Conformational Dynamics of the Pyrene Excimer

- Supporting Information -

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SOAP Descriptors[1]

The SOAP output is represented as the partial power spectrum vector $\boldsymbol{p}$, with its elements defined as follows:

$$p_{nn'l}^{Z_1Z_2} = \pi \sqrt{\frac{8}{2l+1}} \sum_m \left(C_{nlm}^{Z_1}\right)^* C_{n'lm}^{Z_2} \quad (1)$$

where n and n' are indices for the different radial basis functions up to n_{max}, l is the angular degree of the spherical harmonics up to l_{max}. Z_1 and Z_2 are atomic species.

The coefficients $C_{nlm}^{Z_1}$ are defined as the following inner products:

$$C_{nlm}^{Z_1} = \iiint_{R^3} dV \; g_n(r)\, Y_{lm}(\theta, \phi)\, \rho_z(r) \quad (2)$$

where $\rho_Z(\mathbf{r})$ is the Gaussian smoothed atomic density for atoms with atomic number Z defined as,

$$\rho_Z(r) = \sum_i^{|Z_i|} e^{\frac{-|r-R_i|^2}{2\sigma^2}} \quad (3)$$

$Y_{lm}(\theta, \phi)$ are the real spherical harmonics, and $g_n(r)$ is the radial basis function.

We have used a polynomial basis function, for which $g_n(r)$ is defined as:

$$g(r) = \sum_{n'=1}^{n_{max}} \beta_{nn'} (r - r_{cut})^{n'+2} \quad (4)$$

Increasing the arguments n_{max} and l_{max} makes SOAP more accurate, but also increases the number of features. In our case, using $n_{max} = 8$, $l_{max} = 6$, and $r_{cut} = 14$ Å, the resulting SOAP descriptor in our case has 952 features.

Dimensionality Reduction and Choice of RBF Kernel

We applied Kernel PCA with an RBF kernel for dimensionality reduction, which enabled effective separation of clusters in the reduced space. The RBF kernel, with its distance sensitivity, was particularly advantageous in capturing nonlinear relationships between atomic environments, enhancing the distinction between clusters. Specifically, the RBF kernel emphasizes similarity based on Euclidean distance: the closer two points are in high-dimensional space, the higher their similarity score in the transformed space. This sensitivity allows the RBF kernel to capture subtle, nonlinear patterns, making it effective for clustering distinct structures or atomic environments.

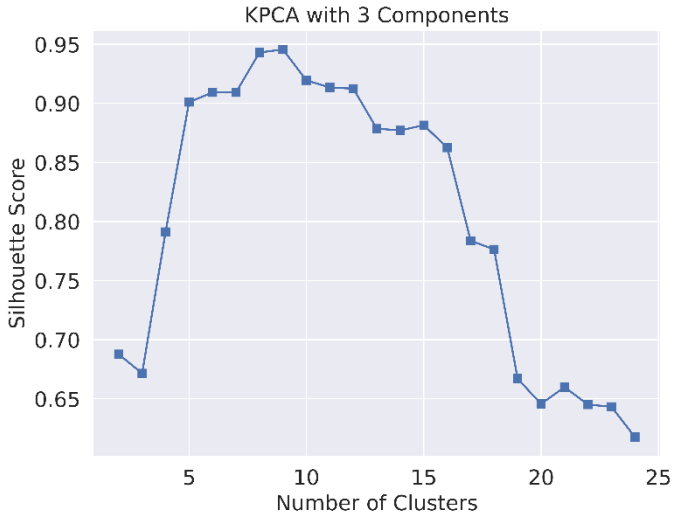

Figure S1. Silhouette score,[1] measuring the goodness of the clustering outcome as a function of the number of clusters identified among the optimized geometries of the pyrene excimer in the S_1 state, at the TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane) level, using SOAP descriptors.[2] The maximum value (0.9456) was found for 9 clusters.

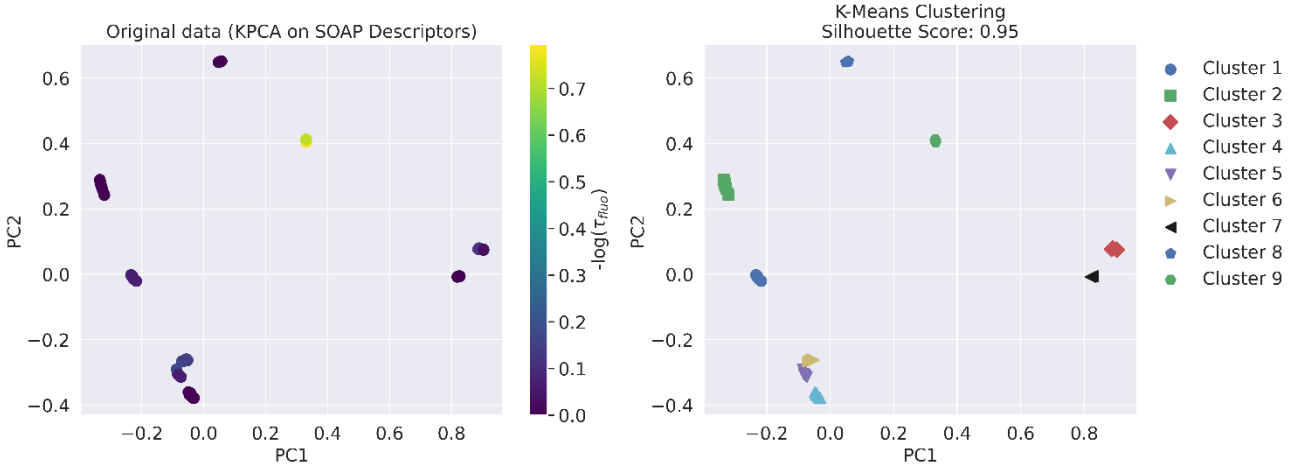

Figure S2. Plots of the optimized geometries on the Cartesian plane are defined by the first two principal components obtained using SOAP descriptors.[2] We note, however, that the first three principal components were considered in the kernel principal component analysis (KPCA). The left panel shows the oscillator strength of each structure, mapped by the color bar. The right panel labels the initially defined nine clusters.

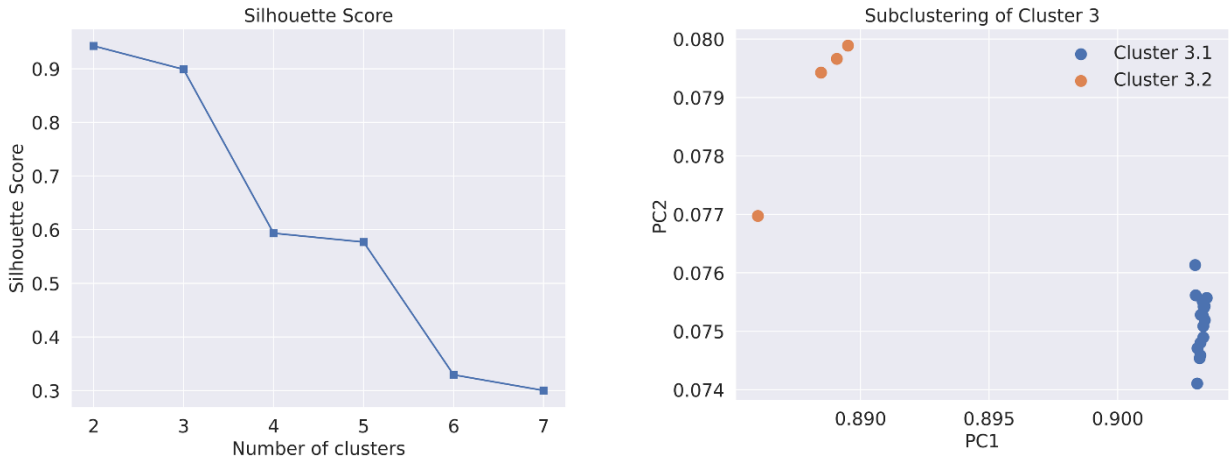

Figure S3. In the left panel, optimized geometries belonging to the two clusters **3.1** (17 structures) and **3.2** (4 structures) are plotted on the Cartesian plane defined by the first two principal components obtained using SOAP descriptors[2]. The right panel displays the silhouette score[1] for the subclustering of the initially defined cluster 3. The highest value (0.9426) was observed for two clusters, supporting our initial choice based on visual inspection of the corresponding structures and their electronic properties, as well as available literature.[3,4]

