

过氧烷基自由基分子内氢迁移反应类速率常数的计算

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Calculation of Rate Constants for Intramolecular Hydrogen Migration Reactions of Alkylperoxy Radicals

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R56	(1,7)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO}^\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2)\text{OOH}$
R57	(1,7)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO}^\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2)\text{OOH}$
R58	(1,8)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO}^\cdot \rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OOH}$
R59	(1,8)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO}^\cdot \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2)\text{OOH}$
R60	(1,8)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO}^\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2)\text{OOH}$
R61	(1,8)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO}^\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2)\text{OOH}$
R62	(1,8)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO}^\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2)\text{OOH}$

表S2 过渡态反应中心几何结构参数

Table S2 Optimized geometrical parameters of the reaction centers of the transition states

TS	Type	d_1/nm	$A_1/(\text{^\circ})$	d_2/nm	$A_2/(\text{^\circ})$	d_3/nm	$A_3/(\text{^\circ})$	d_4/nm
R1	(1,3)	0.1380	88.6	0.1509	83.5	0.1273	101.5	0.1335
R2	(1,3)	0.1390	89.4	0.1499	82.8	0.1286	102.0	0.1331
R3	(1,3)	0.1390	89.4	0.1500	82.9	0.1286	102.0	0.1332
R4	(1,3)	0.1390	89.4	0.1500	82.9	0.1286	102.0	0.1332
R5	(1,3)	0.1390	89.4	0.1500	82.9	0.1286	102.0	0.1332
R6	(1,3)	0.1390	89.4	0.1500	82.9	0.1286	102.0	0.1332
R7	(1,3)	0.1390	89.4	0.1500	82.9	0.1286	102.0	0.1332
R8	(1,3)	0.1390	89.4	0.1500	82.9	0.1286	102.0	0.1332
R9	(1,3)	0.1390	89.4	0.1500	82.9	0.1286	102.0	0.1332
R10	(1,3)	0.1390	89.4	0.1500	82.9	0.1286	102.0	0.1332
R11	(1,4)	0.1435	102.6	0.1420	94.6	0.1207	134.0	0.1382
R12	(1,4)	0.1432	102.7	0.1421	93.9	0.1232	134.6	0.1362
R13	(1,4)	0.1443	103.3	0.1421	94.8	0.1205	133.9	0.1376
R14	(1,4)	0.1431	102.7	0.1423	93.7	0.1234	134.3	0.1361
R15	(1,4)	0.1459	104.1	0.1422	94.9	0.1203	134.0	0.1372
R16	(1,4)	0.1459	104.1	0.1422	94.9	0.1203	134.0	0.1372
R17	(1,4)	0.1433	102.8	0.1421	93.9	0.1232	134.5	0.1363
R18	(1,4)	0.1433	102.8	0.1421	93.9	0.1232	134.6	0.1362
R19	(1,4)	0.1432	102.8	0.1421	93.8	0.1234	134.7	0.1359
R20	(1,4)	0.1433	102.8	0.1421	93.8	0.1234	134.7	0.1359
R21	(1,4)	0.1433	102.8	0.1421	93.8	0.1234	134.7	0.1359
R22	(1,4)	0.1433	102.8	0.1421	93.8	0.1234	134.7	0.1359
R23	(1,5)	0.1422	107.5	0.1414	101.3	0.1162	152.5	0.1399
R24	(1,5)	0.1423	107.3	0.1416	101.0	0.1185	153.9	0.1371
R25	(1,5)	0.142	107.6	0.1415	100.9	0.1159	153.0	0.1398
R26	(1,5)	0.1423	107.4	0.1416	100.9	0.1185	154.0	0.1372
R27	(1,5)	0.1423	107.2	0.1415	100.6	0.1205	155.0	0.1350

