SUPPLEMENTARY MATERIAL

Theoretical studies on triacetonetriperoxide (TATP) derivatives to improve their performance

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Table 1S. Standard orientations of every atom in TATP

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1	−1.727473	−0.972077	0.073655
2	−2.83783	−1.513781	−0.830822
3	−1.929784	−1.308508	1.544841
4	−0.55064	−1.557811	−0.480495
5	−1.786307	0.433984	−0.17584
6	0.550708	−1.557767	0.480549
7	1.727509	−0.972036	−0.073653
8	2.837918	−1.513636	0.830823
9	1.92979	−1.308494	−1.544833
10	1.78632	0.434055	0.175793
11	0.912802	1.153957	−0.744413
12	−0.000029	1.953221	−0.000007
13	−0.684255	2.79501	−1.075554
14	0.684149	2.795025	1.075552
15	−0.912868	1.153924	0.744402
16	−2.616992	−1.288048	−1.875092
17	−2.908808	−2.594563	−0.707678
18	−3.787849	−1.052823	−0.559687
19	−1.9042	−2.39108	1.679638
20	−1.153094	−0.857729	2.156245
21	−2.901747	−0.928954	1.864974
22	3.787943	−1.052767	0.559552
23	2.617165	−1.287729	1.875075
24	2.908836	−2.59444	0.707834
25	1.904133	−2.391063	−1.679629
26	1.153123	−0.857664	−2.15623
27	2.901778	−0.929007	−1.864977
28	−1.085177	2.159032	−1.862837
29	−1.503634	3.353559	−0.620505
30	0.031965	3.494773	−1.508164
31	1.503445	3.353695	0.62050
32	−0.032141	3.494682	1.508217
33	1.085168	2.159051	1.862786

Table 2S. Standard orientations of every atom in TATP3F

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1	−2.1352	−0.26912	0.611137
2	−3.25821	−0.43419	1.640057
3	−2.73996	−0.10577	−0.82453
4	−1.45284	0.879504	1.051302
5	−1.40004	−1.47076	0.739837
6	−0.53486	1.37538	0.028536
7	0.753842	1.581935	0.578333
8	1.343133	2.688043	−0.36218
9	0.76434	2.035876	2.029959
10	1.617868	0.486552	0.321837
11	1.329556	−0.59207	1.254598
12	0.904548	−1.73426	0.539533
13	0.811428	−2.82048	1.608301
14	1.921108	−2.14911	−0.58144
15	−0.27849	−1.51282	−0.19274
16	−2.81931	−0.43557	2.637261
17	−3.95681	0.396397	1.55266
18	−3.77793	−1.37459	1.467574
19	0.096641	2.886725	2.158526
20	0.43937	1.223441	2.673133
21	1.780434	2.321609	2.300936
22	0.221975	−2.45447	2.446063
23	0.331106	−3.70132	1.185655
24	1.810628	−3.07895	1.9571
25	−3.44813	1.039161	−0.88129
26	−1.85596	−0.09618	−1.81809
27	−3.59528	−1.12666	−1.0527
28	1.685392	−3.42339	−0.95773
29	1.858178	−1.38845	−1.67387
30	3.1717	−2.09323	−0.09368
31	1.294388	2.331848	−1.64839
32	0.648587	3.82878	−0.21379
33	2.622692	2.942891	−0.04277

Table 3S. Standard orientations of every atom in $TATPNH_2$

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1	1.021948	−1.745909	−0.157073
2	1.579866	−2.906721	−0.978487
3	1.450317	−1.779519	1.318704
4	1.488072	−0.593704	−0.851266
5	−0.393023	−1.909032	−0.289146
6	1.521536	0.571724	0.036612
7	0.873306	1.685072	−0.5573
8	1.407424	2.906432	0.224307
9	1.149748	1.813151	−2.049683
10	−0.52445	1.715943	−0.260476
11	−1.248946	0.764337	−1.097382
12	−1.97285	−0.15281	−0.28009
13	−2.777314	−0.963021	−1.290088
14	−2.845781	0.574618	0.76204
15	−1.108945	−0.934625	0.530091
16	1.384153	−2.746831	−2.039711
17	2.653231	−2.963143	−0.803455
18	1.105705	−3.837385	−0.664493
19	0.881283	−1.021385	1.859883
20	1.155224	−2.760264	1.700193
21	0.951466	3.79141	−0.241037
22	2.483515	2.949359	0.043923
23	2.226929	1.817419	−2.22467
24	0.709048	0.982604	−2.593386
25	0.719213	2.746569	−2.416096
26	−2.114538	−1.425779	−2.018588
27	−3.337504	−1.729944	−0.758188
28	−3.480126	−0.306357	−1.804467
29	−3.460858	1.288831	0.20966
30	−2.180239	1.14319	1.41936
31	2.902764	−1.638322	1.445319
32	3.162729	−0.665533	1.316188
33	3.198592	−1.908687	2.376429
34	1.179898	2.798638	1.663428
35	1.622036	3.570996	2.148906
36	0.188382	2.827367	1.873903
37	−3.723031	−0.365258	1.462987
38	−3.181214	−0.958421	2.082801
39	−4.398382	0.135663	2.029263