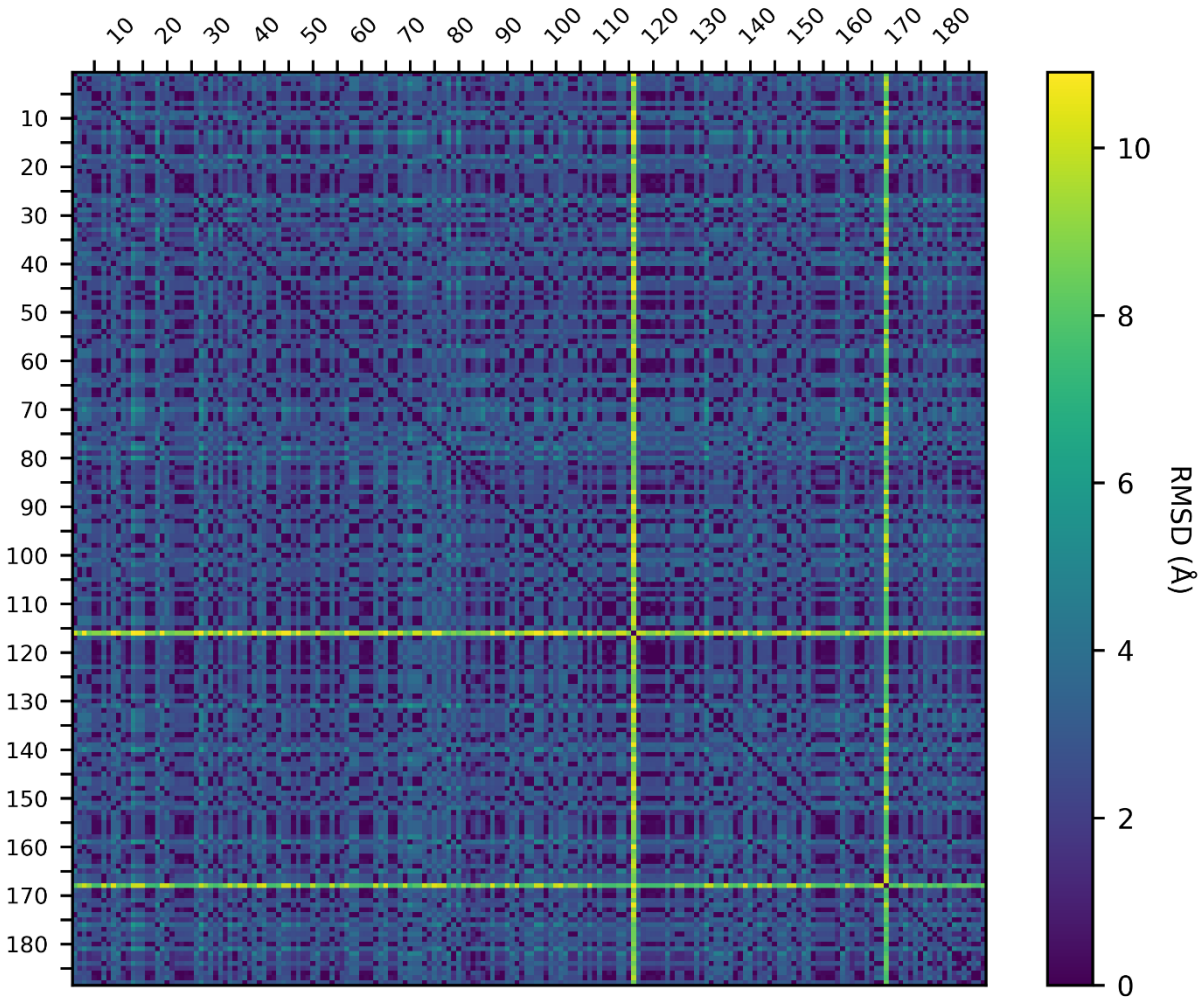

Figure S4. Heatmap representing the RMSD between pairs of optimized structures of the pyrene excimer in the S_1 state, at the TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane) level.

Table S1. Energy data for all the identified clusters at the TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane) level. Each value corresponds to the average over all structures belonging to that particular cluster. The total electronic energy in the S_1 state is obtained as the sum of SCF energy, vertical excitation energy ($\Delta E_{S_1S_0}$), and empirical dispersion correction (D3BJ). The last column provides the total electronic energy including the geometrical counterpoise correction,[5] which was used to reduce the basis set superposition error when calculating the binding energy for the cluster. In the last two columns, the relative values with respect to the global minimum conformation (cluster **3.1**) are shown in parentheses.

Cluster	SCF Energy (Ha)	$\Delta E_{S_1S_0}$ (Ha)	D3BJ correction (Ha)	Total Electronic Energy (Ha)	Total Electronic Energy + gCP correction (Ha)
1	-1230.776634	0.111134	-0.089778	-1230.755278 (*0.539 eV*)	-1230.652293 (*0.509 eV*)
2	-1230.778445	0.110904	-0.087596	-1230.755137 (*0.543 eV*)	-1230.652600 (*0.501 eV*)
3.1	-1230.769401	0.090392	-0.096098	-1230.775106 (*0 eV*)	-1230.671005 (*0 eV*)
3.2	-1230.777777	0.112704	-0.093785	-1230.758857 (*0.442 eV*)	-1230.655824 (*0.413 eV*)
4	-1230.783041	0.120588	-0.089824	-1230.752277 (*0.606 eV*)	-1230.649954 (*0.573 eV*)
5	-1230.781778	0.120361	-0.089778	-1230.751195 (*0.651 eV*)	-1230.648712 (*0.607 eV*)
6	-1230.784700	0.123486	-0.089830	-1230.751044 (*0.655 eV*)	-1230.648690 (*0.607 eV*)
7	-1230.770612	0.095369	-0.093235	-1230.768478 (*0.180 eV*)	-1230.665710 (*0.144 eV*)
8	-1230.779870	0.115029	-0.080318	-1230.745159 (*0.815 eV*)	-1230.643685 (*0.743 eV*)
9	-1230.793575	0.129247	-0.065827	-1230.730155 (*1.223 eV*)	-1230.631395 (*1.078 eV*)

Table S2. Geometrical and electronic properties for a representative geometry of each conformational cluster, optimized at the TD-CAM-B3LYP+D3BJ/def2-TZVP/C-PCM(cyclohexane) level. R is the total distance between the centers of mass of the two pyrene monomers. R_{PA1}, R_{PA2} and R_{PA3} represents its absolute components along the first, second, and third principal axes, respectively, of the reference monomer. α_{PA1}, α_{PA2} and α_{PA3} are the angles between pairs of equivalent principal axes on the two monomers. ΔE_{bind} is the binding energy level, including the geometrical counterpoise correction. $\Delta E_{S_1S_0}$ is the S_0-S_1 vertical excitation energy, while $f_{S_1S_0}$ is the associated oscillator strength. τ_{fluo} is the fluorescence lifetime from Eq. 2 in the main text. CT is the charge transfer character[6] of the S_0-S_1 transition, calculated with the TheoDORE toolbox[7]. a) Ref. [8]; b) Ref. [9]; c) Ref. [10,11]