R28	(1,5)	0.1434	108.1	0.1414	100.8	0.1182	154.0	0.1370
R29	(1,5)	0.1423	107.4	0.1416	100.9	0.1187	153.9	0.1369
R30	(1,5)	0.1423	107.3	0.1416	100.9	0.1184	154.2	0.1373
R31	(1,5)	0.1419	107.6	0.1416	100.9	0.1161	153.2	0.1396
R32	(1,5)	0.1423	107.3	0.1416	100.9	0.1187	154.0	0.1370
R33	(1,5)	0.1423	107.1	0.1415	100.3	0.1208	155.7	0.1347
R34	(1,5)	0.1423	107.3	0.1416	100.9	0.1187	153.9	0.1370
R35	(1,5)	0.1423	107.3	0.1416	100.8	0.1187	154.0	0.1369
R36	(1,5)	0.1423	107.3	0.1416	100.9	0.1187	154.0	0.1369
R37	(1,6)	0.1435	109.2	0.1414	104.2	0.1151	161.3	0.1388
R38	(1,6)	0.1434	109.2	0.1413	103.8	0.1176	163.0	0.1359
R39	(1,6)	0.1433	109.2	0.1414	103.9	0.1145	162.1	0.1394
R40	(1,6)	0.1434	109.2	0.1413	103.9	0.1176	162.8	0.1362
R41	(1,6)	0.1449	110.1	0.1412	104.0	0.1147	160.5	0.1389
R42	(1,6)	0.1435	109.2	0.1411	103.8	0.1197	164.6	0.1340
R43	(1,6)	0.1434	109.0	0.1415	103.7	0.1146	162.6	0.1394
R44	(1,6)	0.1434	109.2	0.1413	103.8	0.1177	163.2	0.1360
R45	(1,6)	0.1435	109.2	0.1412	103.9	0.1197	164.3	0.1343
R46	(1,6)	0.1434	109.2	0.1413	103.9	0.1177	163.0	0.1360
R47	(1,6)	0.1434	109.2	0.1413	103.9	0.1177	163.0	0.1360
R48	(1,6)	0.1434	109.2	0.1413	103.8	0.1178	162.9	0.1360
R49	(1,7)	0.1432	109.6	0.1412	102.6	0.1151	168.5	0.1395
R50	(1,7)	0.1447	110.2	0.1412	103.9	0.1148	160.7	0.1389
R51	(1,7)	0.1432	109.4	0.1412	102.5	0.1146	168.8	0.1399
R52	(1,7)	0.1432	109.6	0.1411	102.2	0.1176	169.2	0.1368
R53	(1,7)	0.1432	109.7	0.1409	102.6	0.1194	172.0	0.1350
R54	(1,7)	0.1433	109.5	0.1412	102.3	0.1149	167.3	0.1397
R55	(1,7)	0.1432	109.6	0.1411	102.3	0.1176	170.3	0.1367
R56	(1,7)	0.1432	109.6	0.1411	102.3	0.1177	169.6	0.1368
R57	(1,7)	0.1432	109.6	0.1411	102.2	0.1177	169.4	0.1367
R58	(1,8)	0.1438	109.6	0.1409	103.0	0.1142	175.4	0.1416
R59	(1,8)	0.1439	109.9	0.1408	103.8	0.1164	175.6	0.1391
R60	(1,8)	0.1438	109.7	0.1409	103.2	0.1166	176.6	0.1390
R61	(1,8)	0.1439	109.9	0.1408	103.6	0.1166	175.3	0.1392
R62	(1,8)	0.1438	109.8	0.1409	103.4	0.1166	176.2	0.1391

表S3 反应势垒和反应焓变

Table S3 Reaction barriers, reaction enthalpy changes^a

Reaction	ΔV_p^{\ddagger}	$\Delta V_p^{\ddagger'}$	ΔH_p^{\ddagger}	$\Delta H_p^{\ddagger'}$	Reaction	ΔV_p^{\ddagger}	$\Delta V_p^{\ddagger'}$	ΔH_p^{\ddagger}	$\Delta H_p^{\ddagger'}$
R1	193.26	182.20	61.00	52.55	R32	91.85	86.96	63.39	52.84
R2	181.22	170.16	54.22	45.77	R33	75.91	71.03	47.61	37.07
R3	179.79	168.74	54.52	46.07	R34	91.83	86.94	63.39	52.84

