Electronic Supporting Information for

FB-REDA: Fragment-Based Decomposition Analysis of the Reorganization Energy for Organic Semiconductors

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Fragment-based Decomposition Analysis of the Reorganization Energy

Within the context of the normal mode analysis, the reorganization energy is expressed in terms of internal coordinate (*S*), as proposed by Shuai, Coropceanu *et al.* Equation S1 shows an expansion of ΔQ in terms of the internal coordinate change ΔS during the nuclei reorganization. The following expression is for λ_N but is equivalent for λ_C:

$$\lambda_N = \sum_i \frac{1}{2} k_i^N (\Delta Q_i^N)^2 \tag{S1}$$

$$= \sum_j \sum_i \frac{1}{2\omega_i} \left(\alpha_{ij}^2 \Delta S_j^2 + \sum_{m(\neq j)} \alpha_{ij} \alpha_{im} \Delta S_j \Delta S_m \right)$$

$$\Delta Q_i^N = \sum_j \alpha_{ij} \, \Delta S_j$$

where k_i^N is the eigenvalue of the mass-weighted Hessian matrix, ΔQ_i^N is projection of the eigenvector of the normal mode onto the Cartesian coordinate difference (see **Scheme 1**) and α_{ij} is the coefficient of the expansion of the normal mode *i* and internal coordinate *j*. As shown in **Equation (S1)**, the squared terms (*i.e.*, diagonal terms) can be easily assigned to the corresponding internal coordinate. However, the partitioning of the cross terms ($\alpha_{ij}\alpha_{im}\Delta S_j \Delta S_m$) into individual internal coordinate is not trivial.

Alternatively, the reorganization energy can be represented in terms of vibronic coupling constants:

$$\lambda_N = \sum_i \frac{V_i^2}{2\omega_i^2} \tag{S2}$$

where ω_i and V_i are the frequency and the vibronic coupling constant of the normal mode *i*. The concept of atomic vibronic coupling constants (AVCC) proposed by Sato *et. al.*, defined the total vibronic coupling constant as a sum of AVCC for each atom:

$$V_i = \sum_j V_{i,j} \tag{S3}$$

where $V_{i,j}$ is the AVCC of atom *j* and normal mode *i*. Inserting **Equation (S3)** into **Equation (S2)** gives an equation similar to **Equation (S1)**.

$$\lambda_N = \sum_i \frac{1}{2\omega_i^2}\left(\sum_j V_{i,j}\right)^2 \tag{S4}$$

$$= \sum_j \sum_i \frac{1}{2\omega_i^2}\left(\Delta V_{i,j}^2 + \sum_{m(\neq j)} V_{ij}V_{im}\right)$$

This expression contains both squared (diagonal) terms and cross terms ($V_{ij}V_{im}$). While the diagonal terms can be easily assigned to the corresponding atomic contribution, the cross terms ($V_{ij}V_{im}$) are not decomposable into individual atomic contribution.

As mentioned in the main text, λ_N can be expressed in terms of inter fragment modes by inserting **Equation (2)** and **(3)** into **Equation (4)**:

$$\lambda_N = \sum_i \frac{1}{2} k_i^N (\Delta Q_i^N)^2 \tag{S5}$$

$$= \sum_N \frac{1}{2} k_i^N \left[(C_i^N)^T m^{1/2}(R_C - R_N)\right]^2$$

$$= \sum_N \frac{1}{2} k_i^N \left[\left(\sum_j \sum_k d_{jk}^i C_{frag,jk}\right)^T m^{1/2}(R_C - R_N)\right]^2$$

We define the projection of the eigenvector of a fragment mode ($\Delta q_{f,jk}^N$) and a fragment ($\Delta q_{f,k}^N$) onto the Cartesian coordinate difference between the cationic and neutral ground states as:

$$\Delta q_{f,jk}^N = \left(C_{frag,jk}^N\right)^T m^{1/2}(R_C - R_N) \tag{S6}$$

$$\Delta q_{f,k}^N = \sum_j \Delta q_{f,jk}^N$$

The **Equation (S1)** then becomes:

$$\lambda_N = \sum_N \frac{1}{2} k_i^N \left(\Delta q_{f,k}^N \sum_j d_{jk}^i\right)^2$$

$$= \sum_N \frac{1}{2} k_i^N \left(\Delta q_{f,k}^N d_k^i\right)^2$$

$$= \sum_N \frac{1}{2} k_i^N \left\{ \left[\left(d_1^i \Delta q_{f,1}^N \right)^2 + \left(d_2^i \Delta q_{f,2}^N \right)^2 + \cdots \right] \right.$$

$$\left. + \left[\left(d_1^i d_2^i \Delta q_{f,1}^N \Delta q_{f,2}^N \right) + \left(d_1^i d_3^i \Delta q_{f,1}^N \Delta q_{f,3}^N \right) + \cdots \right] \right\}$$

$$= \sum_N \frac{1}{2} k_i^N [(square\ terms) + (cross\ terms)]$$

$$d_k^i = \sum_j d_{jk}^i$$

where d_k^i the sum of the coefficients of all fragment modes belonging to fragment *k*. The cross terms make the decomposition of λ_N into fragment contributions non-trivial.

Validity of Harmonic Approximation

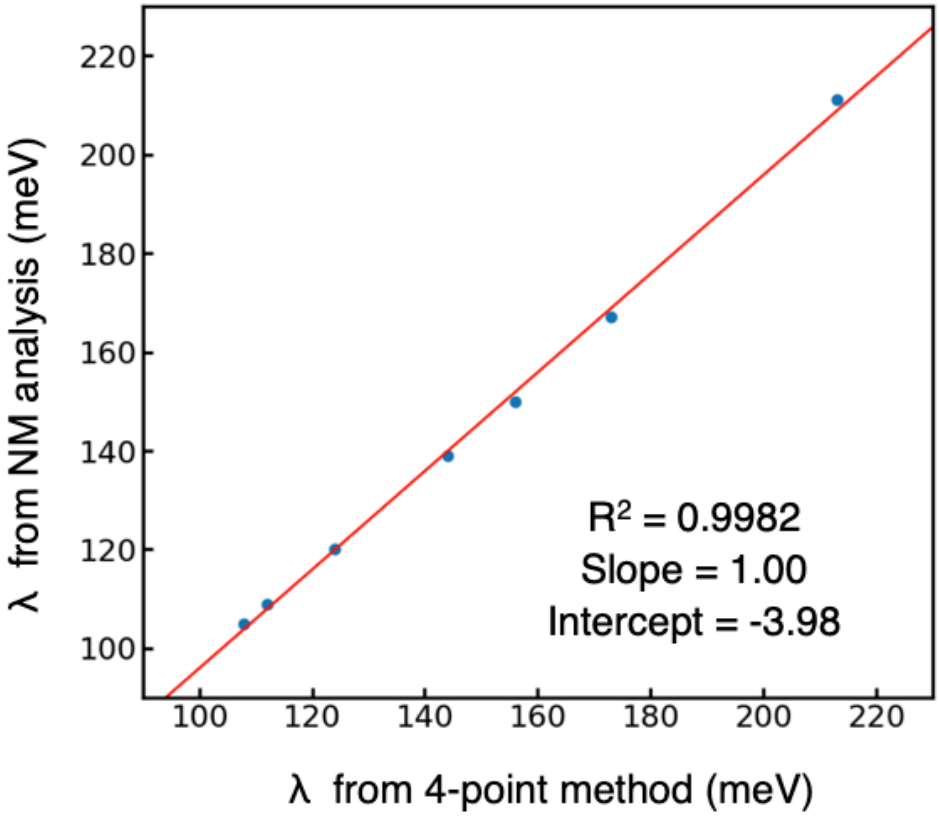
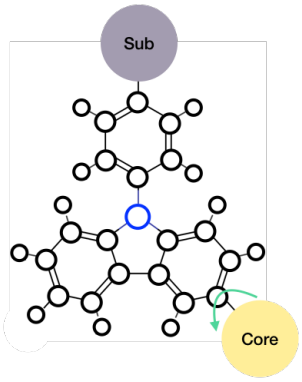
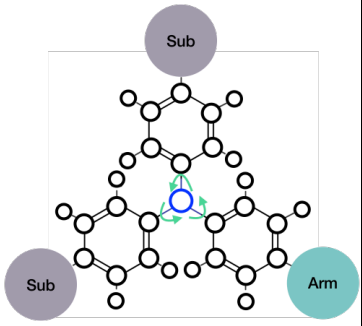
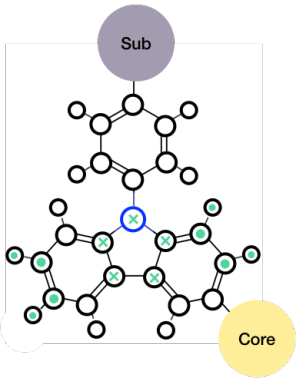
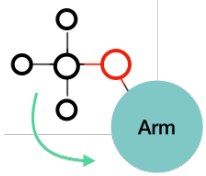
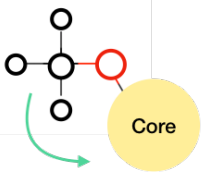
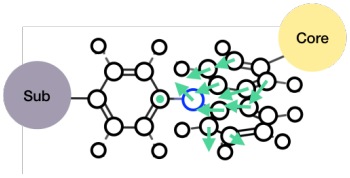
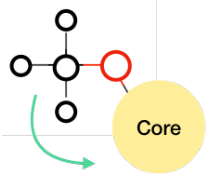


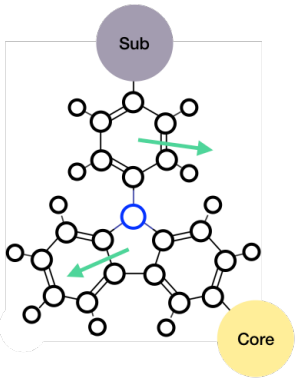
Figure S1. The reorganization energies obtained from the 4-point method and the NM analysis for all compounds considered in this work.

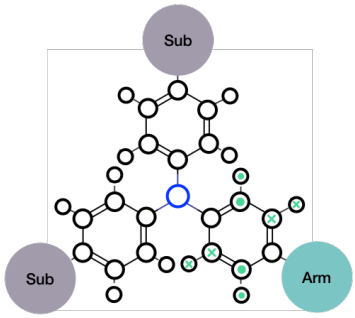
Composition Analysis of Normal Modes in Terms of Fragment Modes

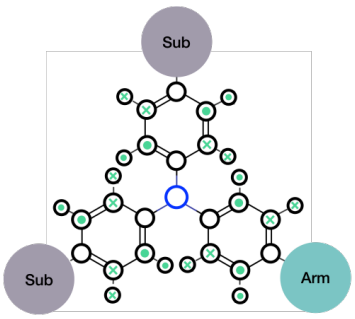
The decomposition analysis of the normal modes delivers useful insights as it identifies the fragments that contribute the most to the total reorganization energy. **Table S1** and **S3** regroup the composition of the 10 most contributing peaks in $\lambda_{tot}(\omega)$ (in terms of total normal and fragment modes) for TPA1PM and TPA3PM. The contribution of each normal mode (λ_i^N, in meV), the weight and the illustration of each fragment mode are present in the tables. Due to symmetry, the contribution of degenerated Arm and Sub fragment modes are summed up. **Table S2** and **S4** give the most relevant fragment modes (with $\lambda_{jk} > 1.2$ meV (10 cm^{-1})) of TPA1PM and TPA3PM.

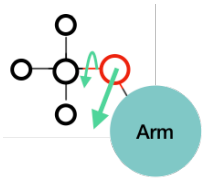
Table S1. The composition of 10 most important peaks in $\lambda_N(\omega)$ of TPA1PM in terms of fragment modes. Only the fragment modes with a weight larger than 0.10 are listed.

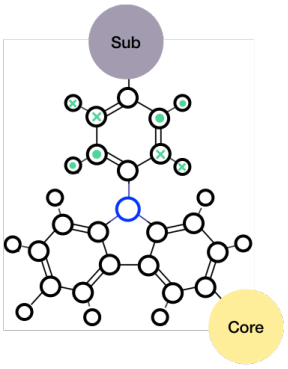
Peak #	1	2	3
Mode Frequency (cm^{-1})	8.29	49.81	140.10
λ_i^N (meV)	8.06	4.49	8.49
Fragment mode and weight	 weight = 0.19	 weight = 0.19	 weight = 0.19
	 weight = 0.12	 weight = 0.10	 weight = 0.10
	 weight = 0.11		

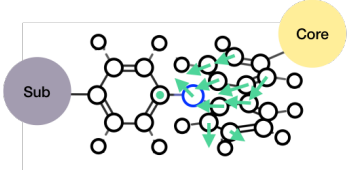
<table>
<tr><th>Peak #</th><th>4</th><th colspan="2">5</th></tr>
<tr><td>Mode Frequency (cm^{-1})</td><td>179.27</td><td>423.51</td><td>432.89</td></tr>
<tr><td>λ_i^N(meV)</td><td>2.34</td><td>1.35</td><td>2.42</td></tr>
<tr><td rowspan="3">Fragment mode and weight</td><td> 

weight = 0.31</td><td rowspan="3"> 

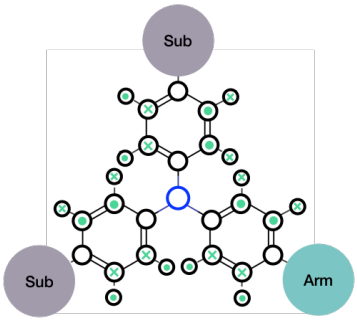
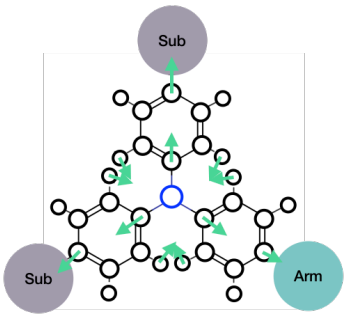
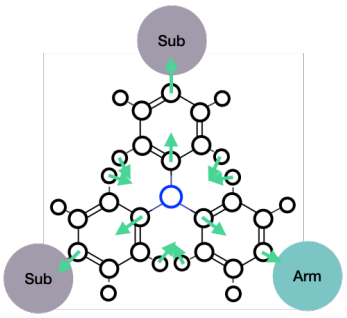
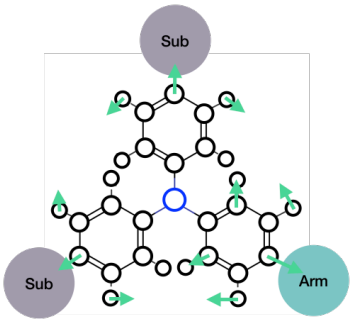
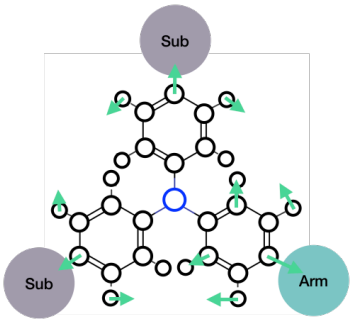
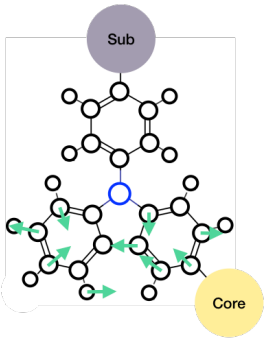
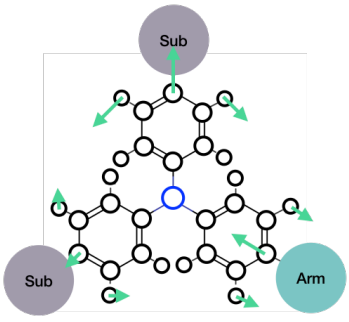
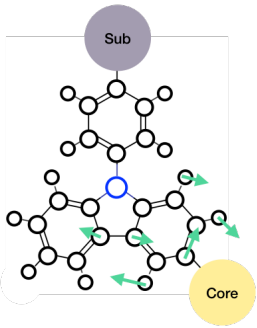
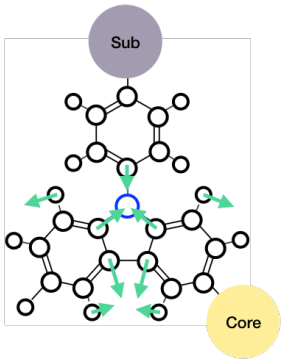
weight = 0.95</td><td> 

weight = 0.83</td></tr>
<tr><td> 

weight = 0.29</td><td rowspan="2"> 

weight = 0.11</td></tr>
<tr><td> 

weight = 0.11</td></tr>
</table>

Peak #	6	7	8
Mode Frequency (cm^{-1})	839.77	1197.51	1293.67
λ_i^N (meV)	1.92	4.41	9.30
Fragment mode and weight	 weight = 0.60	 weight = 0.53	 weight = 0.17
		 weight = 0.21	 weight = 0.15
	 weight = 0.18	 weight = 0.16	 weight = 0.13
			 weight = 0.10