Cluster	R (Å)	R_{PA1} (Å)	R_{PA2} (Å)	R_{PA3} (Å)	α_{PA1} (°)	α_{PA2} (°)	α_{PA3} (°)	ΔE_{bind} (eV)	$\Delta E_{S_1S_0}$ (eV)	$f_{S_1S_0}$	τ_{fluo} (s)	CT
1	4.06	3.24	1.45	1.98	4.97	47.0	46.8	0.646	3.062	0.087	2.83×10^{-8}	0.371
2	4.22	3.14	2.82	0.00	0.01	0.04	0.04	0.643	3.042	5.9×10^{-8}	4.22×10^{-2}	0.366
3.1	3.17	3.17	0.00	0.00	0.04	49.8	49.8	1.150	2.489	0.034	1.14×10^{-7}	0.457
3.2	3.27	3.27	0.00	0.00	0.01	78.4	78.4	0.744	3.053	0.139	1.78×10^{-8}	0.435
4	4.07	3.27	0.63	2.33	0.01	0.01	0.01	0.580	3.283	4.2×10^{-7}	4.79×10^{-3}	0.346
5	4.06	3.19	1.24	2.18	4.76	53.1	52.8	0.544	3.268	0.074	2.91×10^{-8}	0.367
6	4.04	3.27	1.98	1.31	1.06	59.3	59.3	0.557	3.339	0.309	6.69×10^{-9}	0.188
7	3.34	3.34	0.00	0.00	0.00	0.00	0.00	1.005	2.596	0.000	∞	0.438
8	5.35	3.00	2.17	3.87	0.09	0.25	0.26	0.400	3.170	8.4×10^{-6}	2.74×10^{-4}	0.338
9	10.04	0.09	3.46	9.43	78.2	72.4	25.7	0.079	3.436	0.802	2.43×10^{-9}	0.004
Exp.	-	-	-	-	-	-	-	0.73-0.86 [a]	2.61 [b]	0.038	0.9×10^{-7} [c]	-

Table S3. Calculated reaction barriers for the conformational rearrangements between different starting clusters and the global minimum **3.1**, at the TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane) level. Both backward and forward processes are considered.

Starting Cluster	Final Cluster	$\Delta G^{\ddagger}_{forward}$ (Ha)	$\Delta G^{\ddagger}_{backward}$ (Ha)
1	**3.1**	3.8483×10^{-3}	2.0997×10^{-2}
2		3.6068×10^{-3}	2.0913×10^{-2}
3.2		0 [a)]	1.4008×10^{-2}
4		1.5158×10^{-3}	2.0367×10^{-2}
5		1.4147×10^{-3}	2.1407×10^{-2}
6		1.1967×10^{-3}	2.0342×10^{-2}
7		1.4231×10^{-2}	2.0087×10^{-2}
8		1.1703×10^{-3}	2.6638×10^{-2}

[a)] In this specific case, we assumed $\Delta G^{\ddagger} = 0$, as thermochemical corrections, and in particular vibrational zero-point energy contributions, overcompensate for the small electronic energy barrier for the rearrangement from cluster **3.2** to cluster **3.1**.

Table S4. Calculated reaction times for some additional rearrangement pathways between different starting and final clusters, at the TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane) level. Both backward and forward processes are considered. The corresponding reaction barriers are given in parentheses. Fluorescence lifetimes for the starting and final clusters should be compared with $k^{-1}_{forward}$ and $k^{-1}_{backward}$, respectively. These results further confirm the existence of a rich network of conformational rearrangement pathways in the S_1 state of the pyrene excimer, which can occur before it reaches the global minimum geometry and decays radiatively *via* fluorescence emission.

Starting Cluster		Final Cluster		$k^{-1}_{forward}$ (s)	$k^{-1}_{backward}$ (s)
#	τ_{fluo} (s)	#	τ_{fluo} (s)		
1	3.66×10^{-8}	**2**	2.06×10^{-1}	2.50×10^{-11} (4.7650×10^{-3} Ha)	2.12×10^{-11} (4.6067×10^{-3} Ha)
		6	1.28×10^{-8}	5.22×10^{-12} (3.2849×10^{-3} Ha)	6.30×10^{-13} (1.2879×10^{-3} Ha)
3.2	1.96×10^{-8}	**5**	3.25×10^{-8}	2.53×10^{-10} (6.9481×10^{-3} Ha)	8.87×10^{-13} (1.6113×10^{-3} Ha)
		6	1.28×10^{-8}	1.74×10^{-10} (6.5971×10^{-3} Ha)	1.50×10^{-12} (2.1073×10^{-3} Ha)
5	3.25×10^{-8}	**6**	1.28×10^{-8}	2.55×10^{-13} (4.3541×10^{-4} Ha)	6.26×10^{-13} (1.2834×10^{-3} Ha)

Cluster 1 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	0.003555	-3.520041	-0.001714
C	1.208237	-2.833615	-0.019565
C	1.229266	-1.426882	-0.032074
C	0.001055	-0.714753	-0.042297
C	-1.232629	-1.427505	-0.012208
C	-1.204432	-2.831295	0.006931
C	2.449660	-0.684495	-0.006752
C	0.003381	0.709097	-0.044705
C	1.226023	1.418900	-0.007837
C	2.445182	0.677781	0.013509
C	1.207206	2.831487	0.043207
C	-0.009640	3.521656	-0.008868
C	-1.204846	2.841928	-0.035338
C	-1.236682	1.419953	-0.039693
C	-2.440451	0.693306	-0.008307
C	-2.448320	-0.688084	0.034566
H	2.146507	3.373771	0.032379
H	-3.388731	-1.228127	0.044182
H	-3.378312	1.239036	0.022532
H	3.387994	-1.231369	0.005025
H	0.002266	-4.605602	0.011269
H	2.149534	-3.375094	-0.015365
H	-2.144073	-3.375631	0.032297
H	3.382193	1.227004	0.043841
H	-0.007604	4.606140	0.014549
H	-2.146347	3.382441	-0.029565
C	-4.001116	-0.464801	3.080309
C	-2.666190	-0.861717	2.976832
C	-1.621768	0.088509	3.109803
C	-1.957928	1.464598	3.242642
C	-3.322645	1.862326	3.325439
C	-4.332828	0.862535	3.254022
C	-0.258046	-0.280511	3.069879
C	-0.933937	2.446007	3.238661
C	0.426046	2.050644	3.097646
C	0.736977	0.672853	3.064081
C	1.415216	3.052864	2.941145
C	1.079285	4.406924	3.057422
C	-0.226952	4.793629	3.251851
C	-1.270936	3.826486	3.330987
C	-2.626095	4.189183	3.464263
C	-3.623684	3.234413	3.454143
H	2.450587	2.752482	2.818463
H	-4.664290	3.535301	3.534219
H	-2.880834	5.241541	3.548706
H	-0.002957	-1.333300	3.001728
H	-4.786270	-1.211272	3.006705
H	-2.409226	-1.908485	2.851805
H	-5.373214	1.165843	3.324953
H	1.776780	0.372703	2.988770
H	1.858951	5.157886	2.974009
H	-0.484480	5.845442	3.334009

