865759 1.668578 1.100182		6 -1.919905 -1.029668 1.080468
	1 -2.321133 2.506526 1.244049		6 -2.669592 -1.002214 2.270724
	6 -2.619637 -0.707407 0.826539		6 -0.543962 -1.315637 1.144520
	6 -2.189187 0.490927 0.396239		6 -2.108919 -1.203599 3.518350

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 -2.382823 -1.927420 0.014312		1 -3.730588 -0.769524 2.225682
	6 -3.433305 -2.855532 0.028419		6 0.005650 -1.493409 2.433304
	6 -3.479941 -3.954725 -0.811913		6 -0.739643 -1.441653 3.597454
	1 -4.273582 -2.696538 0.696149		1 -2.725531 -1.158537 4.412061
	6 -1.431786 -3.222694 -1.796256		1 1.072499 -1.702066 2.521577
	6 -2.465052 -4.143082 -1.736651		1 -0.259506 -1.592477 4.562149
	1 -4.322096 -4.639531 -0.761062		14 -4.515573 -1.073960 -0.295230
	1 -0.669698 -3.362945 -2.558675		6 -4.735303 -2.841223 0.295997
	1 -2.486400 -4.981651 -2.427150		1 -4.352943 -3.022726 1.302412
	14 -3.749003 -0.763860 2.376952		1 -4.248870 -3.544996 -0.384971
	6 -5.562627 -0.580833 1.908213		1 -5.803397 -3.083312 0.295414
	1 -5.714169 0.111103 1.075493		6 -5.754482 0.007019 0.632147
	1 -6.018031 -1.533137 1.624149		1 -5.524431 1.074476 0.586377
	1 -6.127410 -0.196230 2.762867		1 -5.827212 -0.263670 1.688847
	6 -3.265022 0.598563 3.575802		1 -6.749411 -0.132144 0.196916
	1 -2.179351 0.701604 3.660225		6 -4.987737 -1.103464 -2.116401
	1 -3.675419 1.581243 3.337264		1 -5.878037 -1.728914 -2.239802
	1 -3.639958 0.329119 4.568632		1 -4.192040 -1.545190 -2.722933
	6 -3.501220 -2.364560 3.335491		1 -5.222758 -0.124366 -2.538182
	1 -4.368298 -2.514590 3.987351		28 0.647844 -1.739453 -0.182392
	1 -3.392721 -3.262480 2.725295		15 0.169699 -3.921937 -0.022665
	1 -2.626613 -2.298938 3.987559		6 1.467680 -4.958090 0.739979
	6 -3.301163 3.897469 -0.825971		1 1.183949 -6.014329 0.749129
	1 -3.368796 4.224637 -1.868972		1 1.631125 -4.632925 1.770563
	1 -2.426770 4.398889 -0.396927		1 2.398802 -4.835138 0.185369
	6 -4.559421 4.331421 -0.082305		6 -1.290413 -4.441312 0.939579
	1 -4.480241 4.062228 0.977193		1 -1.211980 -4.070137 1.963830
	1 -5.425118 3.785294 -0.476870		1 -1.393151 -5.530166 0.956095
	6 -4.816947 5.829588 -0.193529		1 -2.189888 -4.005902 0.504722
	1 -4.906933 6.102938 -1.250529		6 -0.117251 -4.764683 -1.616671
	1 -3.948215 6.375006 0.190887		1 -0.976392 -4.312859 -2.117413
	6 -6.067693 6.268827 0.555448		1 -0.307468 -5.833070 -1.480552
	1 -5.990320 6.039655 1.622126		1 0.757356 -4.627849 -2.254174
	1 -6.232032 7.344820 0.458661		6 5.392887 2.044160 1.802830
	1 -6.956939 5.761023 0.171023		19 5.502532 3.699494 -0.714033
	15 0.822072 -2.621352 1.397578		8 5.510074 1.411537 0.722523
	6 0.020500 -4.240761 1.619710		8 5.601106 3.256980 2.018693
	1 0.462865 -4.955131 0.922085		35 2.618579 -2.366470 -1.486004
	1 0.145331 -4.615177 2.639089		8 4.945082 1.275438 2.863274
	1 -1.044465 -4.162340 1.392297		19 3.738512 -0.604891 0.942152
	6 2.520206 -2.923819 1.972023		6 -3.019471 3.247655 0.250370
	1 2.509978 -3.345726 2.980485		1 -3.138122 2.390106 0.921857
	1 3.029846 -3.608835 1.294551		1 -2.299201 3.917584 0.730581
	1 3.078646 -1.985380 1.998029		6 -4.348966 3.979195 0.098361
	6 0.166217 -1.603211 2.753427		1 -4.200144 4.872629 -0.520484
	1 -0.889552 -1.398565 2.589229		1 -5.068067 3.353572 -0.444623
	1 0.289839 -2.103382 3.717748		6 -4.955002 4.388739 1.435150
	1 0.698568 -0.649598 2.781085		1 -4.239494 5.015860 1.978457
	19 4.222433 0.164059 -0.435475		1 -5.107235 3.496384 2.052480
	8 4.309543 1.296737 1.902127		6 -6.273919 5.134012 1.281340
	6 5.325708 2.045817 1.657065		1 -6.687530 5.417778 2.252386
	8 5.907142 1.976176 0.468442		1 -6.144517 6.048364 0.695094
	8 5.795801 2.864190 2.533501		1 -7.018711 4.516608 0.770759
	19 7.696792 3.791400 1.048481		1 -2.617188 3.560196 -1.833059
TS8b	5 0.348754 -0.286159 -2.436401	**TS9b**	5 -0.603393 -0.318007 -2.703370

Species	Cartesian coordinates	Species	Cartesian coordinates
	5 1.324957 1.193520 -2.542737		5 -1.145536 -1.986646 -2.534471
	5 0.331148 2.480548 -3.236174		5 1.719691 -1.991936 -2.877550
	5 -1.252787 1.806624 -3.584742		5 0.301427 -3.036959 -2.664009
	5 -1.015123 2.767817 -2.122045		5 1.352168 -2.673194 -1.292997
	5 -0.814279 1.676399 -0.737949		5 0.542585 -1.437355 -0.332009
	5 0.198500 0.817513 -3.841785		5 0.177803 -1.580568 -3.666117
	5 -1.212854 0.114942 -3.117049		5 1.141072 -0.333087 -2.913607
	1 0.673523 -1.426850 -2.529608		1 -1.173775 0.608476 -3.167338
	1 2.496600 1.147072 -2.716427		1 -2.209370 -2.337217 -2.936175
	1 -2.053548 2.139936 -4.395673		1 2.754601 -2.234808 -3.405838
	1 0.786687 3.362655 -3.892711		1 0.265370 -4.125867 -3.140520
	1 -1.621779 3.775975 -1.965741		1 2.127388 -3.384501 -0.745686
	1 -1.325720 1.866954 0.307358		1 0.837967 -1.215309 0.794308
	1 0.525056 0.467102 -4.929858		1 0.060485 -1.600692 -4.848444
	1 -1.943302 -0.689493 -3.576414		1 1.754457 0.575011 -3.362414
	5 0.638915 0.660931 -0.975366		5 -1.013580 -0.956413 -1.068531
	1 1.525274 0.731848 0.184454		5 -0.415085 -2.684814 -1.081792
	5 0.598886 2.393601 -1.478914		1 -0.931921 -3.530508 -0.423738
	1 1.217136 3.223379 -0.900058		6 1.741966 -1.034401 -1.483469
	6 -1.845774 1.305461 -2.085312		6 0.430865 -0.110457 -1.382487
	6 -0.963266 0.132999 -1.406687		6 -2.191190 0.605076 -0.685494
	28 1.567031 -1.047040 -0.210454		28 -2.013029 -0.717011 0.565587
	35 3.781027 -1.025039 -1.274601		15 -2.254054 -2.135993 2.202301
	8 2.479711 1.441571 0.935315		6 -3.338843 -3.566541 1.864436
	19 4.699779 1.969553 -0.254366		1 -4.329816 -3.213346 1.572414
	6 2.243188 2.604393 1.498505		1 -3.436204 -4.214952 2.739646
	8 3.243334 3.438146 1.556588		1 -2.932289 -4.146701 1.034322
	8 1.095113 2.896708 1.954683		6 -3.022364 -1.434751 3.708109
	19 1.792099 5.248866 2.847313		1 -2.398312 -0.630507 4.103303
	15 1.762124 -3.200225 -0.002075		1 -3.152303 -2.193854 4.484223
	6 3.131437 -3.727688 1.072891		1 -3.998763 -1.011298 3.463664
	1 3.205943 -4.818008 1.102451		6 -0.765390 -2.941116 2.887477
	1 2.959028 -3.356431 2.084848		1 -1.018960 -3.635941 3.693238
	1 4.063916 -3.304761 0.697588		1 -0.082958 -2.182427 3.275872
	6 0.361079 -4.154499 0.658453		1 -0.247349 -3.487929 2.097629
	1 0.146376 -3.846073 1.682101		6 2.912463 -0.226084 -0.925284
	1 0.576227 -5.226734 0.640075		6 2.271687 0.996698 -0.224027
	1 -0.524301 -3.959783 0.049954		1 2.337338 0.857313 0.857490
	6 2.077172 -4.075524 -1.569382		1 2.818900 1.912017 -0.461589
	1 1.224010 -3.942072 -2.237596		6 -0.107379 2.008244 -0.226764
	1 2.221671 -5.144924 -1.392223		6 0.806250 1.108122 -0.612304
	1 2.960994 -3.658631 -2.051578		6 -1.521941 1.851067 -0.684268
	6 -3.317228 1.015193 -1.804692		6 -2.187581 2.975849 -1.173429
	6 -3.327780 -0.475668 -1.400628		6 -3.484842 2.905009 -1.661772
	1 -4.169465 -0.659880 -0.734873		1 -1.669761 3.931796 -1.203754
	1 -3.462645 -1.112668 -2.275644		6 -3.499339 0.552295 -1.199959
	6 -1.938285 -1.329231 0.503787		6 -4.150143 1.685436 -1.665957
	6 -2.001768 -0.715811 -0.690725		1 -3.967278 3.798077 -2.050445
	6 -0.867549 -1.166039 1.528554		1 -4.004633 -0.409360 -1.263993
	6 -1.349605 -1.023181 2.842510		1 -5.163561 1.613347 -2.053197
	6 0.509797 -1.080829 1.311539		14 0.291965 3.462365 0.930803
	6 -0.516208 -0.850615 3.929818		6 -1.263359 3.935354 1.864683
	1 -2.423304 -1.019453 3.014737		1 -1.695591 3.063175 2.364255
	6 1.346689 -0.915156 2.428246		1 -2.040662 4.362080 1.228351
	6 0.857687 -0.814746 3.718227		1 -1.021876 4.672831 2.636642