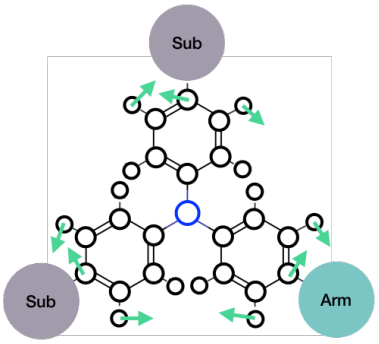
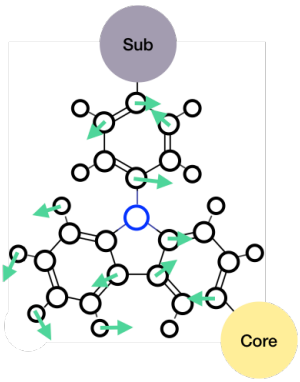
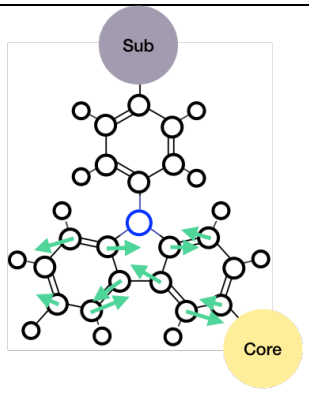
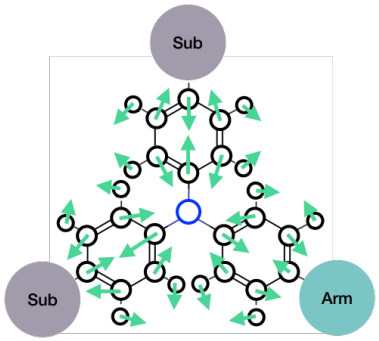
Peak #	9	
Mode Frequency (cm^{-1})	1345.34	1358.82
λ_i^N (meV)	1.23	1.56
Fragment mode and weight	 weight = 0.65	 weight = 0.80
Peak #	10	
Mode Frequency (cm^{-1})	1657.53	1676.93
λ_i^N (meV)	3.72	6.60
Fragment mode and weight	 weight = 0.93	 weight = 0.91

Table S2. Important Core modes with λ_{jk} > 1.2 meV (10 cm^{-1}) of TPA1PM.

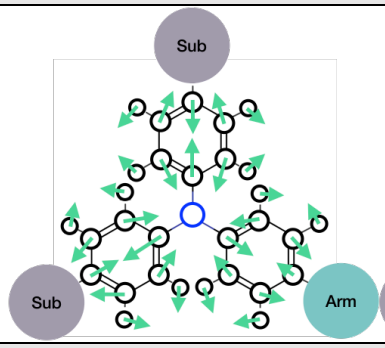
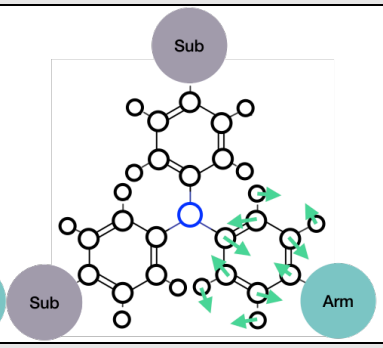
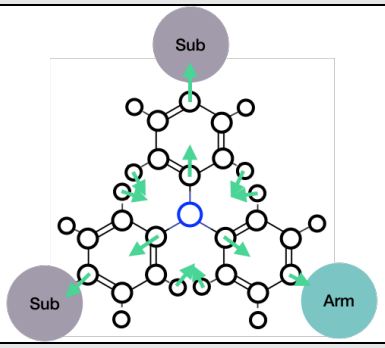
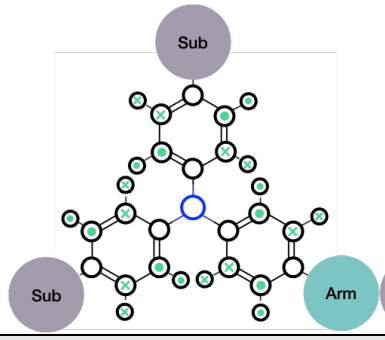
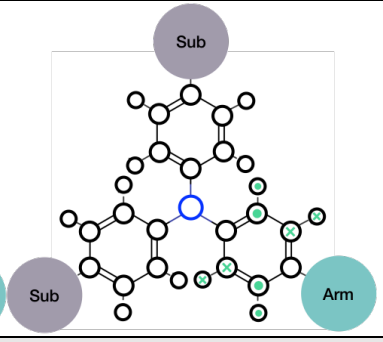
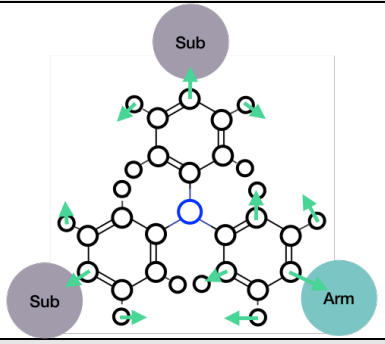
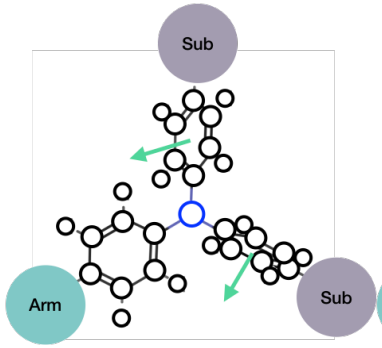
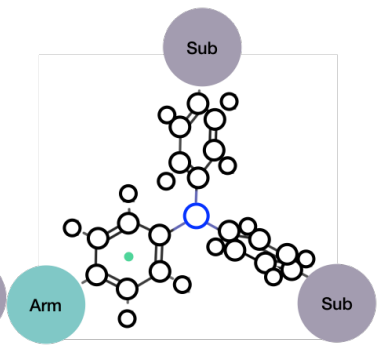
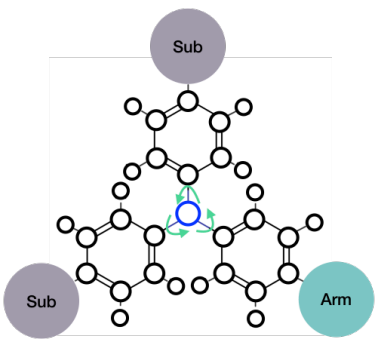
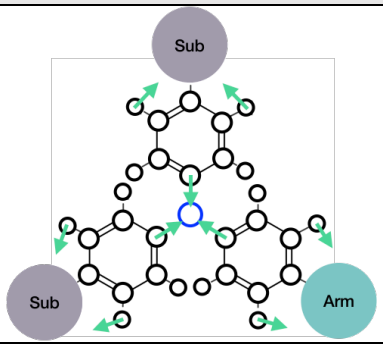
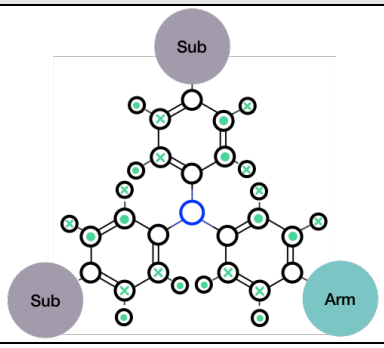
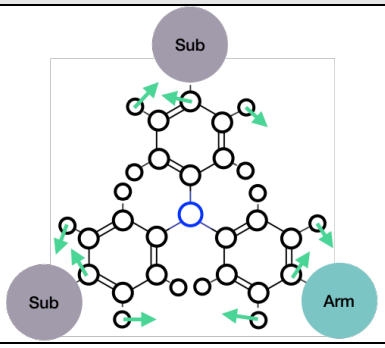
$\lambda_{N,i}$	7.85		4.10
X_f			
$\lambda_{N,i}$	3.38		2.47
X_f			
$\lambda_{N,i}$	2.47		2.03
X_f			
$\lambda_{N,i}$	1.80	1.30	1.25
X_f			

Table S2. (continue) Important Arm modes with λ_{jk} > 1.2 meV (10 cm^{-1}) of TPA1PM.

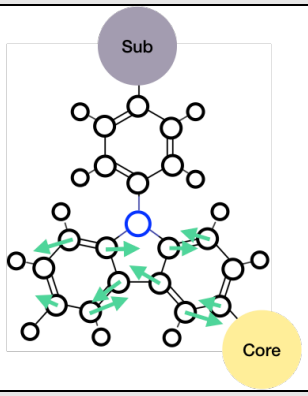
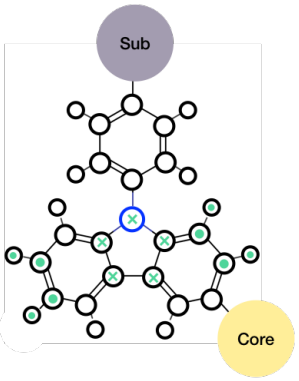
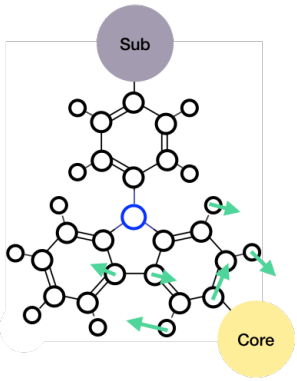
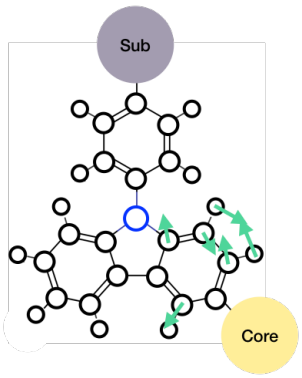
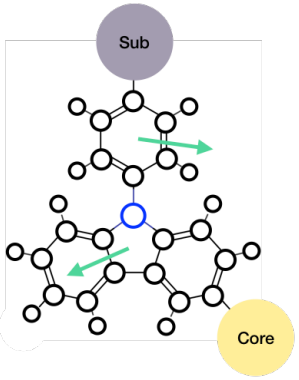
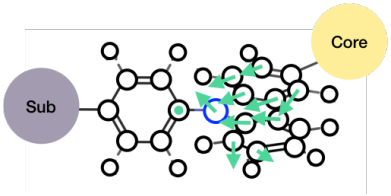
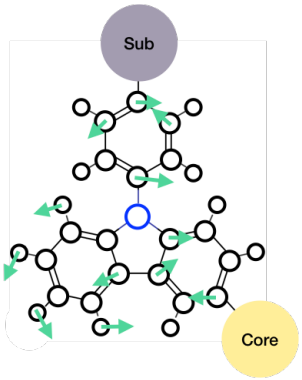
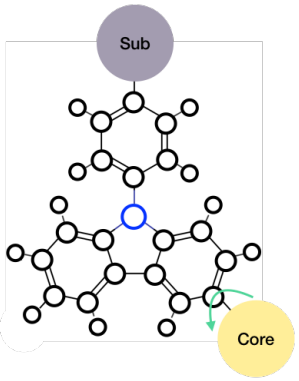
$\lambda_{N,i}$	3.58	2.24	1.50
X_f			
$\lambda_{N,i}$	1.49	1.39	1.38
X_f			
$\lambda_{N,i}$	1.37	1.86	
X_f			

Table S2. (continue) Important Sub modes with λ_{jk} > 1.2 meV (10 cm^{-1}) of TPA1PM.