Cluster 2 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	0.007354	-3.519945	0.078528
C	1.204561	-2.841333	0.021044
C	1.233000	-1.420639	-0.047009
C	0.000330	-0.710245	-0.078968
C	-1.231575	-1.420256	-0.048805
C	-1.209582	-2.829137	0.072876
C	2.440642	-0.688954	-0.056437
C	0.000327	0.710258	-0.078963
C	1.233000	1.420666	-0.047289
C	2.440641	0.688969	-0.056647
C	1.204596	2.841376	0.020416
C	0.007404	3.519957	0.078379
C	-1.209513	2.829097	0.073523
C	-1.231588	1.420241	-0.048409
C	-2.443604	0.685773	-0.088523
C	-2.443593	-0.685799	-0.088897
H	2.146312	3.381911	0.034600
H	-3.382384	-1.230771	-0.078011
H	-3.382407	1.230715	-0.077271
H	3.380793	-1.232701	-0.046081
H	0.003342	-4.603754	0.143936
H	2.146276	-3.381860	0.035695
H	-2.149294	-3.369237	0.091893
H	3.380796	1.232713	-0.046478
H	0.003375	4.603771	0.143692
H	-2.149216	3.369192	0.093204
C	-2.784160	-3.518713	2.989967
C	-1.566506	-2.829173	2.995472
C	-1.543023	-1.420351	3.117595
C	-2.774180	-0.709064	3.148218
C	-4.007592	-1.418160	3.116200
C	-3.980648	-2.838867	3.047856
C	-0.330232	-0.687182	3.157758
C	-2.772687	0.711436	3.148571
C	-1.540028	1.420134	3.118282
C	-0.328779	0.684390	3.158118
C	-1.560616	2.829039	2.996727
C	-2.776810	3.521170	2.991741
C	-3.974714	2.843830	3.049456
C	-4.004611	1.423143	3.116982
C	-5.213022	0.692712	3.126232
C	-5.214467	-0.685208	3.125834
H	-0.620346	3.368162	2.977354
H	-6.155190	-1.227964	3.115444
H	-6.152604	1.237445	3.116131
H	0.607985	-1.233131	3.146380
H	-2.781293	-4.602509	2.924296
H	-0.627359	-3.370231	2.975989
H	-4.922928	-3.378409	3.033256
H	0.610594	1.228353	3.147089
H	-2.771636	4.604987	2.926568
H	-4.915865	3.385346	3.035226

Cluster 3.1 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	0.194982	-3.513490	-0.061509
C	1.355740	-2.767697	-0.031502
C	1.308449	-1.350288	0.038133
C	0.037836	-0.708772	0.059490
C	-1.154535	-1.485075	0.039403
C	-1.052980	-2.890940	-0.049880
C	2.476149	-0.555831	0.056875
C	-0.037242	0.708999	0.057842
C	1.154914	1.485159	0.022663
C	2.405669	0.818070	0.041845
C	1.052384	2.890782	-0.070007
C	-0.195667	3.513326	-0.070320
C	-1.356051	2.767714	-0.025786
C	-1.308005	1.350470	0.048324
C	-2.475458	0.556017	0.081739
C	-2.405050	-0.817833	0.070470
H	1.960998	3.483334	-0.090506
H	-3.312606	-1.412519	0.081442
H	-3.441740	1.051819	0.089782
H	3.442360	-1.051845	0.055822
H	0.251386	-4.596511	-0.115293
H	2.324994	-3.256891	-0.048453
H	-1.961749	-3.483620	-0.058844
H	3.313237	1.412780	0.040904
H	-0.252527	4.596127	-0.127885
H	-2.325495	3.256723	-0.034752
C	-2.570618	-2.421750	-3.031699
C	-1.236052	-2.826588	-3.043923
C	-0.196744	-1.875086	-3.139946
C	-0.530112	-0.491986	-3.166310
C	-1.894152	-0.085324	-3.144333
C	-2.901987	-1.082585	-3.067720
C	1.170338	-2.249293	-3.171807
C	0.498309	0.486810	-3.171566
C	1.862489	0.080163	-3.162650
C	2.165176	-1.299276	-3.189763
C	2.871049	1.077503	-3.095516
C	2.539973	2.416653	-3.057069
C	1.205321	2.821498	-3.056809
C	0.165109	1.869936	-3.142686
C	-1.202146	2.244169	-3.161054
C	-2.197118	1.294030	-3.169361
H	3.911512	0.767025	-3.086997
H	-3.240025	1.597237	-3.167814
H	-1.453229	3.299775	-3.164915
H	1.421413	-3.304923	-3.177943
H	-3.355421	-3.169817	-2.972627
H	-0.982685	-3.881496	-3.030226
H	-3.942389	-0.772250	-3.050250
H	3.207974	-1.602728	-3.198328
H	3.325178	3.164802	-3.004807
H	0.952047	3.876355	-3.041156

Cluster 3.2 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	0.200380	-3.512676	-0.043460
C	1.359263	-2.771632	0.005898
C	1.311445	-1.352246	0.046005
C	0.038982	-0.707503	0.051373
C	-1.153456	-1.483896	0.017022
C	-1.050114	-2.883785	-0.058485
C	2.478891	-0.559477	0.052906
C	-0.038623	0.707505	0.051605
C	1.153545	1.483897	0.008870
C	2.407782	0.813247	0.011155
C	1.049680	2.883784	-0.065948
C	-0.200679	3.512675	-0.042140
C	-1.359187	2.771633	0.015378
C	-1.311093	1.352248	0.055203
C	-2.478460	0.559477	0.070333
C	-2.407647	-0.813249	0.028113
H	1.957865	3.477321	-0.111199
H	-3.315427	-1.408128	0.023298
H	-3.444120	1.055035	0.075242
H	3.444561	-1.055037	0.051085
H	0.252653	-4.596262	-0.086870
H	2.328918	-3.260402	0.005461
H	-1.958598	-3.477315	-0.097399
H	3.315505	1.408126	-0.000051
H	-0.253255	4.596262	-0.085169
H	-2.328820	3.260406	0.021772
C	-3.500859	0.448032	-3.158581
C	-2.961773	-0.843689	-3.141042
C	-1.572970	-1.045895	-3.221089
C	-0.714462	0.088613	-3.262687
C	-1.267732	1.403439	-3.259897
C	-2.680037	1.551510	-3.214950
C	-0.992593	-2.344347	-3.229800
C	0.691525	-0.088721	-3.267613
C	1.244803	-1.403547	-3.268686
C	0.371540	-2.512064	-3.276590
C	2.657391	-1.551613	-3.233672
C	3.478588	-0.448131	-3.183118
C	2.939636	0.843589	-3.161806
C	1.550302	1.045788	-3.232085
C	0.969878	2.344238	-3.236768
C	-0.394548	2.511956	-3.273972
H	3.076459	-2.553357	-3.238162
H	-0.820681	3.510210	-3.274008
H	1.627398	3.207720	-3.231068
H	-1.650059	-3.207828	-3.219535
H	-4.577878	0.576846	-3.111538
H	-3.617811	-1.707848	-3.096579
H	-3.099122	2.553255	-3.216475
H	0.797662	-3.510318	-3.279604
H	4.555913	-0.576942	-3.143692
H	3.595969	1.707751	-3.122006

Cluster 4 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	0.000792	-3.522820	-0.026390
C	1.206986	-2.838679	-0.011146
C	1.232487	-1.427779	-0.007911
C	-0.000720	-0.714233	-0.029011
C	-1.229193	-1.427627	-0.016245
C	-1.207201	-2.835073	-0.027804
C	2.438913	-0.689338	0.049689
C	-0.000962	0.708093	-0.033601
C	1.234189	1.422215	-0.034852
C	2.438767	0.693421	0.013499
C	1.206519	2.841183	-0.040522
C	0.001974	3.524613	-0.028154
C	-1.204264	2.837711	0.002292
C	-1.227054	1.418815	-0.007794
C	-2.442182	0.682245	0.027779
C	-2.445352	-0.684445	0.025137
H	2.146868	3.382662	-0.037847
H	-3.384594	-1.229545	0.048549
H	-3.378753	1.231329	0.061288
H	3.379928	-1.230145	0.086070
H	-0.000362	-4.608617	-0.032831
H	2.147441	-3.381519	0.002710
H	-2.148111	-3.377182	-0.026606
H	3.377231	1.237661	0.043629
H	0.002199	4.609615	-0.009016
H	-2.145553	3.377447	0.009085
C	0.627921	-1.196305	3.233190
C	1.834047	-0.509205	3.202301
C	1.856622	0.909686	3.212343
C	0.630404	1.620197	3.238286
C	-0.604619	0.905878	3.239859
C	-0.576730	-0.513082	3.245747
C	3.071619	1.646464	3.176374
C	0.629922	3.042531	3.233651
C	1.858271	3.756142	3.220588
C	3.074552	3.013151	3.178920
C	1.836046	5.163566	3.232189
C	0.627928	5.851120	3.231054
C	-0.578143	5.166779	3.216030
C	-0.603401	3.755869	3.212828
C	-1.809719	3.017223	3.155425
C	-1.809336	1.634486	3.191639
H	2.776863	5.705836	3.230803
H	-2.747706	1.090074	3.161612
H	-2.750827	3.557872	3.119096
H	4.008269	1.097526	3.142708
H	0.627934	-2.281312	3.214289
H	2.775389	-1.048846	3.195394
H	-1.517012	-1.054684	3.243348
H	4.013685	3.558430	3.155287
H	0.628912	6.936917	3.237547
H	-1.518698	5.709452	3.202411