R4	179.79	168.74	54.27	45.81	R35	91.65	86.76	63.26	52.72
R5	179.79	168.74	54.39	45.94	R36	91.73	86.84	63.18	52.63
R6	179.66	168.60	54.35	45.90	R37	98.54	95.85	78.83	68.24
R7	179.52	168.46	54.35	45.90	R38	84.21	81.51	66.44	55.86
R8	179.35	168.29	54.35	45.90	R39	94.35	91.65	78.20	67.61
R9	179.55	168.49	51.88	43.43	R40	84.27	81.57	63.55	52.97
R10	179.28	168.23	51.88	43.43	R41	97.36	94.67	87.24	76.65
R11	157.91	150.26	82.89	72.34	R42	73.41	70.72	52.55	41.97
R12	139.25	131.60	63.26	52.72	R43	94.59	91.90	81.42	70.84
R13	153.41	145.77	85.73	75.19	R44	83.94	81.24	63.26	52.68
R14	138.57	130.92	64.52	53.97	R45	75.07	72.37	51.38	40.79
R15	153.55	145.91	87.61	77.07	R46	83.83	81.13	63.26	52.68
R16	124.32	116.67	48.91	38.37	R47	83.50	80.81	63.14	52.55
R17	138.71	131.06	63.85	53.30	R48	83.64	80.94	63.18	52.59
R18	138.26	130.62	63.89	53.35	R49	101.60	98.90	79.71	69.12
R19	140.88	133.24	63.85	53.30	R50	94.05	91.36	81.17	70.58
R20	140.67	133.02	63.85	53.30	R51	99.96	97.27	82.76	72.17
R21	140.20	132.55	63.89	53.35	R52	92.87	90.18	63.09	52.51
R22	140.25	132.61	63.89	53.35	R53	76.93	74.23	52.17	41.59
R23	102.88	97.99	78.78	68.24	R54	101.90	99.20	82.22	71.63
R24	90.67	85.78	62.84	52.30	R55	88.36	85.66	62.84	52.26
R25	103.22	98.34	82.17	71.63	R56	92.85	90.15	62.80	52.22
R26	92.93	88.04	63.51	52.97	R57	92.44	89.74	62.68	52.09
R27	78.79	73.90	50.67	40.12	R58	122.77	120.07	89.20	78.62
R28	87.46	82.57	64.22	53.68	R59	111.08	108.38	74.06	63.47
R29	95.59	90.70	64.39	53.85	R60	114.48	111.78	62.97	52.38
R30	89.05	84.16	63.26	52.72	R61	114.39	111.70	62.72	52.13
R31	102.36	97.47	83.05	72.51	R62	114.12	111.43	62.63	52.05

Units of the ΔV_p^{\ddagger} , ΔH_p^{\ddagger} are kJ mol^{-1} .

表S4 分子内氢迁移的过渡态

Table S4 Transition States for intramolecular hydrogen migration in ROO radicals

Cartesian Coordinates (\AA)		
X	Y	Z
-0.944004	-0.270961	0.000000
-0.010662	0.745976	0.000000
1.076400	-0.300537	0.000000

0.094522	-1.111130	0.000000
-1.478190	-0.413310	0.939457
-1.478190	-0.413310	-0.939457

TS1

Cartesian Coordinates (Å)

X	Y	Z
-1.526450	-0.477554	-0.142134
-0.656038	0.743064	-0.164354
0.332519	0.032929	0.507505
1.623700	-0.162008	-0.226783
-0.500400	-1.002010	0.428706
0.358813	0.249514	1.579020
2.282220	-0.839052	0.321924
1.444600	-0.559482	-1.227750
2.137360	0.801429	-0.334322

TS2

Cartesian Coordinates (Å)

X	Y	Z
-1.00081	-0.441514	-0.354543
0.21206	-0.090903	0.460072
1.41114	-0.674869	0.070404
1.95691	0.687363	-0.239135
0.778963	1.06383	0.114751
0.109825	-0.005567	1.5467
-2.24294	0.36063	0.043265
-0.763206	-0.305591	-1.41381
-1.18608	-1.51695	-0.21958
-3.10872	0.043572	-0.541712
-2.48815	0.221086	1.1001

-2.09698 1.43039 -0.129358

TS3

Cartesian Coordinates (Å)

X	Y	Z
0.431699	0.427247	-0.149941
-0.869265	0.072175	0.511632
-2.010660	0.682728	0.005269
-2.531640	-0.663227	-0.402697
-1.404910	-1.064690	0.070573
-0.893639	-0.044573	1.599660
1.616430	-0.409580	0.348265
0.312921	0.332336	-1.234340
0.620448	1.494140	0.043399
1.693850	-0.319839	1.438040
1.423520	-1.467960	0.139879
2.942890	0.005917	-0.293337
3.768150	-0.608358	0.075023
2.907080	-0.102210	-1.381330
3.180470	1.050580	-0.071192