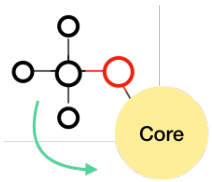
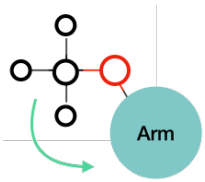
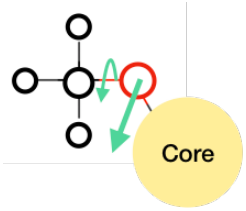
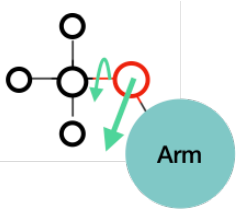
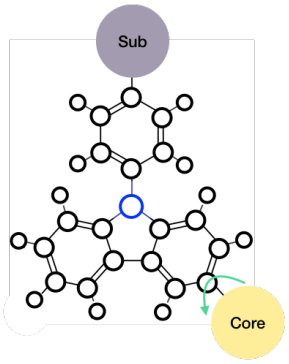
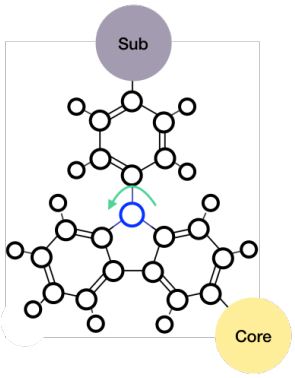
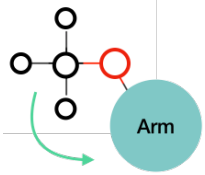
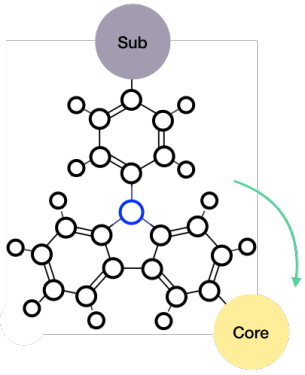
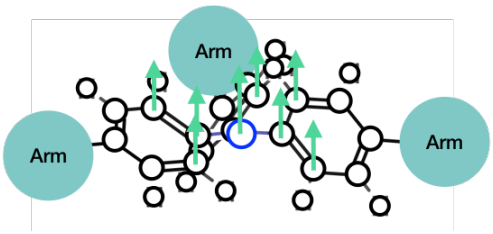
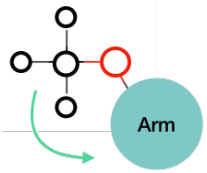
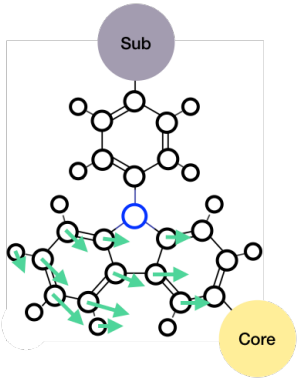
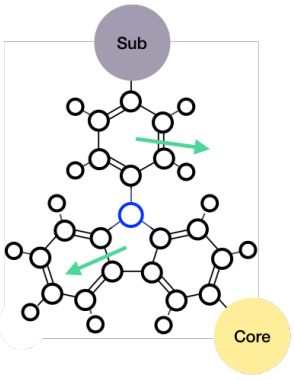
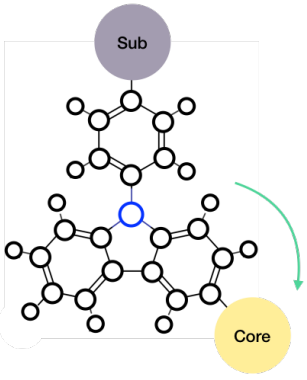
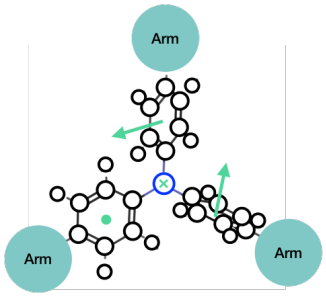
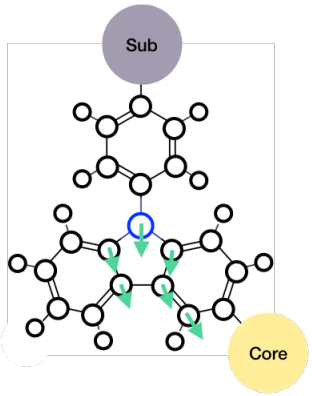
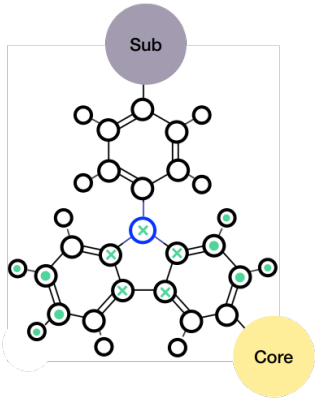
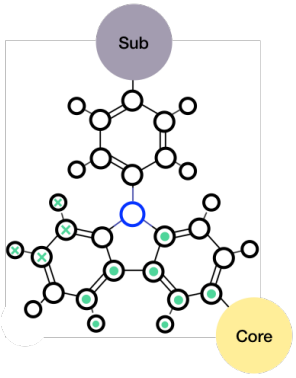
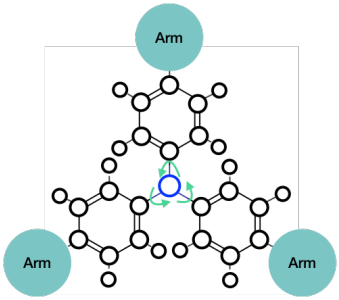
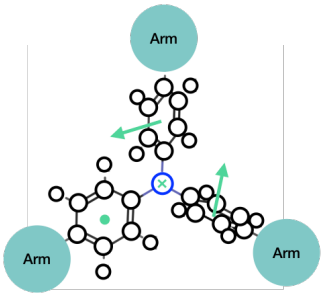
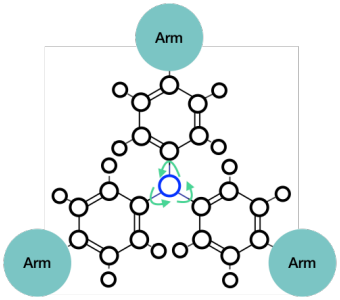
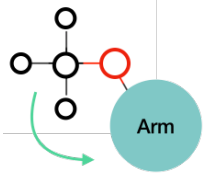
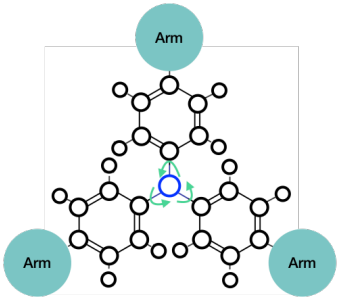
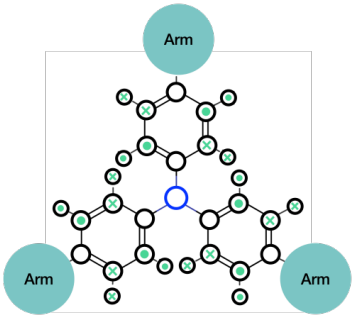
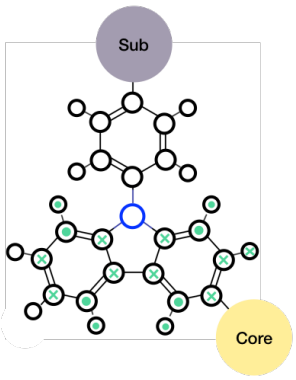
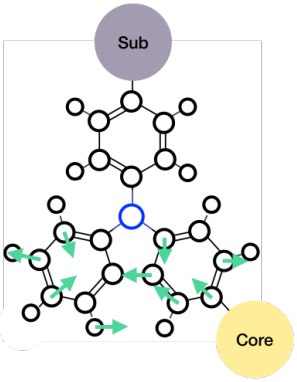
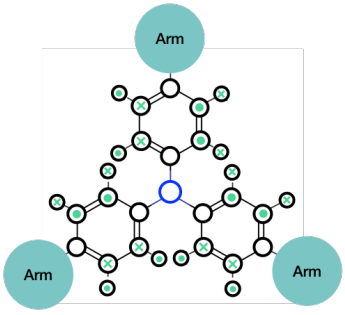
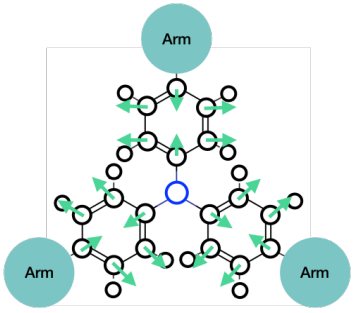
$\lambda_{N,i}$	3.93		2.02
X_f			
$\lambda_{N,i}$	1.74	1.71	
X_f			

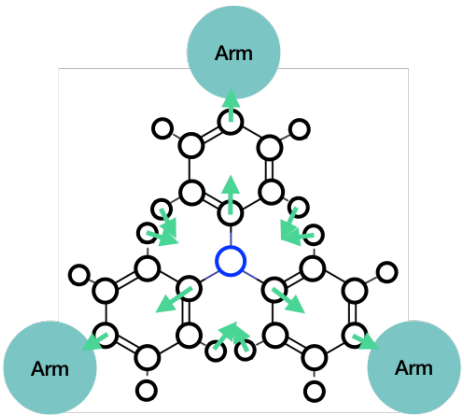
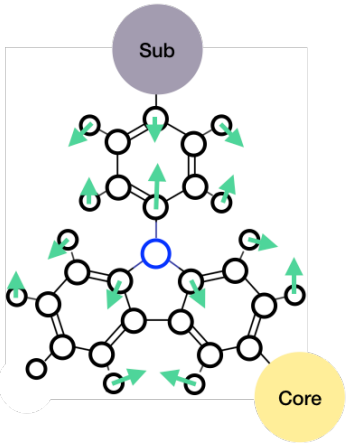
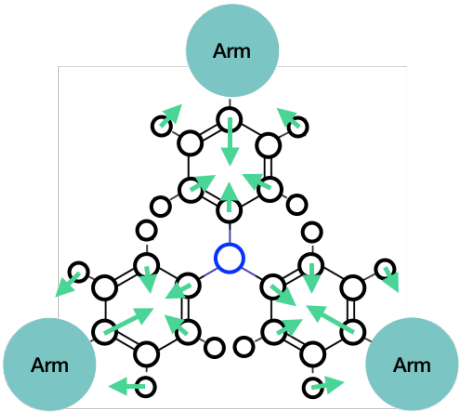
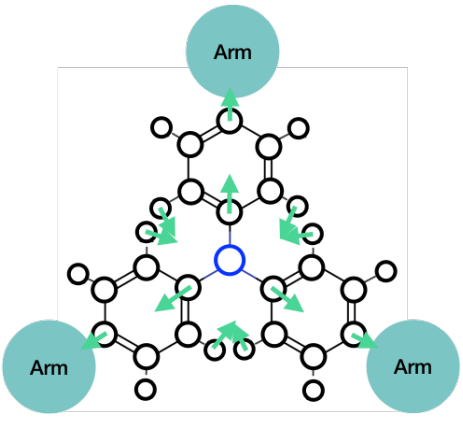
Table S3. The composition of 11 most important peaks in $\lambda_N(\omega)$ of TPA3PM in terms of fragment modes. Only fragment modes with weight more than 0.04 are listed.

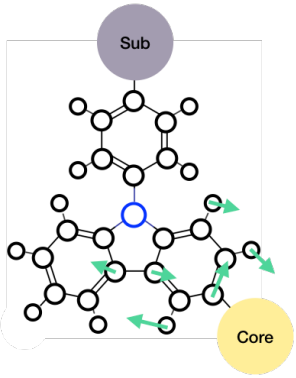
Peak #	1	2
Mode Frequency (cm^{-1})	8.27	46.27
λ_i^N (meV)	10.71	4.18
Fragment mode and weight	 weight = 0.50	 weight = 0.33
	 weight = 0.25	 weight = 0.18

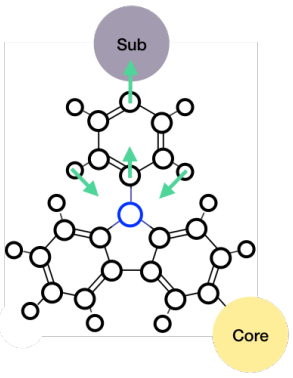
Peak #	*	
Mode Frequency (cm^{-1})	75.16	85.52
λ_i^N(meV)	3.07	1.92
Fragment mode and weight	 weight = 0.29	 weight = 0.25
	 weight = 0.48	 weight = 0.24
		 weight = 0.21

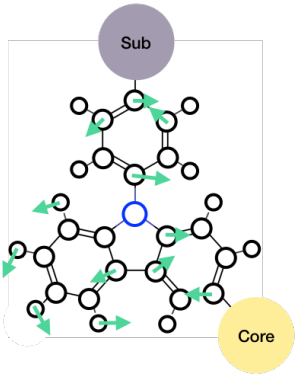
Peak #	3		
Mode Frequency (cm^{-1})	110.35	112.27	135.99
λ_i^N(meV)	2.77	3.11	3.77
Fragment mode and weight	 weight = 0.25	 weight = 0.27	 weight = 0.62
	 weight = 0.40	 weight = 0.09	 weight = 0.19
	 weight = 0.12	 weight = 0.15	 weight = 0.05

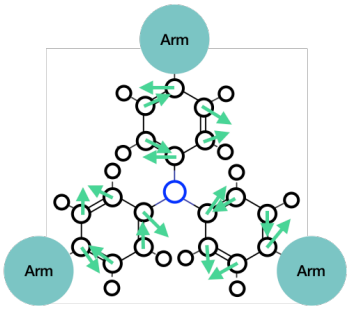
Peak #	5		6
Mode Frequency (cm^{-1})	428.79	437.14	844.93
λ_i^N(meV)	3.57	1.56	2.59
Fragment mode and weight	 weight = 0.92	 weight = 0.92	 weight = 0.61  weight = 0.15  weight = 0.10

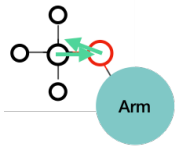
Peak #	7	
Mode Frequency (cm^{-1})	1203.32	1214.65
λ_i^N(meV)	2.00	1.43
Fragment mode and weight	 weight = 0.75	 weight = 0.65
	 weight = 0.75	 weight = 0.04

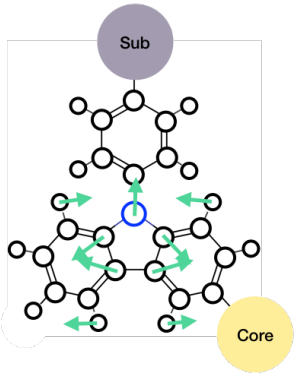
<table>
<tr><th>Peak #</th><th colspan="2">8</th><th>9</th></tr>
<tr><td>Mode Frequency (cm^{-1})</td><td>1290.72</td><td>1299.17</td><td>1359.06</td></tr>
<tr><td>λ_i^N(meV)</td><td>2.36</td><td>1.51</td><td>1.37</td></tr>
<tr><td rowspan="5">Fragment mode and weight</td><td> 

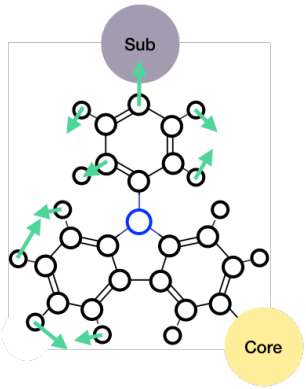
weight = 0.34</td><td> 

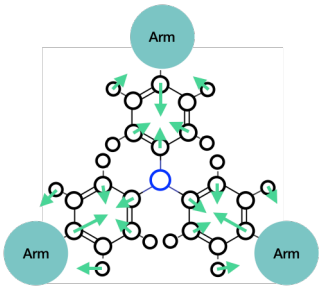
weight = 0.26</td><td rowspan="5"> 

weight = 0.83</td></tr>
<tr><td> 

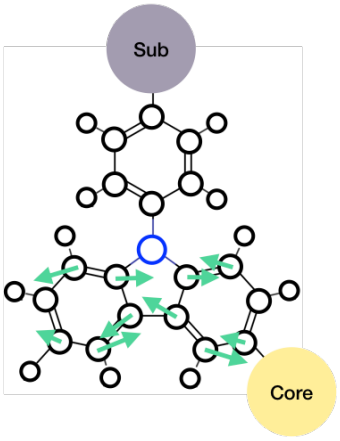
weight = 0.11</td><td> 

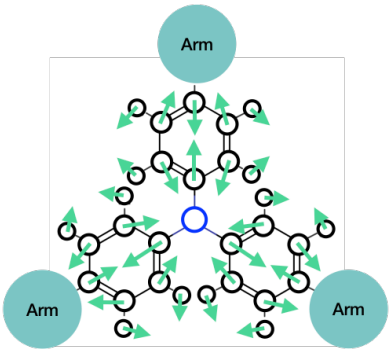
weight = 0.15</td></tr>
<tr><td> 

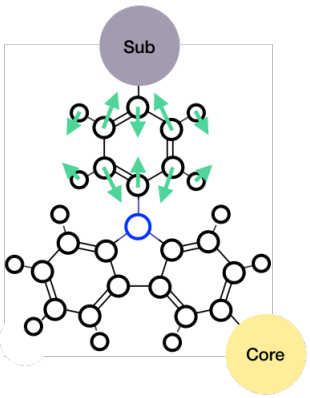
weight = 0.22</td><td rowspan="2"> 

weight = 0.14</td></tr>
<tr><td> 

weight = 0.08</td></tr>
</table>

<table>
<tr><th>Peak #</th><th colspan="2">10</th></tr>
<tr><td>Mode Frequency (cm^{-1})</td><td>1657.57</td><td>1671.64</td></tr>
<tr><td>λ_i^N(meV)</td><td>3.36</td><td>3.96</td></tr>
<tr><td rowspan="2">Fragment mode and weight</td><td rowspan="2"> 

weight = 0.97</td><td> 

weight = 0.48</td></tr>
<tr><td> 

weight = 0.42</td></tr>
</table>

Table S4. Important Core modes with λ_{jk} > 1.2 meV (10 cm^{-1}) of TPA3PM.

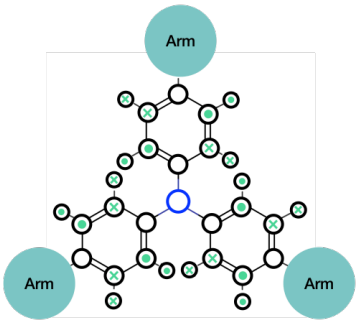
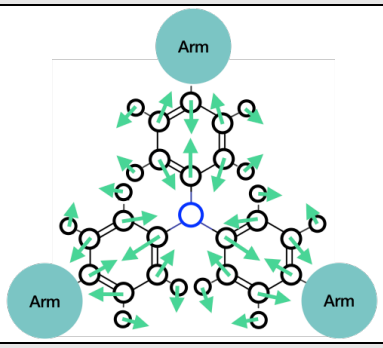
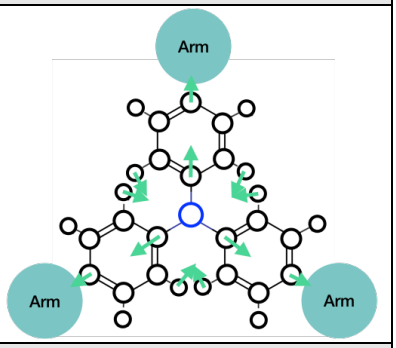
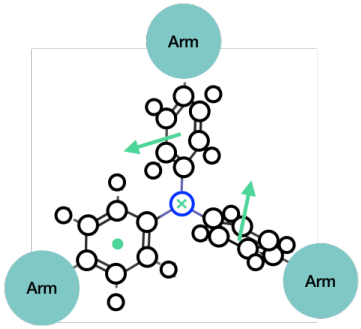
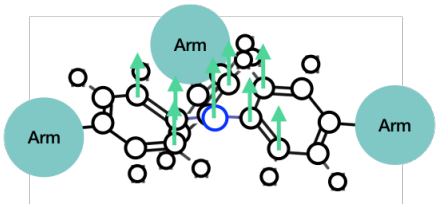
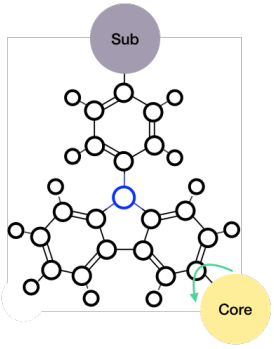
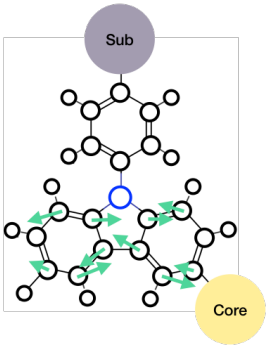
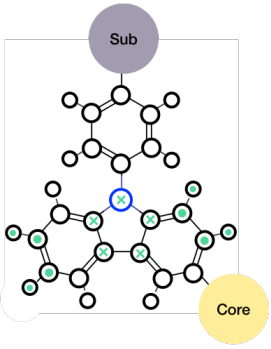
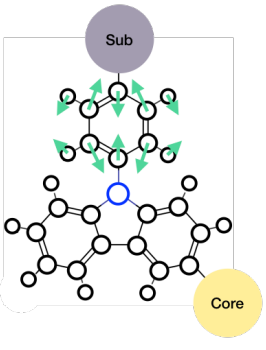
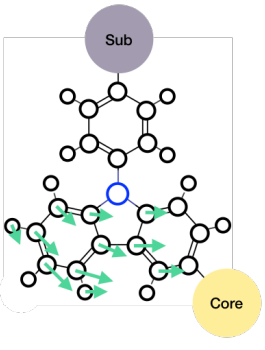
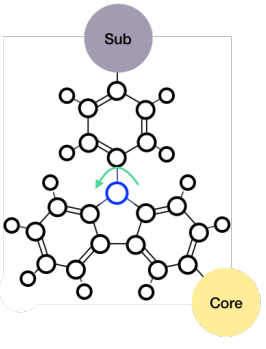
$\lambda_{N,i}$	3.35	2.43	1.69
X_f			
$\lambda_{N,i}$	1.69	1.36	
X_f			

Table S4. (continue) Important Arm modes with λ_{jk} > 1.2 meV (10 cm^{-1}) of TPA3PM.