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -0.933773 -0.740784 4.927356 1 2.418958 -0.824378 2.268347 1 1.544193 -0.682092 4.551249 14 -3.413909 -2.459890 0.989202 6 -2.893820 -3.818030 2.179231 1 -2.330245 -3.469108 3.045647 1 -2.298809 -4.584780 1.677396 1 -3.802265 -4.308336 2.546542 6 -4.832019 -1.508361 1.793278 1 -4.991731 -0.515188 1.365761 1 -4.667612 -1.374575 2.865964 1 -5.763943 -2.071284 1.679152 6 -4.068840 -3.389708 -0.515140 1 -4.533072 -4.320301 -0.172650 1 -3.264100 -3.664304 -1.203655 1 -4.823957 -2.846273 -1.086352 6 -3.957179 1.914875 -0.748385 1 -3.623949 1.605850 0.248085 1 -3.608359 2.943081 -0.884904 6 -5.480700 1.897074 -0.814125 1 -5.804498 2.266078 -1.795057 1 -5.853930 0.868199 -0.740035 6 -6.126855 2.739652 0.279082 1 -5.756366 3.768286 0.207454 1 -5.806626 2.368399 1.259006 6 -7.647774 2.738454 0.204945 1 -8.086381 3.349803 0.997756 1 -7.996516 3.135765 -0.752641 1 -8.047052 1.725245 0.307672 1 -3.854220 1.148726 -2.748010		6 1.568524 3.008148 2.234382 1 2.590021 2.959652 1.851321 1 1.339637 2.058063 2.725854 1 1.555196 3.781687 3.009286 6 0.952721 4.922412 -0.048155 1 1.228465 5.739601 0.625434 1 0.223917 5.316317 -0.761077 1 1.846964 4.646643 -0.614586 1 3.492884 0.117133 -1.785776 6 3.844522 -1.029837 -0.026119 1 4.184548 -1.916553 -0.571332 1 3.290907 -1.392887 0.847063 6 5.060284 -0.228639 0.425974 1 5.600190 0.139930 -0.454770 1 4.740415 0.659644 0.983334 6 6.011576 -1.043525 1.294344 1 5.471394 -1.414726 2.172332 1 6.337704 -1.929816 0.739101 6 7.228876 -0.246822 1.743811 1 6.933895 0.627779 2.330786 1 7.895408 -0.852569 2.362858 1 7.805528 0.109968 0.885638
INT9b	5 -0.694689 -0.422300 -2.498677 5 -1.251493 -2.087258 -2.336783 5 1.597505 -2.128737 -2.780950 5 0.173688 -3.154690 -2.529895 5 1.278852 -2.822271 -1.194036 5 0.523704 -1.580995 -0.194388 5 0.035165 -1.683198 -3.508081 5 1.041515 -0.459230 -2.775258 1 -1.272041 0.508619 -2.941472 1 -2.331686 -2.423051 -2.706095 1 2.609730 -2.377869 -3.349083 1 0.104859 -4.239570 -3.012306 1 2.062220 -3.550503 -0.681909 1 0.840782 -1.388210 0.931179 1 -0.124148 -1.687863 -4.685816 1 1.655636 0.440678 -3.239102 5 -1.051073 -1.086836 -0.861882 5 -0.475730 -2.804736 -0.919235 1 -0.976388 -3.650957 -0.249981 6 1.684514 -1.189481 -1.379226 6 0.390417 -0.232592 -1.215859 6 -2.242933 1.000129 -0.516066 28 -2.207685 -0.499774 0.526879 15 -2.606192 -2.124267 1.976530 6 -3.634119 -3.517006 1.401375	**P1b**	5 1.584932 -2.085319 1.335041 5 1.930114 -3.290213 0.093121 5 -0.847503 -3.508667 0.829613 5 0.423483 -4.190378 -0.213452 5 -0.771556 -3.063981 -0.874440 5 0.005540 -1.504929 -1.000427 5 0.819505 -3.676383 1.438118 5 -0.105018 -2.233444 1.785309 1 3.004873 -3.789899 0.004253 1 -1.817935 -4.039404 1.257476 1 0.405730 -5.337706 -0.521244 1 -1.681237 -3.299269 -1.596300 1 -0.339044 -0.613436 -1.693584 1 1.085666 -4.428938 2.317198 1 -0.564212 -1.813396 2.791543 5 1.650311 -1.591420 -0.368982 5 0.950002 -2.923074 -1.344665 1 1.304896 -3.140024 -2.457417 6 -0.966488 -1.887827 0.349292 6 0.408632 -1.116543 0.610617 6 -2.093292 -0.888868 0.639617 6 -1.374531 0.381143 1.185647 1 -1.869616 1.280571 0.824137 1 -1.443607 0.399393 2.277297 6 0.965826 1.275058 0.426392

Species	Cartesian coordinates	Species	Cartesian coordinates
	1 -4.584093 -3.133795 1.023332		6 0.090142 0.319363 0.787325
	1 -3.834145 -4.225943 2.209221		6 2.316936 0.896971 -0.112562
	1 -3.133589 -4.037196 0.584114		6 3.332044 1.858138 -0.142204
	6 -3.584414 -1.499964 3.392499		6 2.619008 -0.387858 -0.626186
	1 -3.028160 -0.720198 3.917188		6 4.570635 1.608880 -0.713418
	1 -3.818691 -2.299444 4.100328		1 3.164348 2.825060 0.312444
	1 -4.520623 -1.063808 3.037262		6 3.859081 -0.615163 -1.220773
	6 -1.219718 -2.952139 2.823136		6 4.830461 0.372250 -1.286469
	1 -1.581430 -3.682029 3.552572		1 5.330902 2.385632 -0.709993
	1 -0.610368 -2.207681 3.339470		1 4.076678 -1.604266 -1.617685
	1 -0.587479 -3.461371 2.095196		1 5.791268 0.168359 -1.751808
	6 2.894534 -0.425822 -0.848429		14 0.278675 3.064560 0.389627
	6 2.303430 0.764492 -0.063886		6 1.478392 4.461060 0.018405
	1 2.336393 0.534332 1.004648		1 2.014588 4.339828 -0.925493
	1 2.902220 1.664864 -0.216306		1 2.206672 4.645256 0.812278
	6 0.069297 2.018127 -0.163520		1 0.874988 5.371349 -0.070239
	6 0.857054 0.983778 -0.477171		6 -0.972479 3.150265 -1.013074
	6 -1.343651 2.074159 -0.646725		1 -1.780830 2.418545 -0.961292
	6 -1.761554 3.247257 -1.279754		1 -0.460646 2.998996 -1.968312
	6 -3.044241 3.384525 -1.791303		1 -1.430094 4.144068 -1.044580
	1 -1.057456 4.067860 -1.403572		6 -0.474008 3.499337 2.054613
	6 -3.536593 1.161645 -1.039343		1 -0.833899 4.532682 2.031529
	6 -3.945001 2.335556 -1.659842		1 0.288005 3.440039 2.837474
	1 -3.333874 4.302869 -2.295617		1 -1.309843 2.870345 2.363875
	1 -4.242655 0.332279 -0.988307		1 2.330510 -1.578241 2.103158
	1 -4.953357 2.423210 -2.057728		6 -3.011902 -0.615396 -0.549911
	14 0.668457 3.446720 0.939906		1 -3.275457 -1.567039 -1.022020
	6 -0.817988 4.287273 1.713534		1 -2.482379 -0.029984 -1.307814
	1 -1.447551 3.562791 2.238361		6 -4.295561 0.103176 -0.147970
	1 -1.451369 4.800509 0.987791		1 -4.838136 -0.507256 0.583920
	1 -0.482680 5.027151 2.447299		1 -4.062993 1.048298 0.357361
	6 1.726455 2.833447 2.370240		6 -5.203963 0.389192 -1.337927
	1 2.755668 2.602301 2.087774		1 -5.440290 -0.552030 -1.846195
	1 1.296692 1.947625 2.847159		1 -4.663112 1.002661 -2.067006
	1 1.772565 3.619211 3.131254		6 -6.494637 1.091232 -0.938359
	6 1.667486 4.685641 -0.058360		1 -6.289316 2.051714 -0.456977
	1 2.048705 5.479934 0.590798		1 -7.128053 1.284443 -1.807637
	1 1.070940 5.160106 -0.842005		1 -7.072077 0.485015 -0.234608
	1 2.527904 4.215826 -0.543269		1 -2.702614 -1.322617 1.436985
	1 3.434588 -0.048255 -1.720902	**HBr**	35 0.000000 0.000000 0.039666
	6 3.856414 -1.280740 -0.032621		1 0.000000 0.000000 -1.388297
	1 4.168190 -2.139472 -0.636485		
	1 3.335025 -1.686218 0.841909		
	6 5.093706 -0.509857 0.413451		
	1 5.596398 -0.088607 -0.465730		
	1 4.800671 0.342648 1.037367		
	6 6.078752 -1.376985 1.188563		
	1 5.575234 -1.801713 2.064089		
	1 6.378550 -2.227279 0.566240		
	6 7.316256 -0.609827 1.634272		
	1 7.048888 0.226691 2.286378		
	1 8.006909 -1.252847 2.185600		
	1 7.856827 -0.200473 0.776068		