Table 4S. Standard orientations of every atom in $TATPNO_2$

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1	−1.04068	−1.84395	0.377392
2	−1.56793	−3.07616	1.111771
3	−1.46497	−1.71012	−1.09878
4	−1.47896	−0.76078	1.181119
5	0.370061	−2.03464	0.425018
6	−1.32525	0.505781	0.466266
7	−0.68106	1.475074	1.274235
8	−1.1839	2.820612	0.717362
9	−1.01773	1.361765	2.756751
10	0.727206	1.529719	1.049586
11	1.382758	0.360003	1.615437
12	2.006381	−0.36989	0.564259
13	2.893111	−1.37154	1.295521
14	2.754975	0.60283	−0.37533
15	1.055076	−0.96867	−0.29845
16	−1.18563	−3.0729	2.132919
17	−2.65473	−3.06641	1.119842
18	−1.22082	−3.97502	0.602076
19	−0.94965	−0.88605	−1.57721
20	−1.25651	−2.64895	−1.60997
21	−0.53154	3.623691	1.059604
22	−2.20807	2.992456	1.034237
23	−2.09662	1.282988	2.893415
24	−0.54248	0.480452	3.179442
25	−0.6461	2.24636	3.27685
26	2.307668	−1.89797	2.046996
27	3.288376	−2.0978	0.585217
28	3.722795	−0.85516	1.776709
29	3.306438	1.319625	0.226819
30	2.058438	1.096617	−1.04725
31	−2.9468	−1.45352	−1.27633
32	−1.19988	2.922041	−0.79981
33	3.771271	−0.12106	−1.22579
34	−2.22087	3.367919	−1.29205
35	−0.19223	2.606405	−1.40983
36	−3.27115	−0.42441	−1.83866
37	−3.71812	−2.31347	−0.8707
38	3.390737	−0.59291	−2.28285
39	4.911627	−0.18821	−0.78555

Table 5S. Harmonic frequency of TATP

Assignment	Frequency[a]	Intensity[b]
C-H	623/616	31.0
C-H	784/786	181.7
O-O	868/868	236.8
C-H	945/949	93.3
C-O	1197/1101	1275.3
C-O	1260/1276	194.7
C-H	1400/1362	189.1
C-H	1477/1461	41.8
C-H	3059/3013	218.7

[a]Calculated and experimental IR spectra, frequency in cm^{-1}.

[b]Calculated infrared intensity.

Table 6S. Harmonic frequency of the derivatives

Assignment	$TATPNO_2$[a]	$TATPNH_2$[a]	TATP3F[a]
C-H	638 (27.1)	629 (38.5)	652 (30.8)
C-H	768 (211.8)	766 (113.9)	779 (31.0)
O-O	868 (122)	861 (497.1)	880 (42.1)
C-H	938 (177)	925 (148.2)	940 (208.3)
C-O	1155 (477.5)	1144 (372.3)	1170 (1710)
C-O	1268 (163)	1241 (250.7)	1302 (688.6)
C-H	1409 (639.8)	1407 (94.1)	1415 (121.8)
C-H	1486 (111.7)	1490 (41.6)	1491 (115.3)
C-H	3063 (35.0)	3057 (143.2)	3076 (17.3)
NO_2	1352 (254.4)		
NO_2	1622 (1750.1)		
C-N		1144 (372.3)	
N-H		1651 (285.6)	
N-H		3588 (39.3)	
C-F			1108 (1517.5)

[a]Calculated IR spectra frequency (cm^{-1}) and intensity (in brackets).

Table 7S. Calculation summaries of the Gaussian output parameters

	TATP	TATP3F	$TATPNH_2$	$TATPNO_2$
Charge	0	0	0	0
Spin	Singlet	Singlet	Singlet	Singlet
RMS Gradient Norm (au)	0.00001399	0.00000950	0.00000839	0.00000592
Imaginary Freq	0	0	0	0
Dipole Moment (Debye)	0.1369	5.8116	2.9148	6.7908
Point Group	C1	C1	C1	C1