$\lambda_{N,i}$	5.55	3.33	2.64
X_f			
$\lambda_{N,i}$	2.27	2.06	1.95
X_f			

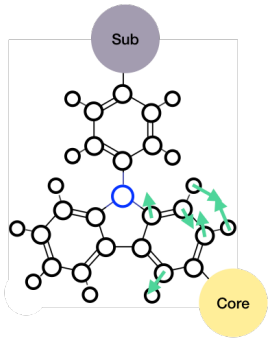
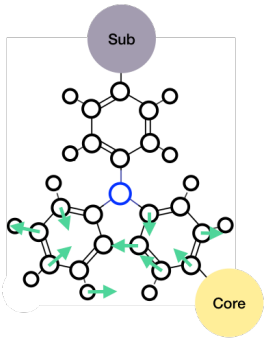
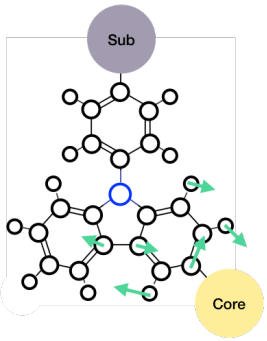
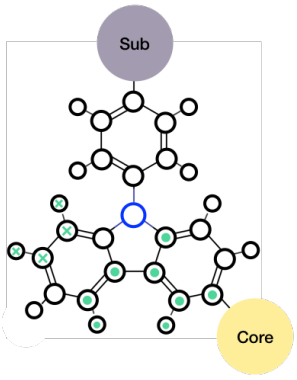
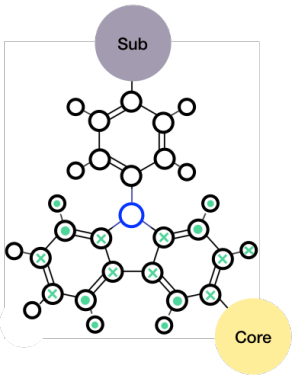
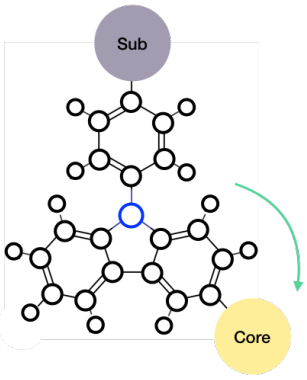
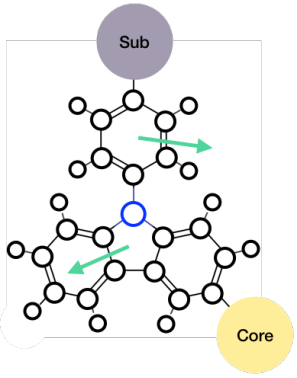
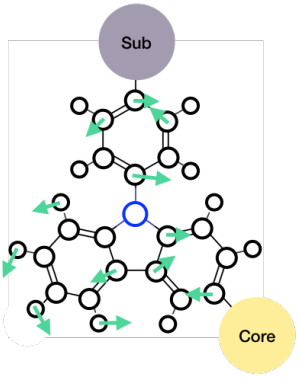
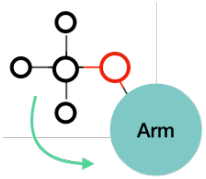
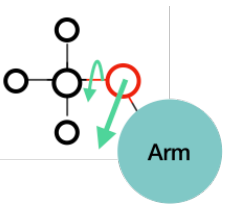
$\lambda_{N,i}$	1.88	1.78	1.72
X_f			
$\lambda_{N,i}$	1.64	1.63	1.52
X_f			
$\lambda_{N,i}$	1.34	1.23	
X_f			

Table S4. (continue) Important Sub modes with λ_{jk} > 1.2 meV (10 cm^{-1}) of TPA3PM.

$\lambda_{N,i}$	2.36 + 1.77 = 4.13	1.43
X_f		

HOMOs and Reorganization in Internal Coordinates

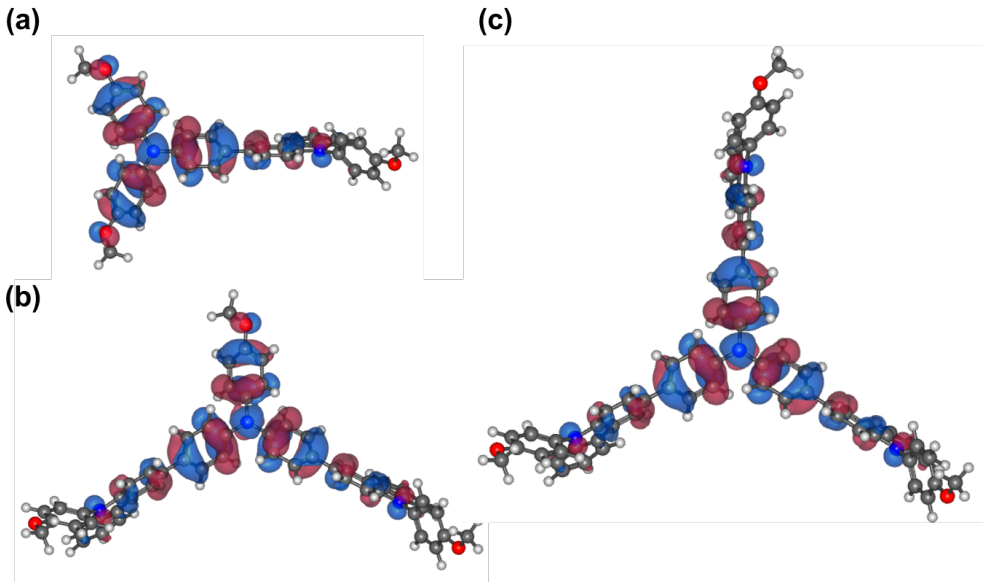


Figure S2. Highest occupied molecular orbital (HOMO) of (a) TPA1PM, (b) TPA2PM and (c) TPA3PM plotted with an isovalue = 0.01 Bohr $^{-3}$.

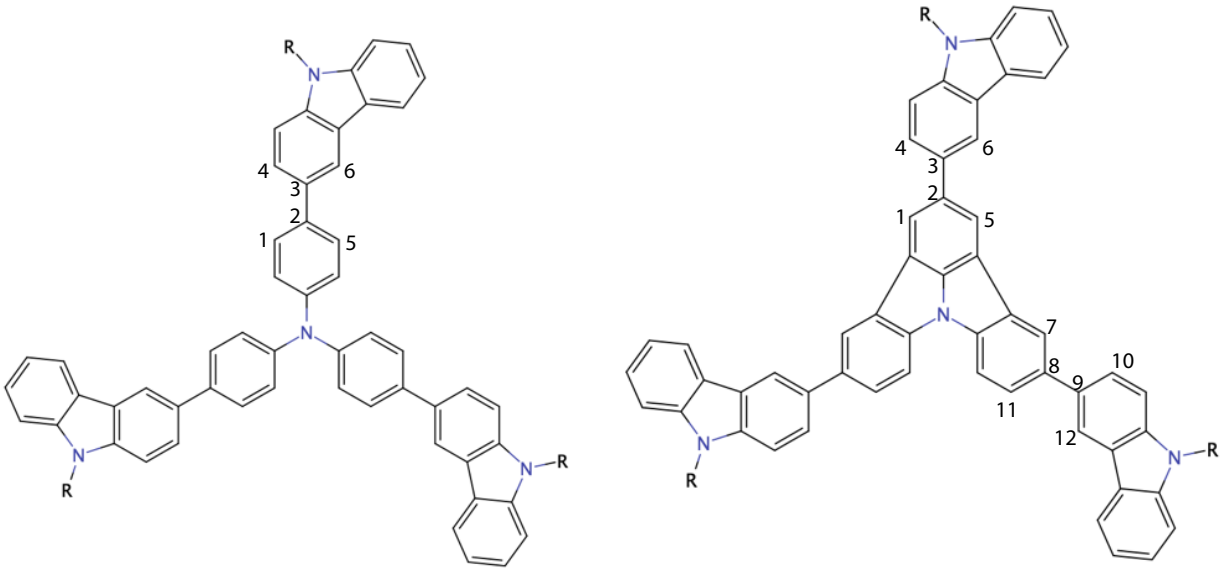


Figure S3. The TPA3PM and ICZ3PM molecules and the indexed atoms used to describe the dihedral and bond angles.

Table S5. Dihedral and bond angles (in °) of neutral and cationic state of TPA3PM and ICZ3PM molecules. The column C – N lists the difference between the internal coordinated of the neutral and cationic states.

Molecule	TPA3PM			ICZ3PM		
Geometry	Neutral (N)	Cation (C)	C – N	Neutral (N)	Cation (C)	C - N
Dihedral 1-2-3-4	-36.688	-29.761	6.927	-41.199	-36.399	4.800
Dihedral 7-8-9-10	-36.688	-29.761	6.927	-38.288	-31.864	6.424
Angle 4-3-2	120.443	120.544	0.101	120.482	120.591	0.109
Angle 6-3-2	120.713	120.547	-0.166	120.621	120.525	-0.096
Angle 10-9-8	120.443	120.544	0.101	120.440	120.526	0.086
Angle 12-9-8	120.713	120.547	-0.166	120.690	120.546	-0.144

Cartesian Coordinates of the Neutral Ground State Geometry

Cartesian coordinates of the neutral ground state geometry of the molecules investigated in this work.

TPA1PM

76

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.399290
C	1.212376	0.000000	2.090508
C	2.424904	0.025173	1.401908
C	2.418691	0.038393	0.000222
C	1.218554	0.013902	-0.694237
N	3.652058	0.039917	2.111312
C	4.023878	0.976293	3.078844
C	5.319870	0.654850	3.557853
C	5.749061	-0.528759	2.840589
C	4.693322	-0.880140	1.958913
C	3.335147	2.095550	3.547972
C	3.953774	2.879066	4.515540
C	5.240086	2.581567	5.022422
C	5.918241	1.461017	4.527029
C	4.768720	-2.002945	1.133359
C	5.932375	-2.766931	1.188489
C	6.992874	-2.427484	2.045628
C	6.905769	-1.313343	2.875401
C	5.855742	3.442671	6.056645
C	6.640521	2.898461	7.086104
C	7.232203	3.701437	8.053452
C	7.040698	5.091895	8.040007
C	6.250260	5.647718	7.021332
C	5.681231	4.836482	6.048018
N	7.625251	5.913847	9.027971
C	7.762530	5.446877	10.360629
C	8.941399	5.666074	11.078196
C	9.072023	5.231905	12.398124
C	8.021390	4.543448	13.012063
C	6.839751	4.310790	12.294495
C	6.707544	4.767080	10.992236

O	8.045896	4.064939	14.292600
C	9.225485	4.271955	15.049164
O	-1.121402	-0.011450	-0.774655
C	-2.380505	-0.028966	-0.121135
C	8.128157	7.196254	8.686363
C	7.892322	8.298781	9.523881
C	8.396959	9.549835	9.204208
C	9.132510	9.738449	8.025796
C	9.362955	8.650009	7.178689
C	8.873295	7.388503	7.519864
O	9.575461	11.011368	7.796943
C	10.327727	11.244331	6.619264
H	7.835567	3.255104	8.835746
H	6.097504	6.720722	6.993259
H	6.780201	1.823073	7.135970
H	5.097205	5.294750	5.255954
H	7.315145	8.160459	10.431500
H	9.064217	6.543604	6.867433
H	8.220863	10.405480	9.847064
H	9.931628	8.764041	6.264085
H	9.762485	6.190387	10.601957
H	5.785813	4.594923	10.447633
H	9.997901	5.424669	12.925761
H	6.030118	3.783048	12.786822
H	3.421313	3.736096	4.914740
H	6.921061	1.238350	4.877571
H	2.347763	2.343601	3.175733
H	7.721710	-1.056678	3.544402
H	3.948880	-2.272124	0.477276
H	7.885962	-3.043889	2.061599
H	6.018065	-3.645173	0.555945
H	1.218187	-0.025136	3.174790
H	3.361080	0.073122	-0.535348
H	-0.926917	-0.015124	1.958483
H	1.196156	0.020610	-1.778319
H	-3.130683	-0.035205	-0.912425
H	-2.500604	-0.926338	0.498744
H	-2.522391	0.860838	0.505088
H	9.043093	3.820799	16.025320

H	10.094430	3.788569	14.584038
H	9.440788	5.340542	15.179368
H	9.747092	11.015897	5.716089
H	10.579922	12.305478	6.625257
H	11.252622	10.653174	6.605995

TPA2PM

106

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.399251
C	1.212353	0.000000	2.090541
C	2.424865	0.025341	1.401952
C	2.418665	0.037833	0.000298
C	1.218598	0.013115	-0.694231
N	3.652095	0.042286	2.111182
C	4.021349	0.978686	3.079380
C	5.319733	0.662709	3.555584
C	5.753177	-0.517864	2.835835
C	4.697456	-0.872802	1.955552
C	3.328419	2.094149	3.551433
C	3.944866	2.878925	4.519303
C	5.233695	2.587192	5.023108
C	5.916037	1.470378	4.524743
C	4.776093	-1.994468	1.128672
C	5.942919	-2.753767	1.180856
C	7.003389	-2.410759	2.036570
C	6.913105	-1.297884	2.867663
C	5.847982	3.450993	6.055838
C	5.655340	4.842253	6.055866
C	6.223890	5.655702	7.028060
C	7.032192	5.105049	8.034164
C	7.243663	3.717750	8.038454
C	6.650955	2.911832	7.074385
N	7.627419	5.933043	9.013229
C	8.104561	7.221331	8.649292
C	8.871891	7.399263	7.495787
C	9.328583	8.664603	7.125045
C	9.039397	9.771529	7.929728