Table S8. Vibrational frequencies for stationary points on **Path a1**, **a2**, **a3** and **b**, obtained at PCM-LC-ωPBE/DZVP level in toluene solution.

Species	Frequencies (cm^{-1})
TS8a1	-238 22 31 36 41 49 62 66 73 74 77 95 102 106 107 116 126 134 154 163 166 175 181 183 185 196 205 207 209 221 227 240 246 248 251 261 269 271 27 284 293 321 339 359 370 389 417 431 472 485 487 498 518 538 561 578 595 597 607 614 617 622 638 652 662 674 686 707 708 716 717 719 722 728 739 741 747 755 760 764 766 769 779 781 782 783 786 791 794 798 801 805 811 820 821 851 859 864 871 878 879 881 884 891 908 909 921 932 934 938 939 946 950 956 958 961 962 966 968 971 978 981 982 985 991 993 995 997 1001 1016 1023 1031 1048 1053 1064 1072 1079 1110 1117 1123 1126 1151 1166 1181 1193 1222 1239 1261 1262 1291 1305 1311 1319 1335 1335 1341 1344 1347 1351 1355 1358 1359 1376 1381 1418 1443 1462 1474 1476 1482 1483 1484 1485 1486 1490 1493 1494 1496 1504 1506 1508 1511 1519 1521 1523 1530 1531 1666 1696 1728 2194 2718 2723 2725 2731 2740 2754 2758 2773 2788 3087 3094 3094 3095 3097 3101 3102 3103 3104 3105 3131 3140 3142 3159 3172 3191 3192 3192 3195 3198 3202 3210 3211 3213 3214 3220 3230 3233 3235 3236 3238 3245 3260 3275
TS8a2	-253 3 7 12 15 26 30 39 43 44 52 55 56 65 68 71 72 78 82 84 90 100 106 113 115 119 127 132 158 166 168 176 182 186 193 201 205 211 214 217 225 235 241 242 247 251 253 254 267 269 275 282 289 320 337 353 368 387 417 430 472 486 489 499 519 538 562 577 597 598 609 614 615 623 638 652 663 673 688 690 700 706 711 716 719 720 723 727 739 741 747 755 762 765 768 771 776 779 783 784 785 791 795 799 801 802 805 811 813 851 854 862 870 875 876 879 882 883 891 910 912 922 932 933 938 941 949 954 956 959 961 963 964 969 971 977 979 982 982 987 992 993 999 1001 1016 1024 1033 1048 1054 1065 1073 1073 1080 1110 1118 1122 1126 1152 1167 1181 1194 1221 1240 1259 1262 1291 1307 1313 1320 1334 1336 1341 1344 1348 1351 1359 1359 1361 1380 1380 1418 1420 1443 1462 1473 1476 1478 1482 1483 1486 1486 1489 1492 1494 1495 1499 1506 1507 1511 1519 1521 1523 1530 1532 1555 1666 1697 1733 2254 2705 2720 2724 2725 2737 2744 2761 2776 2798 3088 3094 3094 3095 3098 3101 3101 3104 3104 3107 3131 3140 3141 3160 3172 3191 3193 3193 3196 3198 3201 3210 3211 3213 3214 3219 3223 3226 3233 3238 3246 3251 3260 3271
TS8a3	-232 6 20 22 24 41 43 47 57 58 63 67 68 70 78 82 86 92 99 103 104 109 115 123 123 125 128 139 155 165 167 179 189 197 200 204 207 209 213 226 237 238 241 248 251 252 260 266 274 282 285 289 291 320 339 357 369 387 417 431 472 486 489 498 520 538 561 577 595 599 607 614 617 623 638 652 664 677 687 692 704 708 710 713 715 717 721 729 739 741 748 756 762 764 768 772 780 781 784 785 788 792 795 799 801 804 812 829 834 851 860 871 878 879 881 886 889 891 897 909 915 922 931 936 939 942 950 957 959 963 964 967 970 975 976 980 984 990 991 995 996 1000 1005 1007 1018 1025 1030 1049 1055 1066 1073 1080 1081 1110 1118 1123 1127 1151 1166 1181 1193 1221 1240 1259 1262 1291 1308 1310 1319 1334 1335 1341 1345 1350 1351 1357 1358 1362 1380 1381 1418 1436 1443 1462 1470 1475 1478 1479 1482 1486 1488 1490 1493 1496 1499 1506 1506 1511 1518 1521 1521 1523 1530 1532 1554 1666 1696 1735 2165 2710 2715 2718 2720 2728

	2740 2756 2773 2796 3051 3088 3093 3094 3094 3096 3099 3100 3101 3103 3131 3140 3141 3159 3169 3172 3193 3193 3194 3196 3197 3203 3203 3208 3210 3217 3225 3227 3229 3231 3234 3245 3260 3275
TS8b	-1243 12 18 22 28 32 37 45 50 58 62 68 73 75 81 82 87 91 99 104 110 114 119 124 135 141 146 156 166 171 174 177 179 189 193 199 205 209 210 218 220 230 239 243 247 248 255 260 266 272 276 284 286 291 335 348 360 376 388 418 472 480 490 499 512 524 529 563 576 598 606 610 621 629 640 641 659 671 681 688 696 708 709 712 713 717 721 736 740 744 756 758 760 763 766 770 775 777 780 784 785 788 792 797 799 805 808 820 820 839 853 862 866 873 875 879 880 887 892 898 903 917 926 931 935 936 941 946 954 957 959 963 964 966 972 975 980 983 984 989 991 997 999 1013 1017 1033 1049 1062 1069 1074 1082 1090 1096 1108 1112 1123 1142 1151 1160 1165 1182 1218 1234 1250 1265 1279 1290 1295 1313 1328 1329 1337 1342 1347 1349 1350 1355 1367 1372 1372 1378 1419 1444 1456 1462 1469 1474 1480 1485 1486 1486 1488 1490 1494 1494 1496 1500 1507 1510 1512 1522 1523 1526 1531 1541 1597 1672 1701 1739 2700 2707 2715 2726 2732 2734 2745 2788 2800 3085 3092 3092 3093 3095 3100 3100 3103 3103 3108 3135 3140 3157 3158 3175 3188 3191 3191 3191 3195 3201 3209 3209 3211 3213 3221 3222 3224 3230 3234 3237 3240 3241 3254
COM1b	15 17 23 28 32 34 37 48 50 58 62 65 68 70 78 81 82 83 88 98 105 112 116 120 129 134 139 143 156 162 170 175 179 181 186 191 197 203 207 211 217 220 226 230 241 247 254 262 264 270 272 287 288 341 346 348 360 382 419 465 476 496 496 521 531 534 561 562 572 583 594 604 612 616 629 638 642 660 673 683 685 698 709 710 711 713 716 736 742 748 754 757 759 761 765 768 771 773 775 784 787 792 795 797 804 805 808 811 817 837 845 857 867 869 871 875 877 880 887 895 902 919 930 933 933 937 946 951 952 958 962 964 965 970 973 977 980 981 982 991 993 995 998 1013 1018 1020 1029 1052 1069 1072 1076 1084 1094 1106 1112 1121 1142 1156 1163 1179 1211 1228 1237 1244 1267 1277 1284 1294 1304 1326 1329 1336 1339 1341 1347 1347 1353 1362 1367 1371 1418 1430 1443 1461 1463 1476 1480 1484 1484 1486 1488 1492 1494 1495 1496 1501 1507 1509 1512 1522 1522 1523 1528 1531 1657 1691 1714 1780 2652 2664 2701 2710 2724 2734 2744 2786 2791 3084 3092 3093 3093 3094 3096 3098 3100 3102 3105 3135 3139 3157 3159 3172 3185 3188 3190 3191 3191 3196 3201 3203 3206 3209 3211 3213 3225 3227 3229 3229 3238 3238 3255 3761
INT9b	22 26 34 41 49 57 61 63 68 90 93 108 116 127 132 142 146 150 159 169 174 178 184 191 195 203 208 218 222 237 244 247 253 257 260 265 281 285 293 319 338 368 380 431 458 470 489 497 504 528 540 560 583 599 608 613 622 623 633 643 656 673 687 691 699 707 709 716 718 730 732 739 752 754 762 763 767 770 774 775 776 779 782 783 788 796 798 803 805 812 825 840 867 869 872 874 877 878 882 891 903 905 921 929 937 938 942 950 951 955 961 962 965 968 970 974 975 979 980 983 986 989 992 1000 1011 1023 1028 1052 1068 1076 1081 1084 1098 1112 1125 1128 1151 1159 1177 1179 1233 1243 1262 1271 1289 1296 1306 1324 1325 1328 1336 1340 1348 1352 1359 1359 1361 1379 1384 1420 1443 1462 1475 1476 1478 1480 1482 1485 1486 1488 1490 1493 1497 1497 1506 1507 1511 1512 1521 1523 1526 1530 1667 1692 1767 2700 2705 2712 2721 2732 2740 2749 2758 2772 3087 3092 3092 3093 3095 3098 3099 3102 3103 3104 3123 3137 3140 3158 3170 3188 3191 3192 3192 3194 3195 3197 3199 3207 3210 3212 3213 3214 3218 3222 3232 3233 3237 3254