Cluster 5 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	0.003587	-3.521000	0.020843
C	1.208260	-2.840458	0.033727
C	1.234439	-1.424998	0.001636
C	-0.002465	-0.712812	-0.019947
C	-1.231672	-1.426234	-0.023716
C	-1.206893	-2.831883	-0.015232
C	2.438343	-0.689981	0.000182
C	-0.001324	0.709163	-0.025286
C	1.234722	1.424698	-0.035655
C	2.443431	0.696604	-0.034642
C	1.208761	2.838319	-0.013628
C	-0.000232	3.522314	0.014165
C	-1.200773	2.834431	0.028947
C	-1.228260	1.417694	0.001499
C	-2.447630	0.680834	-0.006174
C	-2.450466	-0.682633	-0.026048
H	2.148905	3.380771	-0.005900
H	-3.389004	-1.229349	-0.034016
H	-3.383670	1.231702	0.004460
H	3.379565	-1.231524	0.012618
H	0.000172	-4.606717	0.037189
H	2.148728	-3.382788	0.057235
H	-2.146599	-3.375989	-0.023554
H	3.382913	1.238426	-0.050309
H	-0.000630	4.606699	0.045233
H	-2.142216	3.374720	0.056372
C	-1.586726	0.039733	3.263491
C	-0.315435	-0.514449	3.177851
C	0.829492	0.314664	3.141702
C	0.659777	1.732146	3.191943
C	-0.641752	2.285753	3.282512
C	-1.757536	1.412254	3.308596
C	2.133861	-0.211339	3.024055
C	1.793039	2.589251	3.127719
C	3.099659	2.031642	2.986493
C	3.234060	0.628486	2.932179
C	4.210068	2.905829	2.894196
C	4.032498	4.276277	2.963564
C	2.761415	4.826288	3.117067
C	1.626585	3.999589	3.189225
C	0.304344	4.524372	3.311760
C	-0.782932	3.702210	3.348913
H	5.203478	2.482846	2.778656
H	-1.783148	4.117891	3.429704
H	0.179630	5.602084	3.364728
H	2.265401	-1.287595	2.994278
H	-2.454412	-0.611301	3.275075
H	-0.186478	-1.590911	3.124861
H	-2.753916	1.839244	3.370581
H	4.228190	0.203865	2.828406
H	4.894694	4.933205	2.899221
H	2.633522	5.903394	3.168501

Cluster 6 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	0.001702	-3.513584	-0.002016
C	1.206197	-2.830461	0.026403
C	1.235282	-1.422438	0.005186
C	0.001139	-0.710648	-0.005639
C	-1.231264	-1.426771	-0.020235
C	-1.209652	-2.825278	-0.035941
C	2.452575	-0.683013	0.007657
C	0.001884	0.711313	0.000686
C	1.235050	1.424479	-0.013321
C	2.453999	0.682230	-0.008338
C	1.210589	2.828779	-0.021149
C	-0.004848	3.514193	-0.014648
C	-1.207635	2.831293	0.024329
C	-1.230107	1.421995	0.032972
C	-2.452690	0.676698	0.030410
C	-2.455538	-0.680662	-0.010085
H	2.148423	3.374419	-0.041241
H	-3.392687	-1.229821	-0.023637
H	-3.388729	1.228239	0.045294
H	3.389424	-1.231195	0.023492
H	0.000412	-4.599593	0.000375
H	2.145916	-3.374579	0.048706
H	-2.149063	-3.369709	-0.056342
H	3.391319	1.230356	-0.002546
H	-0.003322	4.600056	-0.026709
H	-2.148383	3.373710	0.036336
C	-1.129029	-0.494165	3.198974
C	0.078464	-1.174618	3.209164
C	1.315945	-0.470580	3.233053
C	1.298186	0.948639	3.222814
C	0.050351	1.644331	3.202552
C	-1.159324	0.891356	3.188990
C	2.560371	-1.138066	3.242796
C	2.515814	1.671701	3.205823
C	3.758169	0.978288	3.231967
C	3.746016	-0.435989	3.258593
C	4.962797	1.725886	3.209501
C	4.934097	3.111998	3.147155
C	3.727548	3.797763	3.109635
C	2.497072	3.095685	3.138984
C	1.250248	3.753632	3.102577
C	0.055740	3.046974	3.164265
H	5.909940	1.195641	3.233324
H	-0.890101	3.577240	3.142013
H	1.233011	4.838141	3.050498
H	2.568716	-2.223807	3.237583
H	-2.057927	-1.052975	3.169921
H	0.097200	-2.259608	3.185647
H	-2.104612	1.423053	3.173036
H	4.693256	-0.966774	3.270727
H	5.866692	3.667321	3.126333
H	3.712271	4.882384	3.058790

Cluster 7 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	0.190021	-3.517042	-0.009004
C	1.356471	-2.768307	-0.017546
C	1.306816	-1.352983	0.021067
C	0.038370	-0.708958	0.043184
C	-1.153354	-1.485913	0.024619
C	-1.050333	-2.898354	-0.014059
C	2.474863	-0.554846	0.014279
C	-0.038249	0.709002	0.042573
C	1.153417	1.485937	0.019847
C	2.400663	0.818299	0.013689
C	1.050286	2.898339	-0.019962
C	-0.190053	3.517032	-0.012003
C	-1.356521	2.768289	-0.016501
C	-1.306751	1.353005	0.023387
C	-2.474812	0.554862	0.020742
C	-2.400616	-0.818281	0.021330
H	1.960592	3.489909	-0.027794
H	-3.309387	-1.412752	0.008736
H	-3.442348	1.047938	0.007683
H	3.442362	-1.047931	-0.000988
H	0.248539	-4.600756	-0.035906
H	2.325221	-3.258351	-0.025008
H	-1.960659	-3.489929	-0.018790
H	3.309394	1.412755	-0.002085
H	-0.248649	4.600718	-0.039796
H	-2.325289	3.258326	-0.021697
C	0.185398	-3.518691	-3.276611
C	1.351867	-2.769949	-3.272126
C	1.302101	-1.354666	-3.312029
C	0.033597	-0.710661	-3.331206
C	-1.158069	-1.487595	-3.308485
C	-1.054938	-2.899996	-3.268673
C	2.470162	-0.556524	-3.309353
C	-0.043021	0.707299	-3.331812
C	1.148703	1.484255	-3.313241
C	2.395963	0.816620	-3.309939
C	1.045684	2.896696	-3.274568
C	-0.194674	3.515382	-3.279641
C	-1.361123	2.766647	-3.271088
C	-1.311465	1.351324	-3.309688
C	-2.479513	0.553185	-3.302936
C	-2.405318	-0.819957	-3.302346
H	1.956008	3.488272	-3.269905
H	-3.314049	-1.414413	-3.286586
H	-3.447009	1.046276	-3.287639
H	3.437701	-1.049595	-3.296328
H	0.243993	-4.602377	-3.248783
H	2.320634	-3.259988	-3.266910
H	-1.965246	-3.491563	-3.260771
H	3.304734	1.411090	-3.297337
H	-0.253191	4.599097	-3.252780
H	-2.329873	3.256691	-3.263647