C	8.280354	9.597173	9.095436
C	7.809241	8.340664	9.443679
O	9.443794	11.050288	7.668834
C	10.218180	11.272289	6.503057
O	-1.121438	-0.010472	-0.774558
C	-2.380519	-0.023826	-0.120734
C	7.751895	5.498435	10.353058
C	8.890246	5.824299	11.105507
C	8.999267	5.419721	12.430209
C	7.996159	4.658159	13.051570
C	6.866609	4.330117	12.283729
C	6.735933	4.748789	10.965507
C	8.126914	4.218760	14.458659
C	6.994434	4.176296	15.304577
C	7.072791	3.775292	16.633441
C	8.324719	3.411610	17.131013
C	9.479213	3.432138	16.306893
C	9.370817	3.836393	14.975817
N	8.682694	2.959671	18.403038
C	10.053519	2.685809	18.408712
C	10.582932	2.965714	17.121583
C	10.862904	2.240987	19.455168
C	12.218811	2.061897	19.190306
C	12.758630	2.322227	17.919311
C	11.947650	2.776870	16.883465
C	7.803596	2.804451	19.504278
C	7.038022	3.880554	19.952584
C	6.159689	3.731626	21.026788
C	6.063466	2.496455	21.677249
C	6.841129	1.416251	21.235018
C	7.693700	1.566050	20.151563
O	5.249215	2.242478	22.740375
C	4.441254	3.302320	23.226967
H	9.679818	6.410035	10.648336
H	5.851185	4.486464	10.396380
H	9.876110	5.710573	13.000195
H	6.079961	3.726221	12.724917
H	6.058354	6.726963	7.006500
H	7.862954	3.275886	8.810882

H	5.058720	5.297770	5.271796
H	6.805315	1.838249	7.117493
H	9.104865	6.539718	6.876916
H	7.212528	8.211781	10.339909
H	9.916350	8.768533	6.221553
H	8.059471	10.466985	9.704432
H	6.034695	4.491226	14.908162
H	10.244098	3.827095	14.331282
H	6.190489	3.752024	17.262780
H	12.366919	2.986263	15.903877
H	10.451041	2.046797	20.438940
H	13.819225	2.169687	17.747130
H	12.871119	1.715531	19.986078
H	3.408325	3.732332	4.920637
H	6.920861	1.251633	4.872059
H	2.339150	2.338411	3.181691
H	7.729404	-1.039040	3.535379
H	3.956339	-2.266572	0.473657
H	7.899165	-3.023273	2.050514
H	6.031041	-3.630862	0.547101
H	7.134317	4.842274	19.460488
H	8.277480	0.725382	19.793015
H	5.573374	4.581622	21.351841
H	6.746292	0.465961	21.748559
H	1.217882	-0.025251	3.174797
H	3.361131	0.073368	-0.534984
H	-0.927057	-0.015203	1.958131
H	1.196362	0.020012	-1.778316
H	3.873867	2.889844	24.061754
H	5.049950	4.142917	23.583234
H	3.745223	3.663808	22.459565
H	-2.518472	0.865920	0.506470
H	-3.130892	-0.026322	-0.911855
H	-2.504199	-0.921304	0.498314
H	9.670054	10.993128	5.593895
H	10.431263	12.341693	6.479979
H	11.163897	10.715936	6.533442

TPA3PM

136

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.399306
C	1.212248	0.000000	2.090536
C	2.424665	0.025636	1.401808
C	2.418615	0.038172	0.000231
C	1.218510	0.013621	-0.694349
N	3.651692	0.042167	2.111691
C	4.021410	0.980073	3.077933
C	5.315998	0.658919	3.561213
C	5.746537	-0.526268	2.847583
C	4.693201	-0.878666	1.963527
C	3.332129	2.101281	3.541655
C	3.948962	2.887999	4.507736
C	5.233525	2.590434	5.018581
C	5.911880	1.467049	4.530055
C	4.770706	-2.002634	1.139693
C	5.933853	-2.767015	1.199647
C	6.991844	-2.426798	2.059605
C	6.902898	-1.311210	2.887129
C	5.849547	3.455803	6.049202
C	5.684103	4.850464	6.026764
C	6.256414	5.665219	6.996050
C	7.040029	5.109984	8.017728
C	7.221918	3.719976	8.046895
C	6.626332	2.912503	7.085710
N	7.635948	5.937100	9.001324
C	8.220963	7.170860	8.627151
C	8.955588	7.282133	7.437759
C	9.517873	8.498026	7.069349
C	9.393726	9.640084	7.877585
C	8.664094	9.511414	9.070840
C	8.077144	8.306522	9.437402
C	10.011352	10.926793	7.486199
C	9.351466	12.149020	7.751894
C	9.892838	13.379376	7.397094
C	11.129408	13.384154	6.750347

C	11.823684	12.177189	6.479097
C	11.258050	10.956564	6.849045
N	11.898233	14.460803	6.303264
C	13.081067	13.963223	5.748369
C	13.071844	12.546759	5.842818
C	14.137210	14.652220	5.150261
C	15.202195	13.900214	4.659415
C	15.216754	12.498405	4.756112
C	14.154447	11.816869	5.342928
C	11.532755	15.827884	6.388313
C	10.324577	16.270307	5.832030
C	9.959455	17.604904	5.923701
C	10.807132	18.528039	6.553335
C	12.020161	18.094301	7.099686
C	12.368854	16.744977	7.024651
O	10.362308	19.816115	6.579823
C	11.184096	20.789838	7.203706
O	-1.121671	-0.011237	-0.774233
C	-2.380451	-0.020632	-0.119749
C	7.651258	5.524330	10.355620
C	8.779895	5.741685	11.159118
C	8.782966	5.343135	12.490224
C	7.678391	4.693665	13.065566
C	6.559354	4.472720	12.245960
C	6.536514	4.887736	10.920195
C	7.696408	4.255257	14.478974
C	6.525534	4.333095	15.268166
C	6.497483	3.933398	16.599354
C	7.679993	3.446443	17.157685
C	8.869703	3.345549	16.391410
C	8.868546	3.752109	15.056677
N	7.926920	2.965332	18.445260
C	9.260464	2.552127	18.518001
C	9.878436	2.771619	17.258978
C	9.967045	2.028868	19.601950
C	11.308197	1.708625	19.403379
C	11.933792	1.907808	18.160946
C	11.226169	2.441341	17.087686
C	6.981380	2.899454	19.499443

C	6.302477	4.046113	19.910804
C	5.358603	3.985825	20.936997
C	5.108299	2.767165	21.577538
C	5.798359	1.615195	21.172696
C	6.717162	1.678879	20.135977
O	4.219772	2.596345	22.596901
C	3.504594	3.733935	23.052030
H	9.645934	6.238504	10.736265
H	5.660380	4.708110	10.307209
H	9.656447	5.548415	13.100956
H	5.695914	3.955208	12.651845
H	6.114063	6.739597	6.960090
H	7.819857	3.278871	8.836656
H	5.106414	5.305197	5.228289
H	6.756405	1.836567	7.144572
H	9.068224	6.413088	6.799226
H	7.516091	8.231896	10.362188
H	10.056251	8.567790	6.129454
H	8.564876	10.368499	9.729333
H	8.376496	12.123446	8.227482
H	11.795971	10.030952	6.670136
H	9.366954	14.302987	7.610278
H	14.161801	10.733040	5.409584
H	14.124946	15.732907	5.066585
H	16.063888	11.943919	4.365409
H	16.037296	14.411056	4.189924
H	5.623544	4.741767	14.824526
H	9.766913	3.650428	14.456108
H	5.587681	4.003425	17.184478
H	11.712532	2.602722	16.130301
H	9.489331	1.881721	20.563833
H	12.979890	1.645287	18.040527
H	11.881032	1.298413	20.229394
H	3.416767	3.747424	4.902126
H	6.913317	1.243755	4.884249
H	2.345904	2.348768	3.165990
H	7.717416	-1.053577	3.557513
H	3.953041	-2.272431	0.481112
H	7.884654	-3.043436	2.079233

H	6.021141	-3.646046	0.568458
H	6.518252	4.992900	19.427704
H	7.234212	0.784511	19.806008
H	4.842192	4.889788	21.234157
H	5.584436	0.679737	21.677610
H	9.681631	15.559888	5.323998
H	13.295701	16.398984	7.469094
H	9.027458	17.963109	5.500806
H	12.688937	18.786374	7.595510
H	1.217796	-0.025069	3.174829
H	3.361195	0.073510	-0.534915
H	-0.926935	-0.015205	1.958333
H	1.196179	0.020629	-1.778418
H	2.861889	3.382712	23.859794
H	4.180998	4.507302	23.437142
H	2.883549	4.164990	22.256638
H	12.158843	20.872719	6.706649
H	10.651709	21.737012	7.112324
H	11.341555	20.563846	8.265863
H	-2.516575	0.871287	0.504736
H	-3.131212	-0.024394	-0.910483
H	-2.505200	-0.915956	0.502163

MPD3PM

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N	0.047810	-0.022640	0.123830
C	-1.182500	-0.730740	0.125640
C	-2.252600	-0.293130	0.917600
C	-1.350410	-1.874880	-0.665940
C	-3.459860	-0.980710	0.906700
H	-2.135060	0.596340	1.526520
C	-2.553910	-2.569740	-0.649130
H	-0.529440	-2.223140	-1.283290
C	-3.639060	-2.138470	0.131360
H	-4.285850	-0.607710	1.503650
H	-2.650940	-3.471390	-1.245120
C	1.263780	-0.725700	0.123700
C	2.386000	-0.287650	-0.595500

C	1.443500	-1.917430	0.843220
H	2.338820	0.631520	-1.175130
H	0.623290	-2.334330	1.423320
C	3.611310	-2.083970	0.123400
C	0.047640	1.396860	0.119930
C	0.953540	2.114410	0.912590
C	-0.863010	2.104750	-0.675930
C	0.955340	3.504010	0.893160
H	1.663370	1.577690	1.532630
C	-0.869400	3.494150	-0.667800
H	-1.573530	1.558000	-1.285820
C	0.041640	4.228180	0.109900
H	1.686220	4.039810	1.490150
H	-1.603570	4.022020	-1.267850
C	0.036890	5.708080	0.108910
C	-0.237750	6.422200	-1.080250
C	0.299680	6.424340	1.283200
C	-0.250280	7.811440	-1.126980
H	-0.420450	5.865790	-1.993680
C	0.295440	7.819290	1.264800
H	0.476400	5.893210	2.213150
C	0.026100	8.505010	0.052030
H	-0.461890	8.337270	-2.050910
C	0.498390	8.831530	2.281370
C	0.348970	10.090200	1.642430
C	0.799510	8.784250	3.645940
C	0.511720	11.290260	2.336120
C	0.951220	9.977160	4.346660
H	0.916170	7.828890	4.148760
C	0.811590	11.214000	3.694360
H	0.412850	12.245830	1.833990
H	1.183160	9.954610	5.406550
H	0.942280	12.132230	4.258650
C	-4.922200	-2.875740	0.140170
C	-5.412190	-3.474500	-1.043430
C	-5.669060	-2.995660	1.318680
C	-6.613170	-4.173460	-1.080710
H	-4.842410	-3.363210	-1.960110
C	-6.878950	-3.690140	1.309760

H	-5.290540	-2.574370	2.244620
C	-7.347100	-4.270210	0.102300
H	-6.969400	-4.623010	-2.000460
C	-7.854170	-4.009290	2.332650
C	-8.876880	-4.765500	1.702570
C	-7.955740	-3.716830	3.696140
C	-9.997100	-5.213990	2.403860
C	-9.064230	-4.171360	4.404450
H	-7.180770	-3.140310	4.192320
C	-10.072980	-4.908180	3.760790
H	-10.780790	-5.775590	1.908450
H	-9.154400	-3.953090	5.463650
H	-10.932930	-5.245930	4.330920
C	4.887440	-2.824140	0.124410
C	5.997090	-2.322340	-0.593340
C	5.005700	-4.022500	0.839270
C	7.213080	-2.991050	-0.621160
H	5.876370	-1.388020	-1.127900
C	6.217190	-4.709480	0.826680
H	4.150580	-4.392740	1.392420
C	7.313540	-4.191930	0.086590
H	8.058470	-2.590880	-1.168960
C	6.675380	-5.934890	1.451150
C	8.029040	-6.111370	1.064440
C	6.067280	-6.883740	2.277830
C	8.772180	-7.219480	1.472200
C	6.806080	-7.986270	2.698710
H	5.032270	-6.761070	2.582100
C	8.141680	-8.150500	2.295430
H	9.800240	-7.353060	1.155500
H	6.346400	-8.729630	3.342100
H	8.696640	-9.022040	2.628860
N	8.404610	-5.046340	0.236850
N	-8.558380	-4.918000	0.349700
N	0.062200	9.879800	0.290220
C	-9.333930	-5.617790	-0.609220
C	-9.760160	-4.979000	-1.773260
C	-9.676900	-6.960070	-0.396440
C	-10.510880	-5.665580	-2.728530

H	-9.507090	-3.936020	-1.929830
C	-10.443130	-7.642300	-1.329460
H	-9.332420	-7.460850	0.501700
C	-10.861320	-7.001820	-2.505160
H	-10.825480	-5.147820	-3.625690
H	-10.719450	-8.679990	-1.179250
C	-0.160290	10.893470	-0.676020
C	0.607480	10.939650	-1.839260
C	-1.157310	11.857190	-0.471500
C	0.383620	11.924970	-2.801870
H	1.388940	10.202700	-1.989520
C	-1.369760	12.853950	-1.411910
H	-1.764200	11.812000	0.426140
C	-0.604650	12.892090	-2.586860
H	0.990570	11.935910	-3.698220
H	-2.134970	13.608600	-1.268120
C	9.681290	-4.871330	-0.354690
C	9.804590	-4.726740	-1.736220
C	10.831760	-4.839970	0.445280
C	11.056420	-4.539660	-2.323860
H	8.915170	-4.765250	-2.355610
C	12.081690	-4.678430	-0.133410
H	10.734030	-4.936950	1.520970
C	12.202900	-4.521600	-1.521820
H	11.123970	-4.425030	-3.398230
H	12.981840	-4.654100	0.470640
O	-0.899560	13.903250	-3.451460
O	13.472660	-4.357730	-1.989810
O	-11.599190	-7.762230	-3.362060
C	-12.048180	-7.160850	-4.566200
H	-12.608370	-7.931100	-5.097000
H	-12.706450	-6.305550	-4.368520
H	-11.207740	-6.830000	-5.189260
C	-0.153170	13.987580	-4.655230
H	-0.280240	13.089010	-5.272020
H	-0.545020	14.851490	-5.192780
H	0.915460	14.138340	-4.457220
C	13.649030	-4.193330	-3.387810
H	13.130090	-3.299890	-3.757310

H	14.721810	-4.077160	-3.544710
H	13.294390	-5.069680	-3.944840
N	3.539770	-0.946370	-0.596040
N	2.589050	-2.589020	0.843200

TPD3PM

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N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.327734
C	1.181268	0.000000	2.081590
C	2.370541	-0.007222	1.339354
N	2.383585	-0.018997	0.012377
C	1.194756	-0.011738	-0.626614
N	1.174430	0.007020	3.493119
C	2.100078	-0.783916	4.207335
C	2.741944	-0.322293	5.365032
N	3.609193	-1.062848	6.043733
C	3.877388	-2.300516	5.576927
N	3.314320	-2.829542	4.470885
C	2.439589	-2.083211	3.807021
C	1.203940	-0.016230	-2.099537
C	-0.015419	0.021787	-2.814610
C	-0.048483	0.016207	-4.201629
C	1.171063	-0.031546	-4.883254
C	2.409853	-0.057322	-4.187031
C	2.419648	-0.052201	-2.795083
N	1.422012	-0.033351	-6.252438
C	2.807630	-0.059961	-6.454773
C	3.454181	-0.074979	-5.192299
C	3.525599	-0.097500	-7.650216
C	4.915995	-0.134012	-7.564858
C	5.574355	-0.137681	-6.323816
C	4.850241	-0.111594	-5.135015
C	4.845672	-3.123299	6.321964
C	5.182702	-4.415085	5.855822
C	6.087966	-5.221276	6.530736
C	6.663900	-4.718001	7.700862
C	6.350921	-3.417915	8.182334