TS9b	-103 24 26 30 37 41 53 56 64 73 83 94 112 125 127 141 143 151 155 159 171 179 186 190 192 212 217 220 225 227 244 246 251 257 260 260 268 290 296 320 345 366 381 423 451 462 486 492 501 525 540 559 578 596 606 612 618 623 631 641 655 664 682 690 698 708 708 715 717 725 732 739 746 752 755 764 765 766 769 770 773 778 779 782 789 791 797 803 805 809 810 841 862 870 872 873 874 878 882 889 905 907 922 928 932 936 939 948 950 953 958 960 961 965 969 971 974 977 977 980 982 989 992 997 1010 1025 1025 1050 1064 1070 1076 1082 1095 1112 1123 1126 1151 1162 1178 1178 1234 1244 1259 1270 1290 1296 1306 1325 1326 1328 1336 1341 1349 1356 1356 1357 1360 1377 1381 1420 1443 1462 1476 1477 1478 1479 1481 1485 1486 1488 1490 1494 1496 1498 1506 1507 1511 1512 1517 1521 1523 1530 1660 1693 1756 2700 2704 2713 2722 2732 2739 2748 2755 2764 3087 3092 3092 3093 3094 3098 3099 3100 3100 3103 3127 3138 3141 3158 3171 3187 3191 3192 3193 3193 3197 3201 3208 3208 3209 3210 3214 3220 3221 3225 3226 3230 3243 3257
HBr	2697
P1b	25 30 45 58 66 79 97 110 113 122 150 153 167 183 192 199 225 234 243 248 263 282 303 313 318 327 369 371 415 434 478 480 506 516 528 547 573 580 599 604 614 621 630 634 641 658 665 692 702 706 707 716 718 733 738 749 752 757 760 765 770 773 777 784 787 790 798 799 804 814 818 858 867 869 880 883 886 892 900 911 922 924 930 934 937 939 950 954 957 958 962 963 967 967 971 973 978 991 1000 1003 1021 1029 1034 1050 1064 1071 1085 1099 1109 1113 1128 1148 1165 1167 1183 1230 1243 1252 1279 1284 1290 1308 1318 1327 1330 1332 1338 1343 1349 1361 1369 1376 1419 1443 1461 1477 1482 1485 1492 1499 1501 1505 1505 1512 1515 1521 1523 1531 1541 1670 1722 1730 2716 2719 2726 2732 2743 2754 2755 2770 2785 3087 3090 3094 3095 3097 3102 3113 3129 3139 3146 3160 3180 3185 3191 3192 3193 3198 3210 3211 3218 3226 3230 3243 3259 3313

Table S9. 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 on **Path a1**, **a2**, **a3** and **b**, obtained at PCM-LC-ωPBE/DZVP level in toluene solution.

Species	***E***	***ZPE***	***G***	***G*(sol, 298K)**
TS8a1	-5824.62470	415.19240	-5824.03199	-5824.02176
TS8a2	-7287.89653	425.65829	-7287.30097	-7287.29741
TS8a3	-7287.90424	426.26742	-7287.30874	-7287.29917
TS8b	-7287.91222	424.54605	-7287.31899	-7287.30734
COM1b	-7287.96236	427.51440	-7287.36692	-7287.35729

INT9b	-3250.70169	408.42124	-3250.11870	-3250.10889
TS9b	-3250.69923	407.86181	-3250.11680	-3250.10702
HBr	-2573.91075	3.85604	-2573.92383	-2573.91306
P1b	-1281.96480	335.61221	-1281.48532	-1281.47472

Table S10. 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 on **Path a** and **b**, obtained at PCM- CAM-B3LYP/DZVP level in toluene solution.

Species	***E***	***ZPE***	***G***	***G*(sol, 298K)**
M1	-2535.51736	278.66079	-2535.12631	-2535.11614
R3	-3290.01354	128.19929	-3289.85510	-3289.84523
INT1	-5825.54673	408.88970	-5824.96834	-5824.95824
TS1	-5825.53309	409.22890	-5824.95193	-5824.94192
INT2	-5825.56175	410.33884	-5824.97969	-5824.96957
TS2	-5825.53910	410.48780	-5824.95445	-5824.94403
INT3	-5825.55538	410.42589	-5824.97236	-5824.96248
TS3	-5825.53357	410.53178	-5824.94923	-5824.93869
INT4	-5825.54278	410.79071	-5824.95968	-5824.94944
TS4	-5825.54276	410.69915	-5824.95782	-5824.94789
INT5	-5825.56939	409.98663	-5824.99038	-5824.97996
TS5	-5825.54473	410.25294	-5824.96024	-5824.95009
INT6	-5825.57266	410.25785	-5824.99177	-5824.98172
TS6	-5825.53290	408.60338	-5824.95374	-5824.94370
INT7	-5825.55874	410.68544	-5824.98092	-5824.97039
TS7	-5825.55352	410.35651	-5824.97274	-5824.96191
INT8	-5825.64110	411.69157	-5825.05611	-5825.04020

K_2CO_3	-1463.66945	10.17761	-1463.68791	-1463.67535
$KHCO_3$	-864.33934	17.44052	-864.34175	-864.32654
CAT	-2430.14489	145.40055	-2429.95801	-2429.94772
PMe_3	-460.99165	71.62697	-460.90678	-460.89704
KBr	-3173.77645	0.22480	-3173.80100	-3173.78838
TS8a	-7289.27215	419.87260	-7288.68619	-7288.67608
COM1a	-7289.31858	422.72465	-7288.73100	-7288.72110
INT9a	-3251.17734	403.72804	-3250.60275	-3250.59308
TS9a	-3251.17369	403.19952	-3250.59994	-3250.58966
P1a	-1282.06104	331.97378	-1281.58741	-1281.57627
TS8b	-7289.26993	419.87987	-7288.68422	-7288.67280
COM1b	-7289.31652	422.68653	-7288.72916	-7288.71803
INT9b	-3251.17882	403.89260	-3250.60359	-3250.59262
TS9b	-3251.17302	403.21649	-3250.59893	-3250.58885
P1b	-1282.05857	331.96627	-1281.58512	-1281.57401

Table S11. 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 on **Path a** and **b**, obtained at PCM- B3LYP/DZVP level in toluene solution.