Cluster 8 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	-0.006351	-3.521915	0.006667
C	1.205618	-2.833231	0.000841
C	1.233525	-1.430277	-0.002842
C	-0.001498	-0.714988	-0.008653
C	-1.230983	-1.425046	-0.001406
C	-1.208496	-2.837930	0.007806
C	2.449298	-0.690000	0.011610
C	-0.001250	0.707796	-0.017728
C	1.239294	1.420653	-0.019713
C	2.443863	0.693890	-0.031005
C	1.209174	2.839490	0.032329
C	-0.005162	3.524042	0.009846
C	-1.203582	2.838194	-0.010950
C	-1.225969	1.417539	-0.012909
C	-2.443281	0.681783	-0.006825
C	-2.447187	-0.684512	-0.000805
H	2.147222	3.383683	0.039363
H	-3.386427	-1.229754	0.005089
H	-3.380447	1.230900	-0.005431
H	3.390044	-1.228737	0.002109
H	-0.004475	-4.607562	0.010748
H	2.144932	-3.378380	0.003012
H	-2.150187	-3.378510	0.013620
H	3.383041	1.237238	-0.033599
H	-0.003832	4.609697	0.026857
H	-2.146892	3.375945	-0.018035
C	3.897894	-1.362564	2.926281
C	5.093124	-0.671348	2.946733
C	5.109156	0.749522	2.950736
C	3.881184	1.453732	2.957414
C	2.643937	0.735241	2.959055
C	2.680327	-0.683521	2.905442
C	6.323018	1.490680	2.945135
C	3.875018	2.876492	2.950819
C	5.101333	3.592123	2.944239
C	6.320764	2.857112	2.941560
C	5.072426	5.004958	2.937674
C	3.867165	5.683466	2.940753
C	2.658325	4.989348	2.945813
C	2.636787	3.586205	2.946746
C	1.424500	2.840413	2.931056
C	1.436100	1.456555	2.971561
H	6.011655	5.549806	2.932397
H	0.499382	0.908970	2.973540
H	0.481292	3.374886	2.940366
H	7.262669	0.945833	2.942229
H	3.901507	-2.448203	2.908240
H	6.038870	-1.204821	2.952384
H	1.744759	-1.231943	2.899357
H	7.257571	3.406531	2.936079
H	3.860406	6.769103	2.938765
H	1.716542	5.530218	2.945060

Cluster 9 – Representative Geometry (TD-CAM-B3LYP+D3BJ/6-31G*/C-PCM(cyclohexane))

C	-0.000316	-3.536465	0.001310
C	1.207091	-2.852339	-0.000734
C	1.236133	-1.421440	-0.000273
C	-0.000224	-0.706268	0.000158
C	-1.236696	-1.422028	0.000272
C	-1.206738	-2.852332	0.001583
C	2.436857	-0.697064	-0.000252
C	-0.000095	0.706444	0.000070
C	1.236395	1.422017	0.000436
C	2.437481	0.696763	0.000336
C	1.207008	2.851642	0.000799
C	0.000050	3.535632	0.000385
C	-1.206657	2.852105	-0.000365
C	-1.236650	1.422166	-0.000506
C	-2.437515	0.697140	-0.001141
C	-2.437272	-0.696870	-0.000603
H	2.148428	3.392522	0.001371
H	-3.379256	-1.236792	-0.000811
H	-3.379574	1.236902	-0.001904
H	3.378632	-1.237417	-0.000224
H	-0.001844	-4.622046	0.002529
H	2.150671	-3.389244	-0.005940
H	-2.147694	-3.393883	0.002769
H	3.379581	1.236410	0.000709
H	0.000192	4.621285	0.000669
H	-2.147995	3.393170	-0.000646
C	4.887238	-12.252095	-1.080594
C	4.796651	-12.022393	0.286803
C	4.290610	-10.814568	0.774595
C	3.868319	-9.820499	-0.146448
C	3.963779	-10.061549	-1.542005
C	4.475553	-11.283597	-1.987428
C	4.181489	-10.541262	2.183218
C	3.348451	-8.580649	0.329802
C	3.251827	-8.339448	1.725607
C	3.688323	-9.365655	2.634948
C	2.737447	-7.118839	2.170917
C	2.324545	-6.150278	1.264232
C	2.418698	-6.379526	-0.103169
C	2.926581	-7.586962	-0.591263
C	3.036173	-7.858913	-1.999652
C	3.528499	-9.035077	-2.451341
H	2.662148	-6.933870	3.238429
H	3.605547	-9.228105	-3.517361
H	2.711208	-7.092016	-2.696674
H	4.507020	-11.307575	2.880634
H	5.282784	-13.195616	-1.443004
H	5.120046	-12.783394	0.991002
H	4.548706	-11.468629	-3.055145
H	3.611135	-9.172488	3.700921
H	1.925971	-5.207935	1.626477
H	2.097599	-5.620037	-0.810292

Optimized Transition State for the Rearrangement between Clusters 1 and 3.1

C	-0.000396	-3.509517	0.024851
C	1.206706	-2.820569	0.011829
C	1.228918	-1.423524	-0.019071
C	-0.000300	-0.712991	-0.036806
C	-1.228672	-1.422562	-0.029113
C	-1.206658	-2.819737	0.002884
C	2.457891	-0.675595	-0.013559
C	0.000403	0.712883	-0.036006
C	1.227574	1.423172	-0.025755
C	2.457222	0.677599	-0.018554
C	1.205971	2.819837	-0.001959
C	0.000151	3.508485	0.018069
C	-1.205848	2.819641	0.008114
C	-1.228726	1.422334	-0.020763
C	-2.456538	0.676840	-0.019644
C	-2.457703	-0.676873	-0.024052
H	2.145835	3.363004	0.016423
H	-3.392839	-1.227972	-0.011968
H	-3.391385	1.228594	0.004364
H	3.393423	-1.227680	-0.002731
H	-0.000873	-4.594748	0.051234
H	2.146584	-3.364826	0.029316
H	-2.147324	-3.362845	0.014421
H	3.391794	1.231044	-0.010415
H	0.000413	4.593241	0.050884
H	-2.145630	3.362771	0.038007
C	-3.871252	-0.566508	3.334924
C	-2.629352	-1.180509	3.245437
C	-1.429545	-0.406697	3.292476
C	-1.527201	1.013169	3.409712
C	-2.810196	1.633973	3.491121
C	-3.978205	0.809367	3.456415
C	-0.158943	-0.992804	3.210363
C	-0.355896	1.803504	3.430883
C	0.926400	1.182557	3.335946
C	0.996893	-0.213071	3.237198
C	2.095291	2.006678	3.330626
C	1.988176	3.385921	3.438067
C	0.749172	3.998257	3.540426
C	-0.453561	3.223446	3.534570
C	-1.725547	3.810086	3.619919
C	-2.879640	3.032056	3.597940
H	3.066942	1.530364	3.243894
H	-3.853832	3.507635	3.662397
H	-1.803044	4.890312	3.700076
H	-0.079683	-2.069830	3.101438
H	-4.771376	-1.173188	3.304244
H	-2.549569	-2.258137	3.140921
H	-4.952560	1.283898	3.525306
H	1.968771	-0.688200	3.154161
H	2.887756	3.994178	3.436966
H	0.671923	5.078268	3.623159