TS4

Cartesian Coordinates (Å)

X	Y	Z
0.224480	-0.558909	-0.126555
1.470820	-0.020096	0.515722
2.675420	-0.570823	0.093823
3.080730	0.767838	-0.447754
1.912300	1.110520	-0.032356
1.456460	0.207983	1.586130

-1.041600	0.213963	0.261177
0.363323	-0.566955	-1.212580
0.127355	-1.612590	0.175999
-1.136660	0.237909	1.354070
-0.942583	1.257570	-0.061381
-2.317250	-0.384347	-0.342638
-2.219280	-0.413935	-1.434250
-2.415580	-1.426860	-0.017107
-3.581430	0.391383	0.036766
-4.471940	-0.058927	-0.409202
-3.725640	0.408074	1.121450
-3.527050	1.429120	-0.306163

TS5

Cartesian Coordinates (Å)

X	Y	Z
-0.828299	0.544358	-0.020848
-2.114300	-0.034195	0.496431
-3.285870	0.596192	0.093424
-3.697030	-0.656672	-0.621084
-2.555220	-1.077820	-0.203656
-2.154360	-0.390634	1.530540
0.402593	-0.298565	0.333382
-0.913597	0.680410	-1.103920
-0.726229	1.553730	0.405657
0.447424	-0.441909	1.420210
0.295127	-1.298470	-0.104212
1.715350	0.328317	-0.148576
1.670250	0.472250	-1.235620

1. 820180	1. 330540	0. 286672
2. 953370	-0. 505578	0. 199657
2. 999590	-0. 646477	1. 286350
2. 846110	-1. 507780	-0. 232718
4. 260850	0. 123508	-0. 289566
4. 414620	1. 112610	0. 153298
5. 123280	-0. 495018	-0. 026949
4. 258670	0. 245341	-1. 377270

TS6

Cartesian Coordinates (Å)

X	Y	Z
-1. 477040	0. 569307	-0. 009106
-2. 730900	-0. 083327	0. 498959
-3. 933650	0. 501054	0. 119175
-4. 289120	-0. 750309	-0. 627212
-3. 126010	-1. 127470	-0. 227412
-2. 747470	-0. 468914	1. 523200
-0. 206033	-0. 225961	0. 312254
-1. 576870	0. 732851	-1. 087120
-1. 418310	1. 569400	0. 446498
-0. 148124	-0. 401734	1. 393650
-0. 269142	-1. 215160	-0. 156916
1. 073460	0. 477123	-0. 154713
1. 014660	0. 653718	-1. 236130
1. 132780	1. 468260	0. 312854
2. 349910	-0. 309652	0. 161707
2. 409120	-0. 484969	1. 243830
2. 289010	-1. 302030	-0. 303691

3.632080	0.388048	-0.306517
3.573090	0.562662	-1.387670
3.693470	1.379470	0.158445
4.902480	-0.404973	0.013190
5.797630	0.118509	-0.333535
5.008360	-0.565509	1.090780
4.886280	-1.388430	-0.467122

TS7

Cartesian Coordinates (Å)

X	Y	Z
-2.094200	0.563235	0.046134
-3.372140	-0.104911	0.466292
-4.553790	0.538511	0.116634
-4.915950	-0.630092	-0.751064
-3.771490	-1.069200	-0.360924
-3.419840	-0.581474	1.450490
-0.846948	-0.287898	0.312749
-2.168710	0.831301	-1.012800
-2.023600	1.513660	0.596567
-0.818929	-0.574850	1.371340
-0.916788	-1.222090	-0.257343
0.456355	0.432937	-0.049802
0.425727	0.724942	-1.107090
0.523266	1.367160	0.522187
1.710380	-0.409862	0.207315
1.738040	-0.704820	1.264300
1.643730	-1.342820	-0.367040
3.014980	0.311007	-0.150066