Species	***E***	***ZPE***	***G***	***G*(sol, 298K)**
M1	-2535.97249	274.78715	-2535.58846	-2535.57828
R3	-3290.19354	126.67882	-3290.03818	-3290.02803
INT1	-5826.17336	403.31883	-5825.60542	-5825.59503
TS1	-5826.15764	403.67067	-5825.58622	-5825.57589
INT2	-5826.18425	404.74915	-5825.61237	-5825.60196
TS2	-5826.165004	404.87117	-5825.590546	-5825.57922
INT3	-5826.18193	404.83069	-5825.60919	-5825.59973
TS3	-5826.15820	404.68424	-5825.58514	-5825.57489

INT4	-5826.16773	405.05841	-5825.59502	-5825.58489
TS4	-5826.16656	404.99025	-5825.59189	-5825.58233
INT5	-5826.19400	404.33320	-5825.62542	-5825.61519
TS5	-5826.16971	404.69996	-5825.59486	-5825.58433
INT6	-5826.19586	404.68962	-5825.62503	-5825.61411
TS6	-5826.15792	403.07867	-5825.58861	-5825.57852
INT7	-5826.18544	405.29994	-5825.61707	-5825.60686
M2	-3857.01184	333.04762	-3856.54275	-3856.53220
TS7	-5826.18023	404.84045	-5825.60948	-5825.59922
INT8	-5826.25640	406.52579	-5825.68117	-5825.67165
K_2CO_3	-1463.73100	9.89396	-1463.74990	-1463.73738
$KHCO_3$	-864.41449	17.08055	-864.41765	-864.40130
CAT	-2430.29274	143.78222	-2430.10933	-2430.09940
PMe_3	-461.08854	70.86334	-461.00497	-460.99533
KBr	-3173.66909	0.22638	-3173.69365	-3173.67989
TS8a	-7289.95057	413.84736	-7289.37610	-7289.36640
COM1a	-7289.99412	416.62375	-7289.42020	-7289.40670
INT9a	-3251.89865	398.30904	-3251.33374	-3251.32357
TS9a	-3251.89562	397.77233	-3251.33162	-3251.32052
P1a	-1282.73184	327.48177	-1282.26586	-1282.25535
TS8b	-7289.94815	413.93370	-7289.37231	-7289.36182
COM1b	-7289.99674	416.52729	-7289.41952	-7289.41214
INT9b	-3251.89981	398.45940	-3251.33424	-3251.32479
TS9b	-3251.89486	397.76671	-3251.33085	-3251.32001
P1b	-1282.72936	327.46562	-1282.26356	-1282.25309

Table S12. 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 on **Path a** and **b**, obtained at PCM- B3LYP-D3/DZVP level in toluene solution.

Species	***E***	***ZPE***	***G***	***G*(sol, 298K)**
M1	-2536.04898	275.40980	-2535.662689	-2535.65266

R3	-3290.21227	126.58019	-3290.05639	-3290.04629
INT1	-5826.30578	404.43784	-5825.73357	-5825.72327
TS1	-5826.29115	404.64100	-5825.71724	-5825.70605
INT2	-5826.31861	406.03750	-5825.74265	-5825.73274
TS2	-5826.298414	405.85058	-5825.722599	-5825.71217
INT3	-5826.31507	405.79493	-5825.73919	-5825.72906
TS3	-5826.29295	406.01132	-5825.71540	-5825.70485
INT4	-5826.30320	406.25018	-5825.72708	-5825.71673
TS4	-5826.30173	406.03130	-5825.72396	-5825.71341
INT5	-5826.32544	405.42901	-5825.75306	-5825.74281
TS5	-5826.30179	405.71655	-5825.72477	-5825.71463
INT6	-5826.32862	405.55970	-5825.75464	-5825.74433
TS6	-5826.29254	404.19583	-5825.71891	-5825.70862
INT7	-5826.30597	406.03800	-5825.73357	-5825.72287
TS7	-5826.30492	405.91825	-5825.72987	-5825.71950
INT8	-5826.39251	407.71899	-5825.81334	-5825.80313
K_2CO_3	-1463.73555	9.82043	-1463.75475	-1463.73692
$KHCO_3$	-864.41727	17.00660	-864.42075	-864.40361
CAT	-2430.31503	143.74211	-2430.13166	-2430.12222
PMe_3	-461.09407	70.85339	-461.01049	-461.00023
KBr	-3173.67031	0.21328	-3173.69495	-3173.68125
TS8a	-7290.10807	415.62464	-7289.52624	-7289.51592
COM1a	-7290.14651	417.63641	-7289.56776	-7289.55693
INT9a	-3252.01612	399.06080	-3251.44935	-3251.43867
TS9a	-3252.01423	398.62696	-3251.44710	-3251.43692
P1a	-1282.81671	327.94430	-1282.34964	-1282.33872

TS8b	-7290.10499	414.86273	-7289.52775	-7289.51730
COM1b	-7290.14655	417.75140	-7289.56706	-7289.55728
INT9b	-3252.01778	399.36819	-3251.44978	-3251.43988
TS9b	-3252.01309	398.79236	-3251.44542	-3251.43570
P1b	-1282.81517	327.93862	-1282.34817	-1282.33815

Table S13. Optimized Cartesian coordinates for stationary points involving Cs_2CO_3 on **Path a** and **b**, located at PCM-LC-ωPBE/DZVP (SDD for Cs) level in toluene solution.

Species	Cartesian coordinates	Species	Cartesian coordinates
TS8a	5 0.983423 -1.209975 -2.113189	**COM1a**	5 0.592480 0.611619 -1.980425
	5 -0.429521 -0.372547 -2.790415		5 -1.054460 0.757584 -1.347491
	5 1.877868 1.080271 -3.602508		5 0.151288 3.344595 -1.194089
	5 0.124398 1.044551 -3.687968		5 -1.316100 2.434463 -0.846564
	5 0.927076 2.121203 -2.534621		5 -0.175074 2.799656 0.454016
	5 0.818069 1.372478 -0.930163		5 0.738662 1.323362 0.765727
	5 1.042913 -0.475890 -3.747777		5 -0.386420 2.077452 -2.312027
	5 2.385915 -0.312292 -2.659375		5 1.291630 2.214174 -1.906434
	1 1.161350 -2.367724 -1.908741		1 1.024925 -0.103702 -2.820374
	1 -1.399659 -0.973985 -3.109812		1 -1.953422 0.108827 -1.775776
	1 2.645065 1.550042 -4.374531		1 0.261979 4.502282 -1.428310
	1 -0.455465 1.472212 -4.635899		1 -2.382288 2.970068 -0.893688
	1 1.049186 3.301383 -2.594187		1 -0.293556 3.587408 1.335667
	1 0.971328 1.993797 0.061230		1 1.313261 1.189203 1.790425
	1 1.158985 -1.154488 -4.717007		1 -0.749226 2.336996 -3.414736
	1 3.459305 -0.795070 -2.748098		1 2.183540 2.558393 -2.598078
	5 -0.014169 -0.205517 -1.058896		5 0.236615 -0.013058 -0.354824
	1 -1.069754 -0.337918 -0.126603		1 -5.469719 -0.544977 3.501680
	5 -0.524792 1.218169 -2.040044		5 -0.937809 1.179913 0.360418
	1 -1.540768 1.791186 -1.825020		1 -1.733782 0.875318 1.196231
	6 2.219427 1.219056 -1.956081		6 1.338847 2.597270 -0.259219
	6 1.719811 -0.049041 -1.083983		6 1.576411 1.045911 -0.653036
	28 -0.367146 -1.961362 0.049861		6 2.710586 3.157558 0.128287
	35 -2.040167 -3.142471 -1.289396		1 2.800782 3.070285 1.215817
	8 -2.442286 0.056057 0.270637		6 3.721691 2.175332 -0.515895
	6 2.782720 -0.179760 -0.004014		1 4.664093 2.221864 0.026645
	6 2.657967 -0.493176 1.297376		1 3.919154 2.459691 -1.551805
	6 1.385007 -0.610655 2.064421		6 3.577040 -0.153266 0.405103
	6 0.192532 -1.201362 1.644212		6 3.040534 0.827897 -0.347525
	6 3.523286 1.709608 -1.336952		6 2.798297 -1.046015 1.316660
	1 3.265341 2.502311 -0.627753		6 3.363722 -1.141799 2.601464
	6 4.035147 0.494216 -0.544018		6 1.530067 -1.608787 1.081336
	1 4.680468 0.835291 0.262746		6 2.713128 -1.732660 3.668710
	1 4.632763 -0.150877 -1.192481		1 4.336807 -0.694561 2.788714
	6 1.412970 0.018903 3.322286		6 0.882574 -2.188583 2.194518
	6 0.327367 0.031472 4.175289		6 1.440587 -2.256122 3.458455
	1 2.314768 0.541746 3.632269		1 3.183425 -1.769952 4.647698
	6 -0.900810 -1.191065 2.525420		1 -0.103676 -2.630970 2.052214