Optimized Transition State for the Rearrangement between Clusters 2 and 3.1

C	0.009758	-3.523263	0.039260
C	1.203401	-2.841189	0.044746
C	1.231276	-1.415288	0.002789
C	-0.002327	-0.707248	-0.025450
C	-1.234451	-1.416935	-0.031331
C	-1.213171	-2.836076	0.031878
C	2.440847	-0.685888	-0.010707
C	-0.000196	0.712387	-0.026307
C	1.233086	1.424632	-0.034273
C	2.445663	0.688336	-0.037852
C	1.207164	2.836028	-0.025718
C	0.003090	3.519898	0.029087
C	-1.204487	2.831971	0.051730
C	-1.232699	1.423157	0.003119
C	-2.448172	0.686705	-0.020652
C	-2.445708	-0.685354	-0.058040
H	2.147551	3.379112	-0.041223
H	-3.382718	-1.232529	-0.071330
H	-3.387050	1.231403	-0.001925
H	3.378647	-1.233944	0.000759
H	0.007648	-4.608957	0.057172
H	2.146144	-3.379813	0.062217
H	-2.146977	-3.379203	-0.046815
H	3.385643	1.232206	-0.050102
H	0.001617	4.605163	0.057294
H	-2.143585	3.374694	0.101673
C	-3.038351	-3.291395	2.631503
C	-1.664435	-3.026974	2.732635
C	-1.210854	-1.721454	3.061730
C	-2.165135	-0.680219	3.226050
C	-3.554982	-0.956893	3.100745
C	-3.964513	-2.287752	2.789599
C	0.165013	-1.415595	3.190467
C	-1.731793	0.644649	3.495018
C	-0.340405	0.935111	3.564258
C	0.589302	-0.129355	3.412818
C	0.066319	2.267165	3.783576
C	-0.872179	3.275134	3.971272
C	-2.229051	2.996282	3.931127
C	-2.686831	1.686002	3.673530
C	-4.066302	1.370517	3.573374
C	-4.482358	0.092181	3.287033
H	1.127679	2.494737	3.809588
H	-5.542235	-0.129174	3.199683
H	-4.794091	2.163991	3.715613
H	0.888190	-2.216068	3.072825
H	-3.368797	-4.301522	2.409000
H	-0.945081	-3.835027	2.680073
H	-5.026013	-2.497658	2.698288
H	1.650097	0.094243	3.469937
H	-0.537062	4.292400	4.148674
H	-2.957570	3.788507	4.076561

Optimized Transition State for the Rearrangement between Clusters 3.2 and 3.1

C	0.183105	-3.518725	-0.050912
C	1.357130	-2.766503	-0.053529
C	1.310289	-1.353078	0.018334
C	0.038076	-0.707903	0.049711
C	-1.159091	-1.487498	0.051084
C	-1.053348	-2.908930	-0.005517
C	2.474992	-0.554751	0.030858
C	-0.037594	0.708141	0.046600
C	1.159503	1.487706	0.032175
C	2.399282	0.825699	0.053477
C	1.053171	2.908839	-0.030399
H	1.964045	3.499903	-0.040478
C	-0.183690	3.518437	-0.066428
C	-1.357665	2.766244	-0.053555
C	-1.310075	1.353188	0.024760
C	-2.474578	0.554958	0.052832
C	-2.398608	-0.825369	0.081489
H	-3.307869	-1.418766	0.092197
H	-3.443414	1.046187	0.057037
H	3.443834	-1.045976	0.027812
H	0.246210	-4.602571	-0.095184
H	2.324602	-3.259199	-0.081432
H	-1.964261	-3.500016	-0.003543
H	3.308588	1.419121	0.052237
H	-0.247258	4.602052	-0.115419
H	-2.325381	3.258819	-0.074208
C	-3.307124	-1.236376	-3.178527
C	-2.247601	-2.121510	-3.224211
C	-0.918581	-1.656467	-3.265033
C	-0.679462	-0.254892	-3.271202
C	-1.772766	0.650747	-3.239158
C	-3.074612	0.140532	-3.180064
C	0.191985	-2.542479	-3.277572
C	0.646636	0.238436	-3.279108
C	1.740233	-0.667058	-3.253436
C	1.471365	-2.070596	-3.256468
C	3.042591	-0.156580	-3.210038
H	3.878843	-0.848414	-3.179145
C	3.275071	1.220312	-3.217852
C	2.215117	2.105227	-3.257360
C	0.885767	1.640016	-3.282459
C	-0.224898	2.525980	-3.288356
C	-1.503989	2.054244	-3.252048
H	-2.342073	2.743368	-3.235093
H	-0.036290	3.594410	-3.284886
H	0.003448	-3.610871	-3.266745
H	-4.324718	-1.609723	-3.136474
H	-2.426508	-3.192331	-3.216791
H	-3.910528	0.832535	-3.144279
H	2.309579	-2.759663	-3.244404
H	4.293028	1.593841	-3.187946
H	2.394064	3.176067	-3.257191

Optimized Transition State for the Rearrangement between Clusters 4 and 3.1

C	0.007159	-3.525285	-0.047800
C	1.210444	-2.843202	-0.050480
C	1.229907	-1.427099	-0.009362
C	-0.000711	-0.713963	-0.002707
C	-1.233387	-1.428951	0.013973
C	-1.204016	-2.837727	-0.009333
C	2.437437	-0.689522	0.034457
C	-0.002581	0.705770	-0.000535
C	1.225838	1.417077	0.015145
C	2.434242	0.686725	0.052039
C	1.203662	2.842856	-0.004192
C	0.005292	3.529006	-0.057235
C	-1.206051	2.847432	-0.033364
C	-1.237703	1.421209	-0.006265
C	-2.441064	0.692752	0.033332
C	-2.441531	-0.689652	0.068936
H	2.146556	3.380056	0.018542
H	-3.382225	-1.231569	0.099627
H	-3.380964	1.236385	0.047598
H	3.378926	-1.230799	0.051406
H	0.003878	-4.610857	-0.073921
H	2.152772	-3.382240	-0.070113
H	-2.142782	-3.383717	0.001793
H	3.371967	1.232711	0.091280
H	0.009450	4.613763	-0.076552
H	-2.144524	3.388852	-0.086274
C	-0.595764	-1.484450	3.338376
C	0.748255	-1.174205	3.467507
C	1.179223	0.171817	3.493357
C	0.224388	1.203003	3.344395
C	-1.159006	0.878587	3.188663
C	-1.546559	-0.480051	3.204036
C	2.553221	0.524284	3.661362
C	0.643760	2.564539	3.335755
C	2.012732	2.888916	3.517630
C	2.952017	1.824619	3.684914
C	2.406869	4.240577	3.514907
C	1.474414	5.243240	3.303744
C	0.132627	4.933221	3.101999
C	-0.309954	3.601233	3.126225
C	-1.669786	3.243156	2.912618
C	-2.082527	1.926806	2.986159
H	3.454161	4.485112	3.665509
H	-3.130421	1.677808	2.852541
H	-2.396347	4.033987	2.754246
H	3.279734	-0.275518	3.772387
H	-0.907231	-2.523704	3.319032
H	1.487408	-1.964398	3.556890
H	-2.598378	-0.728026	3.110761
H	3.999872	2.076569	3.820425
H	1.792044	6.281362	3.292695
H	-0.590800	5.725077	2.930477

Optimized Transition State for the Rearrangement between Clusters 5 and 3.1

C	0.004087	-3.524819	0.038369
C	1.208242	-2.837965	-0.016151
C	1.230276	-1.421704	-0.046524
C	0.000404	-0.711443	-0.040642
C	-1.236793	-1.423171	-0.004715
C	-1.203448	-2.838272	0.047158
C	2.442473	-0.688530	-0.051874
C	-0.000037	0.703193	-0.039736
C	1.225808	1.411342	-0.006761
C	2.437851	0.685933	-0.019597
C	1.200857	2.838385	0.043500
C	0.002382	3.527471	0.023583
C	-1.205315	2.844229	-0.004445
C	-1.238147	1.418423	-0.043718
C	-2.439236	0.700112	-0.062248
C	-2.440720	-0.693658	-0.006691
H	2.143792	3.372761	0.097097
H	-3.382594	-1.232692	0.009172
H	-3.378520	1.241540	-0.072649
H	3.382506	-1.231739	-0.056372
H	0.004235	-4.609544	0.073844
H	2.150102	-3.378013	-0.022617
H	-2.142286	-3.382605	0.088785
H	3.374347	1.234114	0.009106
H	0.004992	4.610857	0.067166
H	-2.145266	3.385802	-0.003042
C	-3.329190	0.668500	3.022751
C	-2.356695	-0.326084	3.115881
C	-1.000633	0.020203	3.229522
C	-0.630437	1.392967	3.236840
C	-1.632367	2.402822	3.114452
C	-2.979689	2.009047	3.010722
C	0.028817	-0.966683	3.331331
C	0.738916	1.761506	3.362602
C	1.739605	0.755951	3.472291
C	1.336880	-0.615135	3.445608
C	3.085823	1.139047	3.601830
C	3.433543	2.481409	3.627235
C	2.464053	3.475043	3.525238
C	1.110762	3.140012	3.381666
C	0.080214	4.127660	3.267265
C	-1.227690	3.773992	3.132575
H	3.848494	0.370358	3.682741
H	-1.997322	4.536242	3.047599
H	0.368001	5.174917	3.287533
H	-0.258726	-2.013876	3.303368
H	-4.375579	0.387149	2.946767
H	-2.638619	-1.374087	3.123729
H	-3.746410	2.774315	2.929681
H	2.106686	-1.378495	3.513464
H	4.477328	2.763126	3.732777
H	2.749068	4.522795	3.548608