2.987110	0.608295	-1.206510
3.082790	1.243350	0.425545
4.271420	-0.529866	0.103186
4.298090	-0.830117	1.157830
4.206070	-1.459430	-0.475346
5.569700	0.200940	-0.251481
5.682020	1.116080	0.338177
6.445370	-0.425652	-0.061552
5.587790	0.484823	-1.308360

TS8

Cartesian Coordinates (Å)

X	Y	Z
-2.739420	0.554987	0.047528
-3.996770	-0.150964	0.467982
-5.197190	0.458859	0.122064
-5.527200	-0.717597	-0.747746
-4.369650	-1.124460	-0.360900
-4.028910	-0.631280	1.450990
-1.467810	-0.260979	0.308902
-2.823780	0.824265	-1.010330
-2.695100	1.505190	0.601058
-1.429910	-0.550977	1.366350
-1.512060	-1.194650	-0.264567
-0.186150	0.498023	-0.052866
-0.226251	0.792241	-1.109220
-0.145369	1.432030	0.521921
1.091730	-0.309260	0.200525
1.129050	-0.605973	1.256690

1. 050870	-1. 242290	-0. 376063
2. 374960	0. 449469	-0. 156727
2. 336430	0. 748110	-1. 212300
2. 415910	1. 381850	0. 421116
3. 654310	-0. 356478	0. 093548
3. 692160	-0. 658368	1. 148480
3. 615970	-1. 287630	-0. 486797
4. 938500	0. 403124	-0. 258689
4. 977520	1. 333000	0. 321684
4. 901460	0. 704477	-1. 312680
6. 211500	-0. 409577	-0. 005544
6. 218080	-1. 329820	-0. 598352
7. 107850	0. 159497	-0. 267336
6. 295790	-0. 695377	1. 047770

TS9

Cartesian Coordinates (Å)

X	Y	Z
3. 363580	0. 555995	-0. 094666
4. 637850	-0. 166965	-0. 425581
5. 823060	0. 496596	-0. 129202
6. 160650	-0. 578999	0. 860106
5. 015570	-1. 043970	0. 502548
4. 691780	-0. 744312	-1. 353910
2. 108000	-0. 300926	-0. 295215
3. 426560	0. 927481	0. 933350
3. 315040	1. 447680	-0. 737888
2. 087190	-0. 684631	-1. 322850
2. 159700	-1. 178990	0. 359806

0.811004	0.466523	-0.015613
0.832497	0.849541	1.012440
0.765235	1.348070	-0.667779
-0.452381	-0.377669	-0.215822
-0.473585	-0.759366	-1.244780
-0.404989	-1.260370	0.434872
-1.749710	0.388625	0.066047
-1.727260	0.771044	1.094680
-1.796480	1.271420	-0.584701
-3.015550	-0.452712	-0.132323
-3.037370	-0.836571	-1.160570
-2.969720	-1.334720	0.519657
-4.312370	0.314858	0.147394
-4.358900	1.196950	-0.504692
-4.291390	0.699349	1.175550
-5.579890	-0.524241	-0.050182
-5.535740	-1.403870	0.603659
-5.600340	-0.910264	-1.076700
-6.870060	0.252717	0.227615
-6.961170	1.118310	-0.436270
-7.754030	-0.373684	0.078922
-6.895160	0.622896	1.257490

TS10

Cartesian Coordinates (Å)

X	Y	Z
-1.222550	-0.568778	-0.119138
-0.543279	0.755986	0.210484
0.792901	0.599305	-0.288632
1.141600	-0.701499	0.160721

0.022475	-1.142550	0.058118
-1.938460	-0.972919	0.591417
-1.472890	-0.741086	-1.164370
-0.530337	0.924621	1.292260
-0.961851	1.626240	-0.302214

TS11

Cartesian Coordinates (Å)

X	Y	Z
-0.781108	0.070136	0.619964
0.316555	1.026080	0.137614
1.205450	0.195956	-0.619058
1.345750	-0.949163	0.210346
0.195160	-0.879649	0.644677
-1.116100	0.215653	1.646680
0.840075	1.471210	0.990045
-0.029738	1.807700	-0.545351
-1.850550	-0.321710	-0.360542
-1.421200	-0.581773	-1.331320
-2.438860	-1.167890	0.002442
-2.548350	0.513358	-0.519692

TS12

Cartesian Coordinates (Å)