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 -0.843447 -0.603895 3.775598		1 0.892248 -2.721157 4.275336
	1 0.395141 0.530654 5.138743		14 5.486184 -0.255649 0.438473
	1 -1.841822 -1.624680 2.194016		6 6.027711 -2.033150 0.701002
	1 -1.717163 -0.616932 4.423318		1 5.600628 -2.497510 1.592177
	14 4.279411 -0.717259 2.301340		1 5.768259 -2.652427 -0.162226
	6 4.042242 -1.874221 3.762813		1 7.118035 -2.061960 0.799525
	1 3.194814 -1.623641 4.402561		6 6.306648 0.811712 1.762968
	1 3.923614 -2.911061 3.439504		1 5.819121 1.779300 1.907684
	1 4.949064 -1.832328 4.376352		1 6.329648 0.312654 2.735392
	6 4.968928 0.906801 2.971981		1 7.345583 1.007334 1.478965
	1 4.901223 1.739265 2.267115		6 6.181645 0.226029 -1.242043
	1 4.455228 1.215669 3.886267		1 7.212268 -0.136368 -1.316560
	1 6.025552 0.775227 3.226268		1 5.611829 -0.240742 -2.050482
	6 5.601584 -1.557338 1.251354		1 6.204734 1.301104 -1.430363
	1 6.299979 -2.074252 1.917578		6 2.917600 4.613019 -0.267678
	1 5.169558 -2.311617 0.586920		1 2.121078 5.218569 0.178454
	1 6.190664 -0.872941 0.637771		1 2.815011 4.715151 -1.353639
	6 4.524749 2.258200 -2.343984		6 4.269648 5.162025 0.173913
	1 4.052562 3.067155 -2.911852		1 5.077379 4.602936 -0.311964
	1 4.779828 1.476813 -3.068368		1 4.393042 5.007777 1.252999
	6 5.796809 2.782740 -1.687299		6 4.432602 6.643776 -0.143988
	1 6.309754 1.968898 -1.161923		1 3.632345 7.208555 0.346993
	1 5.535760 3.526339 -0.924154		1 4.300054 6.798865 -1.220468
	6 6.759203 3.407793 -2.690445		6 5.784667 7.195092 0.288047
	1 6.254967 4.229567 -3.210748		1 6.603187 6.671130 -0.213830
	1 7.010270 2.668342 -3.458908		1 5.876377 8.258125 0.051071
	6 8.036850 3.922479 -2.041323		1 5.930900 7.081008 1.366019
	1 8.579799 3.114140 -1.543035		28 0.659126 -1.939202 -0.497494
	1 8.708489 4.367169 -2.780076		15 1.629415 -3.946111 -0.710297
	1 7.817505 4.685980 -1.289362		6 0.544994 -5.414311 -0.607757
	15 0.237904 -3.873537 0.863602		1 1.103543 -6.337659 -0.785969
	6 -1.056758 -4.719815 1.820501		1 0.097559 -5.466059 0.388188
	1 -0.710128 -5.698045 2.164154		1 -0.255070 -5.322677 -1.343209
	1 -1.319173 -4.111012 2.687750		6 2.950195 -4.424672 0.454763
	1 -1.941861 -4.839539 1.194914		1 2.562858 -4.417603 1.476028
	6 1.664437 -3.948741 1.990701		1 3.347171 -5.417873 0.225775
	1 1.462100 -3.371143 2.893211		1 3.761000 -3.697504 0.413411
	1 1.890568 -4.983352 2.264274		6 2.449801 -4.180537 -2.324287
	1 2.535040 -3.514547 1.495118		1 3.233562 -3.429367 -2.445400
	6 0.723537 -5.096607 -0.396729		1 2.894378 -5.175854 -2.413578
	1 1.604316 -4.735580 -0.931673		1 1.715171 -4.034694 -3.117716
	1 0.962912 -6.056751 0.068803		6 -5.563327 0.161516 1.744415
	1 -0.087214 -5.224196 -1.113555		8 -5.267804 -0.058638 0.544823
	6 -2.637167 1.317887 0.575718		8 -6.119985 1.162624 2.246606
	8 -3.817705 1.812238 0.345415		35 -0.857351 -2.597594 -2.300519
	8 -1.692866 2.019945 1.065713		8 -5.192406 -0.851449 2.620812
	55 -4.367647 -0.335034 -1.779268		55 -2.948022 -1.984171 0.513297
	55 -3.305262 4.266103 1.877568		55 -5.612828 2.806034 -0.306567
TS8b	5 0.634711 -1.614261 2.244375	**COM1b**	5 -0.292084 0.393761 -2.195312
	5 -0.859659 -0.796752 2.748411		5 1.259939 0.584839 -1.369290
	5 -0.447958 0.486403 3.892728		5 0.182027 3.200600 -1.773305
	5 1.292734 0.459444 4.124387		5 1.543843 2.311152 -1.096255
	5 0.574403 1.650718 3.036032		5 0.263694 2.911085 -0.034770
	5 0.749547 1.088495 1.361293		5 -0.762347 1.533045 0.367587
	5 0.408166 -1.067706 3.937884		5 0.798617 1.758778 -2.604403

Species	Cartesian coordinates	Species	Cartesian coordinates
	5 1.928632 -0.842990 3.134550		5 -0.907264 2.007661 -2.459680
	1 0.821879 -2.748026 1.940164		1 -0.643611 -0.431892 -2.969123
	1 -1.885679 -1.386827 2.814319		1 2.169126 -0.154775 -1.570279
	1 1.936056 0.812861 5.057808		1 0.142554 4.313003 -2.188337
	1 -1.182974 0.832820 4.763011		1 2.629040 2.808110 -1.069126
	1 0.692694 2.810289 3.260386		1 0.320235 3.820702 0.726024
	1 1.061866 1.800218 0.476059		1 -1.459346 1.560551 1.319640
	1 0.332937 -1.853676 4.826670		1 1.314967 1.832136 -3.673894
	1 2.957007 -1.372765 3.365288		1 -1.679015 2.278876 -3.309598
	5 -0.127405 -0.454884 1.151989		5 -0.191251 0.020359 -0.458698
	1 -0.996352 -0.407150 0.032155		1 4.943940 0.430175 3.838438
	5 -0.778164 0.870882 2.186707		5 0.944436 1.274667 0.221869
	1 -1.723428 1.507779 1.858779		1 1.606932 1.082209 1.196026
	6 1.933277 0.765352 2.592726		6 -1.155198 2.644964 -0.909714
	6 1.575455 -0.377926 1.506940		6 -1.419385 1.061360 -1.095012
	28 -0.312113 -2.028419 -0.224507		6 -2.526249 3.329082 -0.879485
	35 -2.214553 -3.296502 0.635784		6 -3.498201 2.263349 -1.463784
	8 -2.253754 0.114749 -0.545700		1 -4.498974 2.438078 -1.071019
	6 2.821642 -0.432258 0.636666		1 -3.553522 2.341772 -2.550087
	6 2.935998 -0.574457 -0.695347		6 -3.605654 0.124052 -0.148628
	6 1.825735 -0.528543 -1.688865		6 -2.920968 0.947938 -0.967090
	6 0.555598 -1.095187 -1.569403		6 -3.002898 -0.634277 0.989843
	6 -2.403068 1.407526 -0.725611		6 -3.735362 -0.499854 2.183542
	8 -3.603810 1.890844 -0.591817		6 -1.748413 -1.271277 1.022431
	8 -1.405680 2.148002 -1.009126		6 -3.261700 -0.927904 3.409921
	15 0.389252 -3.850821 -1.164242		1 -4.699516 0.002268 2.161786
	6 -0.732311 -4.506772 -2.437098		6 -1.281876 -1.678539 2.291809
	1 -0.351108 -5.446374 -2.845784		6 -2.001974 -1.517921 3.461986
	1 -0.823548 -3.778519 -3.245225		1 -3.856615 -0.788687 4.308626
	1 -1.716923 -4.667180 -1.996776		1 -0.308629 -2.165980 2.356670
	6 1.992321 -3.848878 -2.024729		1 -1.589633 -1.857565 4.410046
	1 1.970854 -3.149229 -2.860893		14 -5.505461 0.085531 -0.366779
	1 2.237544 -4.848974 -2.393564		6 -6.169661 -1.608843 0.090328
	1 2.770285 -3.526791 -1.329766		1 -5.877454 -1.943149 1.087873
	6 0.613140 -5.245971 -0.013325		1 -5.845294 -2.364561 -0.630434
	1 1.389185 -4.995496 0.712864		1 -7.263894 -1.581276 0.054233
	1 0.913957 -6.147868 -0.553675		6 -6.443303 1.370822 0.649526
	1 -0.316465 -5.429171 0.524798		1 -5.947954 2.344316 0.687662
	6 3.368267 1.221588 2.345314		1 -6.598743 1.045790 1.681732
	6 3.972271 0.086656 1.488800		1 -7.434024 1.524663 0.209652
	1 4.769382 0.492843 0.868374		6 -5.947680 0.314813 -2.181343
	1 4.415769 -0.682871 2.121755		1 -6.967437 -0.048805 -2.345500
	6 2.112340 0.238881 -2.832532		1 -5.284767 -0.269599 -2.825638
	6 1.207207 0.411464 -3.860927		1 -5.917159 1.350474 -2.525300
	1 3.074500 0.739989 -2.907198		28 -0.698615 -1.887215 -0.349010
	6 -0.356349 -0.910397 -2.621539		15 -1.728461 -3.876864 -0.349589
	6 -0.043408 -0.187775 -3.757739		6 -0.736713 -5.303494 0.218930
	1 1.472256 1.012331 -4.727307		1 -1.296660 -6.239496 0.137363
	1 -1.358971 -1.320114 -2.521407		1 -0.456475 -5.156390 1.265158
	1 -0.781964 -0.069774 -4.547421		1 0.173136 -5.368834 -0.379085
	14 4.709570 -0.758785 -1.410299		6 -3.239472 -4.096901 0.649801
	6 4.719255 -1.716729 -3.026971		1 -3.025021 -3.883209 1.699239
	1 4.007274 -1.355001 -3.770121		1 -3.635231 -5.112781 0.560946
	1 4.525486 -2.779777 -2.865879		1 -4.001230 -3.388144 0.325426
	1 5.723300 -1.636715 -3.458334		6 -2.291141 -4.427332 -1.996651