Optimized Transition State for the Rearrangement between Clusters 6 and 3.1

C	-0.001791	-3.514829	0.020795
C	1.203234	-2.828677	0.054043
C	1.234963	-1.420683	-0.000059
C	0.001215	-0.710290	-0.023326
C	-1.229629	-1.424826	-0.036916
C	-1.208725	-2.827237	-0.037653
C	2.453129	-0.684652	-0.015449
C	0.002355	0.710543	-0.013146
C	1.235976	1.423304	-0.023403
C	2.453072	0.683322	-0.034974
C	1.210048	2.829582	-0.006884
C	-0.006625	3.515727	0.008540
C	-1.207556	2.832074	0.039093
C	-1.229486	1.419724	0.024607
C	-2.449427	0.677554	0.015162
C	-2.451675	-0.682677	-0.031962
H	2.147619	3.375527	-0.026084
H	-3.389062	-1.231236	-0.048066
H	-3.386006	1.227809	0.032319
H	3.389718	-1.232286	-0.008694
H	-0.002112	-4.600428	0.042563
H	2.142521	-3.372426	0.095742
H	-2.149074	-3.370062	-0.059758
H	3.390684	1.230767	-0.039233
H	-0.004410	4.601552	0.012992
H	-2.148965	3.372830	0.059747
C	-0.793758	-0.840057	3.258987
C	0.447722	-1.463709	3.232945
C	1.645247	-0.698852	3.202592
C	1.558113	0.716714	3.191039
C	0.276973	1.351949	3.219944
C	-0.893979	0.540575	3.255765
C	2.923872	-1.303585	3.155029
C	2.738542	1.499185	3.118500
C	4.013721	0.868287	3.091573
C	4.071514	-0.546972	3.118001
C	5.177531	1.672227	3.013356
C	5.078065	3.054044	2.947188
C	3.837865	3.680200	2.959134
C	2.647795	2.920740	3.045528
C	1.367562	3.516316	3.051525
C	0.213579	2.752192	3.174462
H	6.149472	1.188590	2.996935
H	-0.757018	3.236199	3.183913
H	1.294749	4.598137	2.994650
H	2.984850	-2.387937	3.151119
H	-1.694549	-1.444666	3.268140
H	0.518362	-2.546474	3.227573
H	-1.864430	1.025060	3.270369
H	5.043448	-1.030566	3.088846
H	5.980287	3.654604	2.883376
H	3.767918	4.762475	2.903592

Optimized Transition State for the Rearrangement between Clusters 7 and 3.1

C	0.189396	-3.511489	-0.025339
C	1.356718	-2.759173	-0.026678
C	1.310240	-1.353229	0.012015
C	0.037701	-0.704228	0.035623
C	-1.157143	-1.488409	0.033427
C	-1.055821	-2.889500	0.010416
C	2.482727	-0.550698	0.014582
C	-0.037573	0.704311	0.034191
C	1.157251	1.488477	0.025733
C	2.409383	0.815116	0.024604
C	1.055844	2.889510	-0.000006
C	-0.189502	3.511426	-0.032454
C	-1.356822	2.759115	-0.027717
C	-1.310195	1.353262	0.013946
C	-2.482661	0.550739	0.022741
C	-2.409272	-0.815052	0.035542
H	1.964258	3.483294	-0.004258
H	-3.316722	-1.411644	0.033105
H	-3.448920	1.046213	0.010862
H	3.448936	-1.046203	0.000148
H	0.247843	-4.594875	-0.051547
H	2.324392	-3.251285	-0.053946
H	-1.964242	-3.483290	0.010896
H	3.316816	1.411695	0.017390
H	-0.248049	4.594752	-0.060851
H	-2.324592	3.251174	-0.052429
C	-1.330812	-3.261208	-3.259660
C	0.049194	-3.079723	-3.296599
C	0.602174	-1.788466	-3.323508
C	-0.271360	-0.657313	-3.328465
C	-1.686014	-0.855450	-3.303620
C	-2.188730	-2.169145	-3.260976
C	2.005493	-1.560583	-3.326928
C	0.259439	0.649552	-3.330971
C	1.674172	0.847741	-3.311965
C	2.520565	-0.293479	-3.317948
C	2.177036	2.161530	-3.274259
C	1.319121	3.253595	-3.272189
C	-0.061014	3.072027	-3.303455
C	-0.614077	1.780717	-3.325275
C	-2.017398	1.552831	-3.322830
C	-2.532426	0.285754	-3.308986
H	3.252411	2.310909	-3.250493
H	-3.607431	0.132721	-3.293604
H	-2.680469	2.412892	-3.317723
H	2.668585	-2.420630	-3.322378
H	-1.739586	-4.266135	-3.230420
H	0.714113	-3.937447	-3.294991
H	-3.264006	-2.318460	-3.232762
H	3.595621	-0.140415	-3.307011
H	1.727996	4.258587	-3.246832
H	-0.725928	3.929754	-3.301302

Optimized Transition State for the Rearrangement between Clusters 8 and 3.1

C	-0.001812	-3.525943	-0.006187
C	1.208626	-2.839316	-0.023779
C	1.232290	-1.428556	-0.013444
C	-0.001864	-0.713285	-0.011800
C	-1.234676	-1.424923	0.002338
C	-1.206410	-2.843602	0.011468
C	2.440127	-0.690940	0.009363
C	-0.000784	0.706446	-0.014400
C	1.235689	1.419255	-0.012116
C	2.439788	0.692105	-0.008347
C	1.211070	2.844457	0.028502
C	-0.005038	3.529261	-0.004883
C	-1.202369	2.845455	-0.014905
C	-1.231088	1.418003	-0.009727
C	-2.440140	0.688304	0.001940
C	-2.443890	-0.689050	0.010692
H	2.150513	3.385646	0.017868
H	-3.384629	-1.231450	0.022634
H	-3.378876	1.234595	0.006076
H	3.381127	-1.230624	0.042012
H	-0.000735	-4.611737	-0.006505
H	2.149316	-3.381386	-0.033326
H	-2.146846	-3.386189	0.025375
H	3.379795	1.234014	0.009073
H	-0.004183	4.615066	-0.003321
H	-2.145006	3.384402	-0.024603
C	2.798441	-1.782448	3.291781
C	4.140530	-1.437392	3.296070
C	4.535715	-0.087572	3.175350
C	3.543484	0.916874	3.076953
C	2.159349	0.559421	3.098575
C	1.815197	-0.806276	3.182226
C	5.911361	0.300342	3.137867
C	3.921186	2.283808	2.938570
C	5.294322	2.639999	2.902186
C	6.275219	1.604249	3.005366
C	5.647419	3.996493	2.764819
C	4.669450	4.971954	2.670284
C	3.319011	4.630919	2.704768
C	2.921011	3.294478	2.834807
C	1.546531	2.903298	2.856687
C	1.186302	1.581206	3.010310
H	6.698615	4.267106	2.735932
H	0.137167	1.304755	3.032062
H	0.785365	3.673791	2.815655
H	6.667815	-0.475404	3.215037
H	2.509329	-2.826493	3.359896
H	4.905415	-2.204010	3.378101
H	0.766284	-1.084763	3.167842
H	7.324537	1.882785	2.976024
H	4.955991	6.014008	2.567808
H	2.558504	5.402506	2.627601

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