C	5.438974	-2.626369	7.489903
N	7.597985	-5.302285	8.551585
C	7.895903	-4.398773	9.579450
C	7.139049	-3.215423	9.382090
C	8.751180	-4.552369	10.670733
C	8.852833	-3.487231	11.563468
C	8.120059	-2.303012	11.378183
C	7.259874	-2.161930	10.292628
C	0.439046	-0.011973	-7.275219
C	-0.550392	-0.993271	-7.322633
C	-1.528987	-0.969739	-8.317206
C	-1.502944	0.034566	-9.291407
C	-0.501105	1.015495	-9.251477
C	0.453824	0.998613	-8.246104
C	8.156866	-6.597918	8.404176
C	7.329871	-7.718040	8.329421
C	7.872347	-8.993794	8.169569
C	9.261267	-9.153576	8.108287
C	10.094569	-8.028604	8.195150
C	9.546758	-6.761890	8.330285
O	-2.399216	0.146811	-10.311392
C	-3.434244	-0.820175	-10.396661
O	9.897098	-10.350044	7.965355
C	9.099574	-11.519982	7.871450
C	0.241388	0.804330	4.190433
C	-0.411774	0.354154	5.345603
N	-1.285366	1.101794	6.009476
C	-1.547419	2.334994	5.529041
N	-0.974190	2.852762	4.422246
C	-0.094087	2.100213	3.773975
C	-2.518669	3.169541	6.256923
C	-3.123219	2.683299	7.439157
C	-4.044392	3.437805	8.151286
C	-4.366028	4.707085	7.661773
C	-3.762235	5.222816	6.483026
C	-2.841276	4.448131	5.783496
N	-5.234858	5.663226	8.179993
C	-5.203391	6.793344	7.353292
C	-4.297847	6.555645	6.287651

C	-5.922286	7.984326	7.456858
C	-5.708229	8.952323	6.477578
C	-4.806806	8.739602	5.421253
C	-4.101600	7.543604	5.318641
C	-6.022743	5.519188	9.350998
C	-6.912893	4.453150	9.475007
C	-7.680027	4.297244	10.630251
C	-7.573168	5.233642	11.664718
C	-6.686534	6.312917	11.536091
C	-5.910520	6.447658	10.394785
O	-8.280320	5.185535	12.828279
C	-9.190865	4.112334	13.009279
H	3.333903	-0.013238	1.845651
H	-0.968411	0.010003	1.824225
H	-0.206499	-0.638798	5.740997
H	0.362767	2.526224	2.882771
H	2.532081	0.674142	5.749123
H	1.991084	-2.518242	2.915937
H	4.714203	-4.766493	4.944724
H	5.178747	-1.631822	7.832384
H	6.344590	-6.206544	6.159116
H	6.687143	-1.250013	10.154110
H	9.311326	-5.468284	10.820133
H	8.224695	-1.492314	12.091995
H	9.511761	-3.578260	12.421449
H	-0.937672	0.058965	-2.247921
H	3.347546	-0.072771	-2.235861
H	-0.989150	0.053940	-4.738697
H	5.358833	-0.123038	-4.175843
H	3.019543	-0.102970	-8.608795
H	6.658831	-0.164614	-6.293960
H	5.500699	-0.162614	-8.479142
H	-2.845491	1.694973	7.784331
H	-2.365141	4.812716	4.880995
H	-4.494934	3.057564	9.060767
H	-3.411311	7.375847	4.497573
H	-6.624381	8.147399	8.266461
H	-4.662863	9.515859	4.676670
H	-6.253222	9.889597	6.533379

H	-0.551834	-1.782839	-6.579070
H	1.215032	1.769668	-8.199707
H	-2.289179	-1.740370	-8.329105
H	-0.503385	1.788591	-10.011732
H	6.255172	-7.590893	8.401307
H	10.188391	-5.888659	8.373764
H	7.208455	-9.846740	8.109269
H	11.167574	-8.173940	8.138452
H	-7.009072	3.743622	8.660373
H	-5.207190	7.268094	10.303527
H	-8.360169	3.458262	10.703879
H	-6.614019	7.023029	12.352282
H	-4.030378	-0.547187	-11.267828
H	-3.030919	-1.831012	-10.536036
H	-4.071404	-0.808184	-9.503471
H	8.435253	-11.485768	6.998859
H	9.796337	-12.351347	7.761081
H	8.496566	-11.670328	8.775696
H	-8.679045	3.141994	12.989208
H	-9.641019	4.261665	13.991054
H	-9.978139	4.118514	12.245060

PCZ3PM

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C	1.212327	0.000000	2.090555
C	2.424897	0.025342	1.401989
C	2.418596	0.038067	0.000294
C	1.218516	0.013411	-0.694272
N	3.652022	0.042136	2.111156
C	4.021436	0.978809	3.079860
C	5.320496	0.663785	3.554292
C	5.754480	-0.515652	2.833208
C	4.698281	-0.871310	1.953681
C	3.327685	2.092773	3.553896
C	3.944475	2.876924	4.522358
C	5.234650	2.586867	5.023008

C	5.917681	1.471636	4.523106
C	4.778265	-1.992048	1.125566
C	5.946541	-2.749278	1.175812
C	7.007437	-2.405312	2.030646
C	6.915946	-1.293403	2.862940
C	5.851100	3.456202	6.052576
C	5.675033	4.844763	6.017196
C	6.260438	5.647411	6.996768
C	7.033097	5.052502	8.026417
C	7.236650	3.672740	8.071088
C	6.636665	2.896041	7.085800
C	6.294030	7.078871	7.220828
C	7.079981	7.294459	8.381459
N	7.525711	6.059271	8.863864
C	5.715008	8.165203	6.564362
C	5.911363	9.463358	7.050733
C	6.689113	9.642621	8.217507
C	7.272841	8.577538	8.895046
C	8.339993	5.861577	10.004540
C	9.541237	6.564640	10.144869
C	10.330777	6.376676	11.274013
C	9.964117	5.466263	12.278782
C	8.761197	4.760088	12.114198
C	7.950916	4.961303	11.002057
C	10.819908	5.256709	13.468466
C	10.238303	5.033431	14.737638
C	11.004108	4.835399	15.880647
C	12.392987	4.866269	15.747151
C	13.008461	5.076785	14.485688
C	12.215474	5.272483	13.354883
N	13.384894	4.682918	16.710890
C	14.633521	4.769440	16.087394
C	14.439462	5.011458	14.702377
C	15.909293	4.677954	16.645776
C	16.998903	4.815942	15.788953
C	16.826335	5.043768	14.413013
C	15.551121	5.145793	13.864991
C	5.314059	10.628107	6.356260
C	4.792016	11.714976	7.094731

C	4.216431	12.822995	6.482679
C	4.154301	12.837413	5.088758
C	4.677700	11.768509	4.317278
C	5.255283	10.671540	4.958090
N	3.651800	13.816035	4.227319
C	3.846613	13.391388	2.909637
C	4.484461	12.123115	2.925782
C	3.485136	14.015896	1.714898
C	3.788355	13.357619	0.525119
C	4.430927	12.107997	0.521293
C	4.777729	11.485114	1.716768
C	13.163966	4.441782	18.090968
C	12.409341	5.335001	18.850704
C	12.174772	5.096253	20.205527
C	12.723109	3.961793	20.814375
C	13.492366	3.068669	20.054025
C	13.700633	3.300660	18.702813
C	3.044235	15.033202	4.624851
C	1.944923	15.022425	5.494583
C	1.356398	16.213117	5.893482
C	1.840941	17.437590	5.411041
C	2.929995	17.453827	4.532639
C	3.532070	16.252579	4.155532
O	12.568001	3.637232	22.128441
C	11.797365	4.507687	22.942137
O	1.186005	18.548404	5.853323
C	1.638647	19.812479	5.395466
O	-1.121738	-0.011101	-0.774480
C	-2.380422	-0.022573	-0.120145
H	11.244121	6.951832	11.385467
H	8.462475	4.034921	12.864058
H	5.108494	5.297995	5.209894
H	6.756437	1.818244	7.123005
H	5.087841	8.004199	5.693196
H	6.855987	10.650305	8.583741
H	4.820408	11.670874	8.178550
H	5.685324	9.863412	4.374831
H	3.823250	13.643996	7.071277
H	5.266197	10.515288	1.713700

H	2.981826	14.975954	1.714636
H	4.654714	11.624184	-0.424017
H	3.518905	13.821744	-0.418701
H	9.156951	5.042487	14.826473
H	12.678266	5.405836	12.382172
H	10.536671	4.668341	16.844210
H	15.418674	5.330013	12.803094
H	16.045570	4.510182	17.707980
H	17.697746	5.144001	13.774093
H	18.002910	4.747805	16.196282
H	3.408746	3.729626	4.926479
H	6.923593	1.254369	4.868219
H	2.337709	2.336504	3.185690
H	7.732555	-1.032913	3.529669
H	3.958406	-2.264947	0.471032
H	7.904433	-3.016095	2.042654
H	6.035613	-3.625476	0.540901
H	12.007535	6.225579	18.379731
H	14.275020	2.598800	18.108131
H	11.581794	5.802950	20.771984
H	13.902253	2.192366	20.543698
H	1.555987	14.073633	5.847579
H	4.392222	16.261425	3.495035
H	0.507233	16.222143	6.567747
H	3.325730	18.386175	4.150314
H	1.217947	-0.024821	3.174812
H	3.361063	0.073668	-0.535008
H	-0.927051	-0.014874	1.958154
H	1.196275	0.020570	-1.778350
H	11.798119	4.067031	23.939439
H	12.238413	5.511242	22.989223
H	10.764016	4.586526	22.581690
H	1.561948	19.897238	4.304104
H	0.986898	20.552690	5.860531
H	2.676236	20.002962	5.697415
H	-2.517751	0.868369	0.505508
H	-3.131214	-0.026228	-0.910874
H	-2.504119	-0.918823	0.500743
H	7.862684	8.743136	9.789054

H	9.847713	7.255466	9.367173
H	7.014890	4.423715	10.898011
H	7.836829	3.217020	8.849991

ICZ3PM

132

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.399338
C	1.212328	0.000000	2.090529
C	2.424682	0.025279	1.401749
C	2.418670	0.038225	0.000129
C	1.218567	0.013650	-0.694366
N	3.652061	0.041137	2.111218
C	4.022837	0.978295	3.077728
C	5.319619	0.658963	3.556472
C	5.750508	-0.524056	2.839556
C	4.694776	-0.877477	1.958773
C	3.332084	2.096463	3.546517
C	3.949177	2.881187	4.514130
C	5.236016	2.585580	5.019821
C	5.916634	1.466411	4.525476
C	4.771488	-2.000588	1.133661
C	5.936339	-2.762643	1.188524
C	6.996927	-2.421036	2.044777
C	6.908648	-1.306633	2.873926
C	5.852098	3.452167	6.051920
C	5.685823	4.846324	6.006736
C	6.266368	5.655433	6.977891
C	7.043476	5.042278	8.024137
C	7.219801	3.665966	8.081072
C	6.616611	2.888289	7.093228
C	6.288889	7.108088	7.201785
C	7.054778	7.243168	8.346704
N	7.517818	6.063719	8.860510
C	7.430554	8.366801	9.062233
C	8.238787	7.815784	10.159469
C	8.265815	6.384226	10.003047
C	8.908962	8.388966	11.235112

C	9.606311	7.581901	12.149242
C	9.612187	6.184898	11.961932
C	8.947259	5.572255	10.900271
C	6.953662	9.566306	8.523763
C	6.153488	9.534044	7.350199
C	5.816228	8.321375	6.691143
C	10.327621	8.192175	13.290760
C	10.331829	7.561646	14.556169
C	10.990262	8.103073	15.654580
C	11.657981	9.315934	15.480498
C	11.682276	9.969521	14.221498
C	11.015832	9.401461	13.135124
N	12.402850	10.063825	16.394744
C	12.909143	11.190794	15.740305
C	12.484186	11.164940	14.386112
C	13.682634	12.236047	16.247473
C	14.044046	13.255502	15.369546
C	13.643458	13.240345	14.022699
C	12.861635	12.201171	13.526668
C	5.653583	10.814828	6.787980
C	5.171466	11.832515	7.642721
C	4.693455	13.045786	7.159679
C	4.689959	13.239854	5.777931
C	5.174884	12.243213	4.892750
C	5.654483	11.037123	5.405911
N	4.286515	14.351029	5.033706
C	4.507870	14.083809	3.679485
C	5.061965	12.782839	3.552915
C	4.237040	14.877948	2.564096
C	4.546442	14.356117	1.310043
C	5.107203	13.075700	1.166179
C	5.363620	12.284188	2.281990
C	12.611940	9.734809	17.757777
C	11.526027	9.519890	18.606037
C	11.724085	9.181061	19.945274
C	13.025480	9.080310	20.449562
C	14.118610	9.307493	19.600642
C	13.913537	9.619822	18.265134
C	3.745779	15.548907	5.564829

C	2.611035	15.507650	6.386706
C	2.087826	16.677672	6.916386
C	2.675424	17.914902	6.614736
C	3.800806	17.963246	5.784544
C	4.335758	16.779064	5.275491
O	13.333882	8.768224	21.739918
C	12.263325	8.529538	22.639860
O	2.078711	19.004997	7.174673
C	2.636540	20.280753	6.902660
O	-1.121523	-0.011314	-0.774246
C	-2.380457	-0.023905	-0.120054
H	8.873901	9.463197	11.384959
H	10.175436	5.567374	12.653566
H	5.122551	5.295158	5.195020
H	6.717735	1.809153	7.140423
H	5.177192	8.365029	5.815712
H	7.197172	10.527857	8.962841
H	5.153175	11.649274	8.712101
H	6.055372	10.281078	4.738088
H	4.329133	13.810832	7.835692
H	5.789041	11.291396	2.169872
H	3.797115	15.862824	2.671341
H	5.338584	12.701272	0.174209
H	4.346768	14.953363	0.425621
H	9.780520	6.635207	14.679483
H	11.054107	9.879930	12.161551
H	10.978324	7.601704	16.615560
H	12.545142	12.194321	12.487944
H	13.986353	12.255049	17.287865
H	13.945138	14.049686	13.365695
H	14.646834	14.080122	15.737446
H	3.415507	3.737238	4.913915
H	6.920348	1.246055	4.875085
H	2.344141	2.342731	3.174671
H	7.725122	-1.047909	3.541478
H	3.951892	-2.271426	0.477968
H	7.891217	-3.035658	2.060171
H	6.023080	-3.640855	0.556126
H	10.519184	9.623846	18.216465

H	14.757944	9.771765	17.601831
H	10.863879	9.015022	20.581231
H	15.118784	9.217327	20.009638
H	2.143361	14.552578	6.599443
H	5.222751	16.809004	4.652137
H	1.212452	16.662840	7.556123
H	4.275532	18.905228	5.540979
H	1.218006	-0.024954	3.174815
H	3.361147	0.073679	-0.535196
H	-0.927050	-0.014922	1.958194
H	1.196253	0.020777	-1.778426
H	12.723416	8.298821	23.601105
H	11.622653	9.413758	22.747898
H	11.648962	7.678865	22.318968
H	2.614358	20.510123	5.829808
H	2.016718	21.000967	7.437486
H	3.670188	20.354203	7.263431
H	-2.518738	0.867197	0.505116
H	-3.130997	-0.028698	-0.910968
H	-2.503093	-0.920079	0.501072
H	8.974907	4.495445	10.775667
H	7.796861	3.204913	8.874965

Cartesian Coordinates of Cationic Ground State Geometry

The cartesian coordinates of cationic ground state geometry of all molecules investigated in this work.