Species	Cartesian coordinates	Species	Cartesian coordinates
	6 5.552737 0.899213 -1.731239		1 -3.012423 -3.708924 -2.392657
	1 5.358864 1.647899 -0.958992		1 -2.759731 -5.414724 -1.955057
	1 5.239821 1.331930 -2.685306		1 -1.435095 -4.455566 -2.672298
	1 6.636414 0.753278 -1.784873		6 5.381696 0.501038 1.995111
	6 5.792435 -1.785911 -0.257582		8 5.282091 -0.111886 0.903901
	1 6.584239 -2.254851 -0.850849		8 5.899026 1.615759 2.226061
	1 5.224814 -2.591235 0.218166		35 0.993917 -2.887909 -1.801427
	1 6.280762 -1.212243 0.532465		8 4.809458 -0.159088 3.075886
	6 3.498492 2.590647 1.679319		6 -2.960565 3.822932 0.499252
	1 3.258756 2.504253 0.614175		1 -3.301538 2.973740 1.101752
	1 2.760286 3.276309 2.106438		1 -2.097778 4.245813 1.023632
	6 4.889392 3.192130 1.850459		6 -4.057184 4.879789 0.420679
	1 5.092421 3.336558 2.918709		1 -3.679053 5.752084 -0.126589
	1 5.654358 2.493595 1.489587		1 -4.907302 4.504254 -0.162090
	6 5.048517 4.521880 1.123154		6 -4.550587 5.322085 1.792930
	1 4.287490 5.222911 1.483655		1 -3.703234 5.698690 2.376551
	1 4.847262 4.376511 0.055890		1 -4.932368 4.451760 2.338242
	6 6.431689 5.132759 1.302853		6 -5.632604 6.390637 1.715187
	1 6.519409 6.084850 0.773168		1 -5.968742 6.691402 2.710748
	1 6.646905 5.318880 2.359001		1 -5.267339 7.285584 1.203193
	1 7.209924 4.466622 0.919233		1 -6.506014 6.028403 1.165148
	1 3.864517 1.257897 3.319223		1 -2.469271 4.186087 -1.556894
	55 -4.522534 -0.480297 1.072834		55 2.820256 -1.836465 1.074608
	55 -2.887615 4.561558 -1.572575		55 5.817299 2.335386 -0.781967
Cs_2CO_3	6 -0.000004 1.253440 0.000022	**$CsHCO_3$**	6 -2.077163 0.041895 -0.000095
	8 1.125732 1.881005 0.000412		8 -1.511302 1.156169 -0.000096
	8 -1.125761 1.880968 -0.000481		8 -3.458258 0.070048 -0.000013
	8 0.000032 -0.068990 -0.000129		1 -3.723192 -0.864762 -0.000033
	55 2.897398 -0.336949 -0.000102		8 -1.547605 -1.104141 -0.000162
	55 -2.897398 -0.336951 0.000128		55 1.242245 -0.006604 0.000050
CsBr	35 0.000000 0.000000 -2.100698		
	55 0.000000 0.000000 1.336808		

Table S14. Vibrational frequencies for stationary points involving Cs_2CO_3 on **Path a** and **b**, located at PCM-LC-ωPBE/DZVP (SDD for Cs) level in toluene solution.

Species	Frequencies (cm^{-1})
TS8a	-1006 10 18 21 25 31 42 46 47 49 58 62 64 66 69 69 80 84 89 99 106 112 115 129 134 142 150 156 167 169 174 176 180 185 189 193 199 203 208 211 217 226 229 234 246 249 252 258 267 271 278 284 286 296 307 339 360 378 382 433 481 484 490 498 508 525 537 563 590 598 603 610 617 628 633 644 660 668 683 690 698 704 707 708 711 717 720 727 740 741 748 756 758 761 764 766 775 778 780 784 785 790 793 797 801 803 810 821 821 837 851 858 866 875 879 880 885 887 891 896 905 920 922 931 933 938 941 946 953 954 961 964 966 970 972 980 980 983 985 991 993 999 1002 1013 1017 1028 1050 1066 1073 1075 1081 1092 1102 1109 1116 1127 1143 1151 1159 1180 1182 1221 1225 1258 1266 1284 1291 1296 1325 1329 1330 1338 1342 1349 1350 1353 1355 1361 1373 1384 1419 1443 1447 1462 1469 1473 1479 1483 1485 1486 1486 1487 1489 1494 1494 1496 1500 1506 1510 1511 1520 1523 1524 1530 1543 1589 1673 1703 1739 2696 2710 2716 2722 2733 2741

	2747 2784 2795 3087 3092 3092 3093 3095 3099 3100 3102 3103 3103 3129 3139 3143 3157 3170 3188 3191 3191 3191 3196 3201 3208 3209 3211 3214 3220 3222 3229 3229 3234 3237 3239 3242 3252
COM1a	1 9 11 15 21 23 28 29 40 46 50 56 57 63 67 68 73 75 78 81 95 100 111 113 117 117 130 132 145 147 157 162 175 176 182 185 190 197 198 207 212 217 223 227 241 243 252 261 265 272 278 285 286 313 344 348 359 379 424 469 484 492 502 515 536 542 561 565 581 584 599 601 613 616 623 631 644 660 666 677 685 697 708 709 710 711 716 724 740 742 753 754 756 759 762 766 767 772 776 783 784 792 794 796 800 805 807 810 819 835 848 853 862 868 871 874 876 881 886 896 909 919 931 933 936 939 945 951 953 958 959 963 968 971 976 978 979 980 984 987 990 995 1001 1008 1011 1019 1027 1052 1070 1074 1077 1082 1097 1110 1119 1124 1149 1156 1178 1179 1213 1221 1240 1254 1259 1283 1288 1293 1316 1325 1330 1337 1340 1343 1347 1349 1352 1356 1370 1378 1417 1421 1443 1462 1463 1475 1480 1484 1485 1486 1487 1492 1494 1495 1496 1501 1506 1510 1511 1520 1522 1523 1526 1530 1657 1691 1715 1792 2661 2671 2705 2714 2721 2738 2747 2768 2786 3088 3092 3092 3093 3094 3095 3097 3098 3102 3102 3128 3140 3147 3157 3170 3188 3189 3190 3192 3192 3196 3199 3200 3205 3208 3210 3212 3226 3227 3228 3230 3236 3237 3255 3772
TS8b	-1019 4 18 22 29 30 35 38 48 49 53 62 63 71 74 77 81 84 90 92 109 114 115 131 135 145 147 154 164 167 172 174 176 178 191 194 202 209 211 216 219 221 231 237 245 248 255 258 266 272 278 284 286 294 337 349 361 379 390 418 472 481 492 499 519 525 531 564 576 599 605 610 621 630 640 642 660 673 679 690 696 704 708 710 711 717 720 736 741 744 755 758 761 764 767 770 775 778 780 786 787 791 792 797 799 808 810 820 823 839 854 861 867 875 879 880 882 887 891 896 903 917 924 931 935 936 941 946 954 955 959 962 965 967 973 975 981 983 985 987 991 997 1000 1015 1015 1033 1050 1062 1069 1075 1082 1090 1096 1108 1112 1120 1135 1146 1158 1165 1182 1218 1234 1251 1265 1278 1291 1296 1313 1328 1329 1337 1342 1348 1349 1351 1355 1367 1372 1373 1419 1443 1444 1461 1469 1473 1477 1480 1485 1486 1486 1487 1489 1494 1494 1496 1500 1507 1510 1512 1522 1523 1527 1531 1542 1588 1673 1702 1738 2696 2711 2717 2725 2731 2734 2744 2789 2811 3085 3092 3092 3093 3095 3100 3100 3103 3103 3109 3135 3140 315 3158 3175 3188 3191 3191 3192 3195 3202 3209 3209 3210 3213 3221 3223 3225 3230 3234 3237 3240 3242 3252
COM1b	1 10 15 21 23 27 31 32 33 46 50 56 63 65 68 71 75 78 83 87 94 104 112 113 114 119 128 138 143 153 155 164 170 175 180 185 191 196 201 211 217 220 226 229 241 247 254 262 265 270 271 287 288 342 346 348 359 382 419 465 476 496 497 521 532 534 562 567 571 581 593 604 611 617 629 637 642 660 672 676 683 698 709 710 711 713 716 736 742 748 754 756 759 762 765 767 770 772 775 784 786 791 793 797 803 805 808 810 817 837 849 857 866 869 870 875 877 880 886 895 902 919 930 933 933 937 946 950 952 958 961 962 964 969 973 976 979 980 981 989 992 995 997 1008 1012 1020 1028 1052 1067 1071 1076 1083 1094 1105 1112 1121 1142 1156 1163 1179 1211 1228 1240 1244 1267 1276 1284 1294 1304 1325 1329 1336 1339 1341 1346 1347 1352 1361 1366 1370 1417 1421 1443 1461 1463 1476 1480 1484 1485 1486 1487 1492 1494 1495 1496 1501 1507 1510 1512 1522 1522 1523 1528 1531 1657 1691 1714 1791 2662 2671 2701 2710 2722 2733 2748 2785