X	Y	Z
-0.111654	1.381420	-0.116678
0.419698	0.034621	0.376530
-0.507834	-0.917230	-0.186517
-1.773380	-0.310417	0.034145
-1.366270	0.818125	-0.082471
-0.052764	2.234940	0.553974

0.073458	1.614580	-1.164920
0.342370	-0.002967	1.469860
1.816530	-0.340342	-0.087055
2.546210	0.362464	0.323445
2.077860	-1.343240	0.259438
1.881340	-0.316953	-1.177140

TS13

Cartesian Coordinates (Å)

X	Y	Z
-0.216865	-0.250337	0.388759
1.051900	-0.961434	-0.086111
2.105900	-0.039007	0.205040
1.574190	1.198260	-0.253399
0.415908	0.908182	0.057047
-0.302154	-0.176264	1.475860
0.997226	-1.156190	-1.163990
1.290700	-1.883880	0.451317
-1.512060	-0.464379	-0.340111
-1.831190	-1.508850	-0.190178
-1.346110	-0.361021	-1.418980
-2.637540	0.471294	0.116774
-3.561560	0.265912	-0.428734
-2.844300	0.349473	1.183850
-2.371810	1.517790	-0.055187

TS14

Cartesian Coordinates (Å)

X	Y	Z
0.245433	-0.489963	1.357270
-0.377053	0.008699	0.043061

0.643895	-0.350727	-0.936072
1.869350	-0.007213	-0.301726
1.479870	-0.246206	0.811124
0.094460	0.103107	2.255820
0.225105	-1.566720	1.519470
-0.593339	1.522790	0.059864
-0.954039	1.859020	-0.914567
-1.333010	1.798420	0.816708
0.340986	2.041480	0.280705
-1.629190	-0.757188	-0.368795
-2.434090	-0.574866	0.347948
-1.970270	-0.427226	-1.353680
-1.430050	-1.829520	-0.409544

TS15

Cartesian Coordinates (Å)

X	Y	Z
-0.632749	-0.006491	-0.035054
0.498221	-0.296548	0.970980
1.677280	0.197525	0.335287
1.551220	-0.302301	-0.990161
0.302612	-0.199730	-0.986302
0.581390	-1.374700	1.148710
0.408132	0.238907	1.921620
-1.729040	-1.032950	-0.141712
-2.376140	-1.005340	0.747544
-2.369800	-0.839589	-1.006290
-1.328950	-2.046890	-0.223340
-1.056660	1.440050	-0.121300
-1.654730	1.627870	-1.016850

-1.677180	1.706320	0.746938
-0.191904	2.106960	-0.130526

TS16

Cartesian Coordinates (Å)

X	Y	Z
-0.453448	-0.526977	0.650511
-1.766120	-0.942046	-0.023042
-2.192650	0.229961	-0.728756
-1.984940	1.263370	0.224412
-0.998556	0.719789	0.724838
-0.314222	-0.876333	1.674440
-2.509750	-1.229090	0.727672
-1.662600	-1.730950	-0.774160
0.792735	-0.490427	-0.191384
0.560934	-0.039401	-1.163340
1.091770	-1.530660	-0.405871
1.972030	0.241486	0.463576
2.183530	-0.213184	1.438690
1.680150	1.278300	0.663750
3.237510	0.221931	-0.397733
4.056510	0.756248	0.090650
3.574100	-0.802457	-0.585882
3.062610	0.697314	-1.367600

TS17

Cartesian Coordinates (Å)

X	Y	Z
-1.056300	-0.511077	0.677221
-2.422350	-0.839236	0.064563

-2.752430	0.317379	-0.714520
-2.416680	1.389040	0.156423
-1.474020	0.785668	0.672918
-0.921944	-0.799626	1.720510
-3.168730	-0.998240	0.849857
-2.417690	-1.684750	-0.629953
0.161953	-0.658732	-0.193076
-0.055198	-0.259542	-1.190640
0.352671	-1.736120	-0.334826
1.424190	0.000486	0.378467
1.621220	-0.399233	1.381460
1.240070	1.073890	0.506091
2.663370	-0.201103	-0.500785
2.845190	-1.275310	-0.628345
2.461760	0.195081	-1.503040
3.919020	0.465090	0.068590
4.165740	0.065424	1.057240
4.784160	0.303333	-0.580003
3.780360	1.545550	0.173634