TPA1PM

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C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.401568
C	1.211135	0.000000	2.092079
C	2.420117	0.017816	1.397466
C	2.420057	0.024935	-0.004238
C	1.220521	0.009499	-0.696282
N	3.653426	0.026280	2.106464
C	4.040355	0.960414	3.042156
C	5.340498	0.624917	3.526886
C	5.747134	-0.579503	2.826107
C	4.680473	-0.923497	1.960530
C	3.368055	2.105030	3.491710
C	4.000005	2.898926	4.431203
C	5.287485	2.586908	4.948696
C	5.947273	1.431261	4.475390
C	4.717380	-2.057344	1.152446
C	5.866695	-2.845248	1.209822
C	6.939857	-2.514556	2.051871
C	6.886594	-1.385173	2.867056
C	5.919276	3.449212	5.944516
C	6.896686	2.950370	6.838858
C	7.496401	3.755043	7.785251
C	7.149803	5.120823	7.881207
C	6.180468	5.639643	6.994612
C	5.583892	4.819724	6.058964
N	7.752413	5.941071	8.836178
C	8.156093	5.413547	10.086922
C	9.378114	5.802731	10.652873
C	9.779385	5.298649	11.883232
C	8.954510	4.390049	12.567842
C	7.724064	4.003253	12.001539
C	7.327800	4.509537	10.779591
O	9.245124	3.839506	13.761917

C	10.468934	4.195965	14.405054
O	-1.113409	-0.009056	-0.770412
C	-2.382825	-0.029671	-0.126610
C	7.971688	7.315042	8.571256
C	7.724744	8.274099	9.572078
C	7.945111	9.613066	9.317937
C	8.419884	10.030904	8.059116
C	8.670594	9.076258	7.059261
C	8.449665	7.729737	7.320359
O	8.602534	11.357566	7.916493
C	9.078333	11.856964	6.666719
H	8.246191	3.346037	8.451382
H	5.896800	6.682646	7.064779
H	7.172217	1.903141	6.799646
H	4.853004	5.249892	5.384614
H	7.345719	7.955902	10.536299
H	8.665008	6.990013	6.557692
H	7.747790	10.367719	10.070436
H	9.052520	9.371721	6.090867
H	10.019772	6.491678	10.115751
H	6.370120	4.227718	10.357314
H	10.732402	5.604105	12.294817
H	7.094625	3.317086	12.556204
H	3.473185	3.766603	4.810361
H	6.949022	1.195932	4.816935
H	2.382350	2.355124	3.118379
H	7.715318	-1.139265	3.523605
H	3.884820	-2.318521	0.510173
H	7.819091	-3.149455	2.070119
H	5.928662	-3.734600	0.591574
H	1.216405	-0.029528	3.176474
H	3.362207	0.053375	-0.540591
H	-0.927404	-0.016770	1.959164
H	1.196600	0.016049	-1.779970
H	-3.122388	-0.038348	-0.926614
H	-2.502646	-0.928182	0.489977
H	-2.529410	0.861568	0.494989
H	10.481332	3.642907	15.343057
H	11.333036	3.905898	13.797296

H	10.506732	5.270972	14.612378
H	8.382075	11.618099	5.855294
H	9.142275	12.937542	6.785785
H	10.070252	11.454842	6.433098

TPA2PM

106

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.401024
C	1.211695	0.000000	2.091406
C	2.420995	0.019856	1.397920
C	2.419818	0.027935	-0.003489
C	1.219983	0.010160	-0.696076
N	3.653180	0.030830	2.108128
C	4.044487	0.979402	3.033105
C	5.340256	0.644160	3.524088
C	5.741521	-0.571905	2.842611
C	4.674513	-0.923517	1.979073
C	3.377978	2.132335	3.464494
C	4.014083	2.938057	4.394014
C	5.297269	2.626405	4.915250
C	5.950924	1.463216	4.463248
C	4.710791	-2.069194	1.186342
C	5.855992	-2.860726	1.258228
C	6.928932	-2.523038	2.098915
C	6.877991	-1.382365	2.896960
C	5.935363	3.506087	5.899126
C	5.663596	4.891820	5.933898
C	6.269012	5.727869	6.853543
C	7.178056	5.205988	7.793788
C	7.463333	3.826960	7.776171
C	6.853336	3.003612	6.847965
N	7.799934	6.053930	8.726315
C	8.172523	7.366969	8.337386
C	8.787450	7.588301	7.098848
C	9.151833	8.872057	6.709618
C	8.907507	9.956231	7.567882
C	8.291637	9.732916	8.813886

C	7.926140	8.455727	9.193465
O	9.221389	11.239278	7.293678
C	9.841045	11.541295	6.045065
O	-1.115243	-0.009791	-0.771167
C	-2.382070	-0.032038	-0.124830
C	8.057337	5.620055	10.037157
C	9.219489	6.043077	10.711140
C	9.463544	5.624110	12.005328
C	8.569331	4.772749	12.692229
C	7.408434	4.362329	11.999701
C	7.152192	4.771318	10.704192
C	8.837246	4.338158	14.066030
C	7.768888	4.019374	14.945132
C	7.982502	3.615135	16.252319
C	9.305560	3.517473	16.699352
C	10.402843	3.812314	15.838115
C	10.160923	4.225758	14.536005
N	9.791712	3.122127	17.930293
C	11.195115	3.147642	17.891836
C	11.610287	3.568143	16.604128
C	12.106736	2.854778	18.904446
C	13.461724	2.972949	18.598846
C	13.893443	3.376297	17.324972
C	12.974036	3.679580	16.323221
C	9.005736	2.747729	19.054823
C	8.069016	3.634932	19.583381
C	7.289655	3.269908	20.680670
C	7.464071	2.009444	21.267022
C	8.415071	1.121296	20.738014
C	9.173875	1.484111	19.637071
O	6.770052	1.555360	22.339675
C	5.799949	2.413398	22.928104
H	9.923133	6.694189	10.206279
H	6.248464	4.450159	10.199820
H	10.355311	5.979098	12.508950
H	6.704268	3.696396	12.484888
H	6.042546	6.787486	6.861152
H	8.170745	3.417612	8.487757
H	4.980552	5.320423	5.209717

H	7.075995	1.942852	6.864427
H	8.991371	6.747269	6.445933
H	7.436396	8.287809	10.145772
H	9.635088	9.017609	5.752414
H	8.100258	10.585933	9.454583
H	6.747816	4.131523	14.598668
H	10.994483	4.419324	13.869611
H	7.152682	3.387766	16.910790
H	13.311790	3.999741	15.342426
H	11.774252	2.551732	19.890264
H	14.956071	3.455668	17.121971
H	14.197179	2.750448	19.364958
H	3.494126	3.816278	4.759820
H	6.950834	1.229402	4.812549
H	2.393750	2.382262	3.086715
H	7.706245	-1.129684	3.551727
H	3.879514	-2.334775	0.543935
H	7.805363	-3.161560	2.128204
H	5.916166	-3.758704	0.652107
H	7.957659	4.619992	19.142905
H	9.894705	0.792186	19.215345
H	6.569365	3.974262	21.076126
H	8.529228	0.149167	21.203906
H	1.217859	-0.028179	3.175809
H	3.362209	0.056259	-0.539557
H	-0.927292	-0.016178	1.958933
H	1.196169	0.015798	-1.779835
H	5.374048	1.855385	23.761539
H	6.258095	3.335871	23.304135
H	5.005372	2.666157	22.215844
H	-2.528921	0.858599	0.497938
H	-3.124297	-0.041468	-0.922576
H	-2.499838	-0.930596	0.492453
H	9.196681	11.259024	5.204917
H	9.990897	12.620098	6.042273
H	10.809640	11.037499	5.951541

TPA3PM

136

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.400732
C	1.211962	0.000000	2.091266
C	2.421408	0.021234	1.398272
C	2.419576	0.029918	-0.003107
C	1.219765	0.011216	-0.695883
N	3.654122	0.032816	2.106975
C	4.049073	0.985786	3.028437
C	5.350360	0.658348	3.507333
C	5.752142	-0.556080	2.824151
C	4.679459	-0.914976	1.970271
C	3.380629	2.134682	3.465172
C	4.021255	2.944582	4.389050
C	5.311243	2.641843	4.896343
C	5.966743	1.483244	4.439070
C	4.717418	-2.060622	1.177090
C	5.868467	-2.843964	1.238883
C	6.946806	-2.499051	2.070266
C	6.894758	-1.359060	2.868530
C	5.955818	3.528007	5.873392
C	5.679220	4.911870	5.906905
C	6.288702	5.752668	6.821176
C	7.212635	5.237179	7.748192
C	7.501534	3.860480	7.733130
C	6.882572	3.030996	6.815135
N	7.840959	6.087546	8.679715
C	8.228849	7.388936	8.301383
C	8.754538	7.633001	7.019806
C	9.129483	8.914192	6.656045
C	9.003308	10.003884	7.544310
C	8.476224	9.736371	8.825941
C	8.094995	8.460620	9.202330
C	9.406236	11.359441	7.149464
C	8.761694	12.493618	7.706992
C	9.108861	13.788475	7.356358
C	10.136177	13.959429	6.422016
C	10.815022	12.843165	5.854050
C	10.441449	11.555484	6.216438

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C	11.718745	14.791493	5.031631
C	11.830419	13.379915	4.968822
C	12.532131	15.631550	4.272757
C	13.483309	15.030395	3.450449
C	13.616984	13.633798	3.382935
C	12.792053	12.802040	4.135987
C	10.268556	16.445590	6.244659
C	8.941439	16.836993	6.023655
C	8.531638	18.119931	6.350767
C	9.446907	19.040384	6.886110
C	10.777205	18.654416	7.095748
C	11.177555	17.355834	6.782260
O	8.947618	20.271126	7.163852
C	9.828112	21.249003	7.703411
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C	8.082829	5.636169	9.994447
C	9.281908	5.965911	10.650550
C	9.511761	5.520849	11.940605
C	8.566507	4.732790	12.631339
C	7.369985	4.413806	11.954576
C	7.127293	4.852035	10.664375
C	8.821047	4.261805	13.998830
C	7.745959	4.054987	14.900681
C	7.945130	3.615756	16.199866
C	9.259005	3.368223	16.611694
C	10.360565	3.550369	15.726848
C	10.133890	4.001466	14.432794
N	9.728991	2.908556	17.829073
C	11.123973	2.781608	17.755376
C	11.551632	3.168726	16.460677
C	12.023490	2.379325	18.741431
C	13.375108	2.353116	18.402815
C	13.817708	2.722227	17.121816
C	12.912828	3.134422	16.146838
C	8.933225	2.615676	18.970541
C	8.123370	3.601240	19.532931
C	7.333246	3.318278	20.646927

C	7.370571	2.039265	21.216757
C	8.194557	1.050852	20.654584
C	8.962447	1.333962	19.536282
O	6.653978	1.657655	22.304051
C	5.811018	2.619026	22.926100
H	10.024337	6.566347	10.137692
H	6.198842	4.598896	10.165780
H	10.434253	5.802065	12.435774
H	6.627888	3.795072	12.446073
H	6.054517	6.810756	6.831122
H	8.215794	3.456230	8.440886
H	4.986417	5.335194	5.188802
H	7.106120	1.970489	6.834777
H	8.867278	6.811190	6.322336
H	7.686515	8.280796	10.189871
H	9.512429	9.083724	5.656153
H	8.381998	10.543451	9.543318
H	7.944399	12.347099	8.404287
H	10.978193	10.704644	5.810428
H	8.596865	14.641139	7.786330
H	12.892061	11.722720	4.074597
H	12.423870	16.708840	4.317905
H	14.369935	13.200425	2.733260
H	14.132238	15.657308	2.847589
H	6.735832	4.281916	14.578245
H	10.966636	4.110723	13.746085
H	7.111847	3.473922	16.877811
H	13.259258	3.426689	15.160291
H	11.683755	2.102493	19.732544
H	14.877522	2.687948	16.892813
H	14.100240	2.042725	19.148069
H	3.500241	3.820042	4.760108
H	6.971462	1.254812	4.778183
H	2.391713	2.379504	3.096247
H	7.726589	-1.099495	3.516102
H	3.882803	-2.332061	0.541435
H	7.827908	-3.131521	2.091552
H	5.929598	-3.741468	0.632033
H	8.118866	4.597679	19.104084

H	9.584013	0.565963	19.088911
H	6.711680	4.098433	21.067097
H	8.203593	0.066384	21.108404
H	8.242199	16.132826	5.585781
H	12.200823	17.044916	6.963203
H	7.509846	18.443096	6.187219
H	11.499804	19.345531	7.510020
H	1.218159	-0.027781	3.175709
H	3.362077	0.058580	-0.538937
H	-0.927256	-0.016228	1.958752
H	1.196002	0.016872	-1.779681
H	5.342687	2.106976	23.766378
H	6.386658	3.475436	23.297251
H	5.034060	2.975010	22.238696
H	10.653716	21.467335	7.015504
H	9.227381	22.147410	7.843290
H	10.235914	20.930108	8.670129
H	-2.528531	0.856357	0.499606
H	-3.124673	-0.039655	-0.923142
H	-2.501142	-0.932582	0.489745

MPD3PM

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C	-2.290580	-0.225532	0.824725
C	-1.346786	-1.865940	-0.691579
C	-3.488619	-0.918112	0.815413
H	-2.184405	0.676601	1.415892
C	-2.549631	-2.550947	-0.688695
H	-0.515181	-2.228345	-1.285209
C	-3.655450	-2.100626	0.063258
H	-4.322227	-0.529411	1.389173
H	-2.632146	-3.465010	-1.265382
C	1.233740	-0.702985	0.083283
C	2.361669	-0.265405	-0.636213
C	1.398338	-1.898815	0.808079
H	2.313989	0.646039	-1.228177

H	0.576041	-2.300787	1.395981
C	3.570452	-2.071704	0.093766
C	0.040005	1.418816	0.091225
C	0.986969	2.115208	0.862048
C	-0.893311	2.144289	-0.669182
C	0.996894	3.499283	0.864897
H	1.704727	1.563954	1.458901
C	-0.874331	3.528187	-0.654387
H	-1.624031	1.613243	-1.268111
C	0.068597	4.247617	0.110401
H	1.749240	4.016240	1.449574
H	-1.616057	4.067657	-1.232175
C	0.081994	5.715871	0.125612
C	-0.354005	6.452393	-1.005598
C	0.519725	6.415132	1.265934
C	-0.353736	7.837859	-1.030681
H	-0.665031	5.917398	-1.895935
C	0.521278	7.803751	1.270558
H	0.815152	5.872897	2.157826
C	0.091038	8.512319	0.111748
H	-0.681704	8.382143	-1.908260
C	0.868971	8.801709	2.263779
C	0.643453	10.066127	1.664682
C	1.353567	8.736963	3.572491
C	0.906335	11.259506	2.335413
C	1.607191	9.924313	4.255180
H	1.532242	7.777601	4.048218
C	1.388348	11.167744	3.640018
H	0.746234	12.219391	1.858695
H	1.981615	9.890733	5.272745
H	1.601207	12.078855	4.189583
C	-4.927556	-2.833853	0.067984
C	-5.327561	-3.590902	-1.063057
C	-5.765319	-2.805026	1.198685
C	-6.520246	-4.295384	-1.097086
H	-4.698659	-3.592888	-1.946285
C	-6.961897	-3.509535	1.194194
H	-5.458473	-2.269914	2.091001
C	-7.340057	-4.248065	0.035899

H	-6.811903	-4.860570	-1.974266
C	-8.009003	-3.711520	2.177134
C	-8.975943	-4.553077	1.572740
C	-8.214368	-3.253014	3.480704
C	-10.144436	-4.929754	2.232915
C	-9.373067	-3.634609	4.153048
H	-7.484636	-2.608114	3.960504
C	-10.325234	-4.459718	3.532592
H	-10.883905	-5.559166	1.751991
H	-9.545882	-3.288832	5.166623
H	-11.223893	-4.736674	4.074027
C	4.828436	-2.808646	0.102654
C	5.937601	-2.330385	-0.642512
C	4.945020	-3.992018	0.858769
C	7.144939	-3.004117	-0.657609
H	5.817464	-1.412579	-1.204099
C	6.146406	-4.681236	0.857443
H	4.093123	-4.337623	1.431709
C	7.243487	-4.187546	0.088911
H	7.990176	-2.629633	-1.222503
C	6.609956	-5.888859	1.516484
C	7.956702	-6.075950	1.120681
C	6.011620	-6.811423	2.376468
C	8.710155	-7.166904	1.548234
C	6.760823	-7.899869	2.820709
H	4.980254	-6.684427	2.690026
C	8.090776	-8.074159	2.407627
H	9.733953	-7.307006	1.222096
H	6.310781	-8.624568	3.490846
H	8.650699	-8.933996	2.760492
N	8.322765	-5.031065	0.253726
N	-8.552826	-4.869460	0.272856
N	0.170526	9.871071	0.358150
C	-9.255363	-5.699192	-0.643336
C	-9.625131	-5.208083	-1.894712
C	-9.579951	-7.015810	-0.289372
C	-10.305428	-6.020688	-2.801363
H	-9.390392	-4.181901	-2.156587
C	-10.271639	-7.823031	-1.178047