	2789 3084 3092 3093 3093 3094 3095 3098 3100 3102 3105 3134 3139 3157 3158 3171 3187 3188 3190 3191 3191 3196 3199 3202 3206 3209 3210 3212 3224 3226 3228 3229 3236 3238 3255 3773
Cs_2CO_3	20 48 72 142 180 216 690 691 889 1077 1449 1552
$CsHCO_3$	52 119 132 569 581 676 850 1023 1246 1425 1776 3789
CsBr	13 13 99

Table S15. 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 involving Cs_2CO_3 on **Path a** and **b**, located at PCM-LC-ωPBE/DZVP (SDD for Cs) level in toluene solution.

Species	***E***	***ZPE***	***G***	***G*(sol, 298K)**
TS8a	-6128.84411	424.47249	-6128.25334	-6128.24291
COM1a	-6128.90055	426.86638	-6128.31011	-6128.30344
TS8b	-6128.84210	424.49684	-6128.25194	-6128.24172
COM1b	-6128.89904	426.97318	-6128.31188	-6128.30228
Cs_2CO_3	-304.18624	10.05255	-304.20877	-304.19377
$CsHCO_3$	-284.56996	17.50387	-284.57441	-284.55952
CsBr	-2593.60173	0.14220	-2593.62838	-2593.61614

Table S16. 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 involving Cs_2CO_3 on **Path a** and **b**, located at PCM-LC-ωPBE/TZVP (SDD for Cs) level in toluene solution.

Species	***E***	***ZPE***	***G***	***G*(sol, 298K)**
M1	-2535.68671	280.73570	-2535.29164	-2535.28127
R3	-3290.01013	128.80181	-3289.85038	-3289.84063
INT8	-5825.81033	414.48988	-5825.22087	-5825.21011
Cs_2CO_3	-304.23703	9.96716	-304.25974	-304.24469

TS8a	-6130.02168	422.28220	-6129.43501	-6129.42289
TS8b	-6130.01994	422.34204	-6129.43277	-6129.42207

Table S17. 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 involving K_2CO_3 on **Path a** and **b**, located at PCM-LC-ωPBE/TZVP (SDD for Cs) level in toluene solution.

Species	***E***	***ZPE***	***G***	***G*(sol, 298K)**
K_2CO_3	-1463.45147	10.23808	-1463.47066	-1463.45360
TS8a	-7289.23489	422.59746	-7288.64389	-7288.63338
TS8b	-7289.23296	422.72850	-7288.64128	-7288.63114

Table S18. Single-point energies (*E*: a.u.) and Gibbs free energies [*G*(sol,298K): a.u.] for stationary points involving in the formation of **P1a/b** from **M1+R3**, obtained at PCM- METHOD/TZVP//DZVP levels in toluene solution (METHOD = LC-ωPBE, CAM-B3LYP, B3LYP and B3LYP-D3 respectively).

Species	**LC-ωPBE**		**CAM-B3LYP**	
	E	***G*(sol, 298K)**	***E***	***G*(sol, 298K)**
R3	-3290.00983	-3289.20705	-3290.65372	-3289.84468
CAT	-2430.09945	-2429.45804	-2430.59248	-2429.94810
PMe3	-460.96707	-460.79258	-461.07104	-460.89713
K_2CO_3	-1463.45132	-1463.26419	-1463.86120	-1463.67270
$KHCO_3$	-864.22672	-864.08816	-864.46650	-864.32847
KBr	-3173.69088	-3173.14245	-3174.33780	-3173.78906
M1	-2535.68627	-2534.77752	-2536.03379	-2535.11584
INT1	-5825.71616	-5823.99144	-5826.69787	-5824.95809
TS1	-5825.70698	-5823.98194	-5826.68143	-5824.94144
INT2	-5825.73428	-5824.00847	-5826.70984	-5824.96915

TS2	-5825.71139	-5823.98554	-5826.68535	-5824.94393
INT3	-5825.72482	-5824.00060	-5826.70081	-5824.96148
TS3	-5825.71064	-5823.98454	-5826.68143	-5824.93826
INT4	-5825.72107	-5823.99420	-5826.69231	-5824.94933
TS4	-5825.72067	-5823.99064	-5826.69221	-5824.94767
INT5	-5825.73773	-5824.01362	-5826.71681	-5824.98036
TS5	-5825.71776	-5823.99174	-5826.69121	-5824.94959
INT6	-5825.74320	-5824.01786	-5826.72127	-5824.98201
TS6	-5825.70880	-5823.98963	-5826.67700	-5824.94319
INT7	-5825.72195	-5824.00563	-5826.70389	-5824.97052
TS7	-5825.71995	-5823.99842	-5826.69974	-5824.96280
INT8	-5825.80963	-5824.07954	-5826.78545	-5825.04368
TS8a	-7289.23401	-7287.30916	-7290.61435	-7288.67548
COM1a	-7289.28358	-7287.35848	-7290.66214	-7288.71966
INT9a	-3251.33385	-3250.10879	-3251.83189	-3250.59283
TS9a	-3251.33199	-3250.10730	-3251.82646	-3250.59049
P1a	-1282.23004	-1281.47680	-1282.34240	-1281.57606
TS8b	-7289.23164	-7287.30743	-7290.61220	-7288.67315
COM1b	-7289.28358	-7287.35584	-7290.66002	-7288.71811
INT9b	-3251.33595	-3250.10865	-3251.83377	-3250.59317
TS9b	-3251.33153	-3250.10721	-3251.82571	-3250.58800
P1b	-1282.22754	-1281.47535	-1282.34008	-1281.57443

Species	**B3LYP**		**B3LYP-D3**	
	E	***G*(sol, 298K)**	***E***	***G*(sol, 298K)**
R3	-3290.83407	-3290.02805	-3290.85284	-3290.04619

CAT	-2430.74187	-2430.09911	-2430.76411	-2430.12211
PMe3	-461.16845	-460.99512	-461.17397	-461.00000
K_2CO_3	-1463.92333	-1463.73858	-1463.92793	-1463.74175
$KHCO_3$	-864.54206	-864.40495	-864.54491	-864.40361
KBr	-3174.23157	-3173.67641	-3174.23285	-3173.68263
M1	-2536.49067	-2535.57719	-2536.56701	-2535.65181
INT1	-5827.32681	-5825.59469	-5827.45855	-5825.72287
TS1	-5827.30980	-5825.57576	-5827.44246	-5825.70713
INT2	-5827.33461	-5825.60253	-5827.46821	-5825.73298
TS2	-5827.31446	-5825.57927	-5827.44765	-5825.71239
INT3	-5827.33016	-5825.59846	-5827.46241	-5825.72883
TS3	-5827.30900	-5825.57520	-5827.44283	-5825.70473
INT4	-5827.32025	-5825.58501	-5827.45507	-5825.71714
TS4	-5827.31867	-5825.58172	-5827.45328	-5825.71385
INT5	-5827.34382	-5825.61510	-5827.47472	-5825.74302
TS5	-5827.31920	-5825.58454	-5827.45103	-5825.71396
INT6	-5827.34692	-5825.61506	-5827.47909	-5825.74445
TS6	-5827.30482	-5825.57864	-5827.43893	-5825.70805
INT7	-5827.33290	-5825.60649	-5827.45326	-5825.72340
TS7	-5827.32870	-5825.59893	-5827.45285	-5825.71957
INT8	-5827.40686	-5825.67146	-5827.54197	-5825.80309
TS8a	-7291.29534	-7289.36507	-7291.45213	-7289.51509
COM1a	-7291.34568	-7289.40176	-7291.49255	-7289.55752
INT9a	-3252.55515	-3251.32379	-3252.67205	-3251.43910
TS9a	-3252.55051	-3251.32134	-3252.66774	-3251.43600
P1a	-1283.01449	-1282.25546	-1283.09929	-1282.33877

TS8b	-7291.29295	-7289.36219	-7291.45006	-7289.51547
COM1b	-7291.34351	-7289.41218	-7291.49283	-7289.55672
INT9b	-3252.55667	-3251.32369	-3252.67410	-3251.43994
TS9b	-3252.54958	-3251.32087	-3252.66743	-3251.43525
P1b	-1283.01217	-1282.25310	-1283.09799	-1282.33727