H	-9.279197	-7.398801	0.679678
C	-10.636702	-7.333777	-2.442892
H	-10.583287	-5.619062	-3.767236
H	-10.532823	-8.844023	-0.924046
C	-0.171703	10.903872	-0.557092
C	0.457945	10.978894	-1.798783
C	-1.143560	11.852706	-0.211768
C	0.119912	11.984221	-2.704411
H	1.224524	10.254906	-2.053587
C	-1.471445	12.865020	-1.099238
H	-1.640576	11.783713	0.749701
C	-0.845462	12.937103	-2.354377
H	0.621592	12.024211	-3.662612
H	-2.219761	13.609290	-0.851748
C	9.598530	-4.879152	-0.355159
C	9.709913	-4.806040	-1.743156
C	10.749837	-4.805373	0.440705
C	10.957843	-4.649255	-2.345165
H	8.818318	-4.884591	-2.355869
C	11.994456	-4.666105	-0.151614
H	10.657890	-4.848273	1.520417
C	12.108855	-4.583417	-1.549109
H	11.021931	-4.595940	-3.424242
H	12.897492	-4.606049	0.445067
O	-1.243229	13.960754	-3.150747
O	13.369982	-4.441721	-2.027189
O	-11.303341	-8.206150	-3.239574
C	-11.708366	-7.766195	-4.529829
H	-12.219362	-8.612897	-4.987526
H	-12.398879	-6.916869	-4.464325
H	-10.845559	-7.485907	-5.146061
C	-0.637227	14.093526	-4.430382
H	-0.826412	13.212900	-5.056048
H	-1.097022	14.968344	-4.889510
H	0.444355	14.253260	-4.346035
C	13.551953	-4.360684	-3.435482
H	13.033646	-3.490649	-3.856184
H	14.624912	-4.252936	-3.592328
H	13.200534	-5.270363	-3.936826

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TPD3PM

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C	1.197398	0.000998	-0.632945
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C	2.133441	-0.755599	4.187303
C	2.739717	-0.283144	5.365089
N	3.634762	-0.991239	6.031104
C	3.965443	-2.212181	5.545963
N	3.431897	-2.747992	4.422326
C	2.537824	-2.033130	3.761410
C	1.204329	0.005390	-2.092209
C	-0.020259	0.009556	-2.808369
C	-0.050666	0.014003	-4.190969
C	1.175272	0.009846	-4.872470
C	2.419835	0.020463	-4.173808
C	2.429048	0.015652	-2.789003
N	1.422557	0.028879	-6.230228
C	2.813008	0.052362	-6.440456
C	3.463747	0.049125	-5.182784
C	3.520041	0.045685	-7.640855
C	4.912764	0.056355	-7.562613
C	5.575688	0.066150	-6.326000
C	4.858170	0.058198	-5.130106
C	4.956299	-2.994488	6.277892
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C	6.272402	-5.045952	6.476014
C	6.837564	-4.517606	7.645983
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C	5.542245	-2.469359	7.446854
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C	-0.516643	-0.994664	-7.303842
C	-1.489030	-1.003138	-8.302675
C	-1.495337	0.006997	-9.273928
C	-0.527036	1.023881	-9.227133
C	0.427176	1.034730	-8.223273
C	8.392746	-6.341896	8.334351
C	7.599497	-7.487172	8.265928
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N	-1.054498	2.769208	4.396990
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C	-3.158042	2.540085	7.441656
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C	-4.445580	4.535596	7.665242
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C	-2.926234	4.323362	5.778614
N	-5.325872	5.461719	8.187163
C	-5.328825	6.602479	7.364510
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C	-5.899156	8.749228	6.507527

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C	-4.261731	7.388924	5.329185
C	-6.109317	5.295303	9.360913
C	-6.970006	4.204373	9.482011
C	-7.735058	4.032193	10.634540
C	-7.650330	4.971761	11.670771
C	-6.788657	6.073986	11.542432
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H	-0.129649	-0.673083	5.759021
H	0.264433	2.477222	2.839646
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H	2.111202	-2.474619	2.862795
H	4.875861	-4.646440	4.899957
H	5.250450	-1.482788	7.785880
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H	6.766212	-1.044065	10.105246
H	9.529297	-5.180150	10.735304
H	8.331960	-1.243097	12.024950
H	9.686896	-3.285178	12.338294
H	-0.943119	0.013473	-2.242275
H	3.355392	0.025110	-2.227575
H	-0.989380	0.026647	-4.731586
H	5.374126	0.054919	-4.175215
H	3.009001	0.027194	-8.596101
H	6.660145	0.075258	-6.301758
H	5.493151	0.053562	-8.479321
H	-2.854046	1.559319	7.784926
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H	-4.527604	2.882909	9.068009
H	-3.574875	7.246294	4.500981
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H	-4.881920	9.350165	4.705427
H	-6.468794	9.670416	6.571813
H	-0.490422	-1.789411	-6.566214
H	1.161218	1.831360	-8.173184

H	-2.219173	-1.801735	-8.323638
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H	6.521644	-7.396872	8.346450
H	10.401038	-5.561618	8.297534
H	7.550113	-9.619640	8.065702
H	11.452303	-7.812544	8.062277
H	-7.052702	3.495100	8.665616
H	-5.338112	7.069376	10.310297
H	-8.398462	3.180161	10.706942
H	-6.733242	6.784134	12.359549
H	-3.983939	-0.647826	-11.271515
H	-2.947447	-1.903927	-10.543123
H	-4.033672	-0.926501	-9.510013
H	8.833926	-11.230279	6.959539
H	10.233546	-12.031542	7.722472
H	8.912913	-11.396008	8.739669
H	-8.715921	2.858493	13.000776
H	-9.695535	3.966504	13.998620
H	-10.034259	3.810798	12.254004

PCZ3PM

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C	0.000000	0.000000	0.000000
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C	1.211208	0.000000	2.091777
C	2.421305	0.018227	1.398436
C	2.419816	0.026554	-0.003403
C	1.220158	0.010230	-0.695932
N	3.652203	0.025456	2.107807
C	4.031833	0.953182	3.061158
C	5.327805	0.615955	3.547749
C	5.742731	-0.577968	2.834729
C	4.682789	-0.916355	1.957345
C	3.355777	2.090534	3.518341
C	3.981740	2.874346	4.473894
C	5.264180	2.558380	4.992626
C	5.929531	1.414394	4.510325
C	4.732112	-2.042148	1.137301

C	5.884595	-2.825211	1.193648
C	6.950649	-2.498905	2.046449
C	6.885576	-1.378904	2.873771
C	5.890243	3.416848	6.006821
C	5.638688	4.805167	6.029089
C	6.242601	5.602372	6.989131
C	7.104781	5.018586	7.954264
C	7.388731	3.650257	7.941244
C	6.773521	2.872050	6.971554
C	6.230972	7.034098	7.251482
C	7.076210	7.249882	8.371424
N	7.599190	6.024277	8.784997
C	5.572122	8.104317	6.666463
C	5.736271	9.404476	7.189778
C	6.569376	9.579159	8.322321
C	7.237819	8.522914	8.924566
C	8.490040	5.832611	9.868300
C	9.647303	6.614083	9.972710
C	10.515326	6.422443	11.038279
C	10.266486	5.446848	12.022876
C	9.097655	4.672065	11.894177
C	8.217257	4.860073	10.838010
C	11.199526	5.242149	13.144281
C	10.718804	4.837130	14.413642
C	11.564930	4.634846	15.494016
C	12.933974	4.841455	15.298631
C	13.450836	5.234758	14.031982
C	12.579899	5.437229	12.967483
N	13.985959	4.690186	16.188461
C	15.185057	4.975351	15.520699
C	14.891446	5.315006	14.175967
C	16.488586	4.981179	16.016084
C	17.509647	5.318335	15.129561
C	17.239844	5.645898	13.790663
C	15.933354	5.650242	13.307701
C	5.046651	10.547552	6.576385
C	4.646481	11.658367	7.363205
C	3.991221	12.751919	6.820836
C	3.725871	12.739577	5.446422

C	4.127555	11.648071	4.624167
C	4.777487	10.561915	5.193981
N	3.114815	13.698446	4.657669
C	3.111951	13.253702	3.326334
C	3.738320	11.983722	3.267137
C	2.579495	13.868668	2.194527
C	2.703483	13.194173	0.980522
C	3.333378	11.942298	0.899405
C	3.849594	11.328364	2.039328
C	13.872579	4.302866	17.550822
C	13.079991	5.042167	18.428169
C	12.956661	4.661124	19.764095
C	13.651134	3.538217	20.232050
C	14.456377	2.800458	19.349238
C	14.559362	3.174269	18.018973
C	2.569732	14.926986	5.118449
C	1.599568	14.929667	6.130188
C	1.074814	16.128217	6.585875
C	1.497324	17.345015	6.025828
C	2.459455	17.342993	5.007013
C	2.995940	16.134495	4.565351
O	13.612318	3.084182	21.510312
C	12.821467	3.795729	22.453607
O	0.916344	18.458833	6.535593
C	1.296352	19.722236	6.002806
O	-1.115163	-0.009343	-0.771109
C	-2.382201	-0.034383	-0.124924
H	11.396755	7.048712	11.119753
H	8.885899	3.900209	12.625596
H	5.007679	5.252532	5.269116
H	6.954045	1.803355	6.971561
H	4.898393	7.938843	5.832995
H	6.714966	10.577812	8.717248
H	4.827854	11.638746	8.431816
H	5.116537	9.744464	4.566635
H	3.688335	13.586604	7.441636
H	4.327870	10.355984	1.974024
H	2.084009	14.830196	2.257691
H	3.415003	11.446920	-0.062216

H	2.301008	13.647910	0.080803
H	9.651155	4.711782	14.557465
H	12.971160	5.705426	11.991625
H	11.177337	4.331683	16.459363
H	15.727499	5.912590	12.274506
H	16.697466	4.737573	17.051138
H	18.059733	5.901722	13.127948
H	18.534926	5.330119	15.484829
H	3.456014	3.738870	4.863629
H	6.929713	1.180688	4.858775
H	2.372381	2.345195	3.141571
H	7.707948	-1.135694	3.539304
H	3.905522	-2.301248	0.486367
H	7.833010	-3.129629	2.063638
H	5.954735	-3.707366	0.565819
H	12.566397	5.926801	18.067223
H	15.163874	2.593098	17.331256
H	12.336414	5.249977	20.427440
H	14.979750	1.931323	19.731216
H	1.253850	13.988152	6.542912
H	3.758586	16.129733	3.794266
H	0.321831	16.152285	7.365349
H	2.804854	18.268131	4.564146
H	1.216805	-0.029270	3.176057
H	3.362025	0.055858	-0.539516
H	-0.927308	-0.017053	1.959012
H	1.196562	0.016949	-1.779684
H	12.936242	3.266906	23.399539
H	13.170380	4.828825	22.569955
H	11.763104	3.800610	22.166050
H	1.066932	19.789662	4.932744
H	0.710598	20.463506	6.545729
H	2.364092	19.916905	6.158780
H	-2.529832	0.854469	0.500153
H	-3.124229	-0.042455	-0.922865
H	-2.499230	-0.934631	0.489951
H	7.866197	8.685564	9.791655
H	9.866037	7.354850	9.211847
H	7.311600	4.268442	10.765520

H	8.062392	3.206978	8.664305

ICZ3PM

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C	1.211071	0.000000	2.091873
C	2.421377	0.017894	1.398578
C	2.419816	0.025794	-0.003398
C	1.220257	0.009700	-0.695916
N	3.651978	0.025830	2.107757
C	4.028622	0.950744	3.066080
C	5.326409	0.616857	3.549153
C	5.745923	-0.571524	2.829528
C	4.686507	-0.910290	1.951506
C	3.348395	2.082801	3.529397
C	3.971923	2.864524	4.488749
C	5.256011	2.551504	5.003552
C	5.926160	1.413667	4.514736
C	4.739947	-2.032370	1.126409
C	5.895947	-2.810577	1.177750
C	6.961468	-2.483426	2.030780
C	6.892246	-1.367542	2.863556
C	5.880830	3.406962	6.023048
C	5.629307	4.797807	6.044869
C	6.227745	5.601004	7.000045
C	7.105852	4.998506	7.972043
C	7.364762	3.631934	7.968127
C	6.748164	2.855240	6.993040
C	6.187720	7.049584	7.275593
C	7.016609	7.186448	8.373486
N	7.574913	6.014261	8.810480
C	7.382176	8.300867	9.105346
C	8.295747	7.751089	10.124742
C	8.381820	6.328191	9.908407
C	9.010538	8.317202	11.165863
C	9.811198	7.508969	12.004930
C	9.867778	6.118202	11.760230

C	9.163968	5.516006	10.722644
C	6.811640	9.489655	8.650949
C	5.938049	9.457859	7.524635
C	5.623782	8.248013	6.838786
C	10.571002	8.110047	13.110986
C	10.816775	7.376992	14.300071
C	11.528426	7.908800	15.363507
C	12.012322	9.216049	15.237645
C	11.796576	9.974825	14.051874
C	11.075434	9.420252	13.003218
N	12.762659	9.968396	16.124930
C	13.046798	11.210504	15.536546
C	12.464732	11.248482	14.244898
C	13.743970	12.295452	16.065619
C	13.870717	13.428475	15.262878
C	13.313219	13.479850	13.975671
C	12.604654	12.395201	13.461068
C	5.340257	10.721128	7.047983
C	4.951503	11.725708	7.968467
C	4.383753	12.923909	7.561101
C	4.196397	13.124436	6.189570
C	4.590465	12.142982	5.237473
C	5.154375	10.949704	5.673004
N	3.678555	14.222429	5.519111
C	3.731061	13.974001	4.139786
C	4.297092	12.691736	3.926938
C	3.294919	14.772870	3.083467
C	3.455583	14.272906	1.792064
C	4.027692	13.011897	1.560840
C	4.446667	12.213490	2.623670
C	13.179790	9.555723	17.418580
C	12.239753	9.131926	18.357945
C	12.644177	8.716390	19.625818
C	14.003793	8.742179	19.963811
C	14.947670	9.177638	19.018877
C	14.540583	9.573723	17.755504
C	3.168806	15.399794	6.127303
C	2.151948	15.311084	7.088363
C	1.659980	16.459197	7.687841

C	2.162538	17.719248	7.324284
C	3.171739	17.810721	6.356586
C	3.674701	16.650070	5.770546
O	14.506548	8.370014	21.166437
C	13.600291	7.924337	22.168380
O	1.607341	18.779341	7.962547
C	2.064617	20.083715	7.626267
O	-1.115016	-0.008582	-0.771060
C	-2.382265	-0.030204	-0.125022
H	8.930448	9.380928	11.360174
H	10.508867	5.501997	12.379675
H	4.992334	5.242202	5.288343
H	6.912951	1.784051	6.999801
H	4.927391	8.284262	6.008945
H	7.037765	10.444999	9.110287
H	5.070775	11.538657	9.030041
H	5.488241	10.211453	4.951389
H	4.087954	13.675980	8.282800
H	4.879509	11.234669	2.441676
H	2.843140	15.741668	3.260642
H	4.140173	12.654984	0.542617
H	3.127678	14.872380	0.949121
H	10.406766	6.377932	14.395921
H	10.939079	9.980724	12.084517
H	11.700069	7.333401	16.265297
H	12.167000	12.442427	12.468747
H	14.165996	12.261009	17.063001
H	13.433144	14.376685	13.377292
H	14.410175	14.288773	15.645207
H	3.442948	3.725072	4.882879
H	6.928046	1.183576	4.860891
H	2.363919	2.335933	3.154506
H	7.714187	-1.123961	3.529475
H	3.913651	-2.292506	0.475549
H	7.846681	-3.110236	2.044087
H	5.969200	-3.689551	0.545839
H	11.185944	9.140686	18.101209
H	15.270653	9.887967	17.017790
H	11.897899	8.393439	20.340063

H	15.994826	9.182041	19.299136
H	1.744510	14.340100	7.347972
H	4.472911	16.714522	5.039201
H	0.871722	16.412217	8.430570
H	3.578953	18.769967	6.064290
H	1.216493	-0.029402	3.176125
H	3.361955	0.055543	-0.539550
H	-0.927337	-0.016971	1.959027
H	1.196706	0.016826	-1.779664
H	14.211665	7.680743	23.036841
H	12.883606	8.709634	22.436562
H	13.055200	7.029644	21.844585
H	1.889274	20.307849	6.567349
H	1.485493	20.771279	8.242165
H	3.131089	20.204087	7.851260
H	-2.527512	0.859182	0.499809
H	-3.124150	-0.036510	-0.923100
H	-2.501737	-0.930014	0.490020
H	9.237637	4.448369	10.550574
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