TS18

Cartesian Coordinates (Å)

X	Y	Z
1.694010	-0.019094	0.850047
2.415500	1.024560	-0.013145
3.135810	0.252123	-0.980763
3.709130	-0.782780	-0.193032
2.757210	-0.825873	0.591025
1.692160	0.180138	1.922450

3.106780	1.614800	0.597446
1.755740	1.686790	-0.581263
0.435883	-0.650377	0.314763
0.571827	-0.893043	-0.744569
0.253875	-1.595410	0.839000
-0.809408	0.250579	0.480813
-0.640553	1.206750	-0.028675
-0.945563	0.486330	1.543200
-2.086190	-0.396317	-0.068443
-2.257510	-1.351470	0.444215
-1.940600	-0.641087	-1.128080
-3.329550	0.488281	0.080773
-3.157480	1.441940	-0.432816
-3.472930	0.734328	1.139920
-4.601940	-0.163816	-0.468097
-4.820720	-1.102860	0.049938
-5.469040	0.491232	-0.347414
-4.502540	-0.390164	-1.534270

TS19

Cartesian Coordinates (Å)

X	Y	Z
2.299490	-0.106748	0.831651
2.970760	1.067010	0.106353
3.717430	0.454357	-0.951511
4.338050	-0.646876	-0.301650
3.393190	-0.828972	0.471190
2.297990	-0.045825	1.920720
3.640080	1.604540	0.786160
2.280130	1.766560	-0.373527

1.063790	-0.716920	0.224413
1.195030	-0.805649	-0.859342
0.932672	-1.732650	0.614679
-0.218648	0.092142	0.524964
-0.101247	1.117970	0.155993
-0.350712	0.167680	1.611100
-1.471970	-0.530472	-0.101688
-1.584490	-1.559360	0.262840
-1.333450	-0.605070	-1.187500
-2.754100	0.255765	0.194027
-2.639990	1.286120	-0.167249
-2.893120	0.328450	1.280580
-4.009170	-0.361399	-0.434212
-4.123270	-1.391080	-0.074217
-3.870590	-0.432740	-1.519790
-5.286290	0.428479	-0.133937
-6.161230	-0.036915	-0.596015
-5.471630	0.486992	0.943296
-5.216400	1.452970	-0.513043

TS20

Cartesian Coordinates (Å)

X	Y	Z
0.131305	0.446356	0.000040
0.139465	1.105700	0.877097
0.139430	1.105870	-0.876889
1.403620	-0.409050	-0.000070
1.396060	-1.067780	0.877304
1.396010	-1.067620	-0.877561
2.689660	0.428549	-0.000030

2.709810	1.080260	0.879774
2.709770	1.080400	-0.879729
3.931890	-0.442600	-0.000133
4.006450	-1.070440	-0.891202
4.006530	-1.070540	0.890852
5.097360	0.442939	-0.000140
6.230200	-0.228931	-0.000011
-1.158690	-0.381554	-0.000016
-1.164980	-1.041740	0.876865
-1.165020	-1.041570	-0.877029
-2.433110	0.470414	0.000097
-2.426700	1.130600	0.877021
-2.426730	1.130780	-0.876687
-3.723620	-0.356862	0.000030
-3.730490	-1.017660	0.876788
-3.730530	-1.017460	-0.876875
-4.999570	0.492590	0.000150
-4.993440	1.152330	-0.876071
-4.993410	1.152120	0.876526
-6.282980	-0.342997	0.000074
-6.335000	-0.988174	0.883106
-7.173700	0.291735	0.000171
-6.335040	-0.987955	-0.883117

TS21

Cartesian Coordinates (Å)

X	Y	Z
3.544650	-0.017056	0.803320
4.173800	1.100700	-0.038907
4.893960	0.411599	-1.067720

5. 551920	-0. 624698	-0. 351139
4. 635660	-0. 753765	0. 465583
3. 579110	0. 133640	1. 883090
4. 857060	1. 701380	0. 570564
3. 456710	1. 749050	-0. 550821
2. 297860	-0. 689240	0. 291927
2. 391360	-0. 860903	-0. 785734
2. 197020	-1. 672910	0. 764774
1. 014620	0. 124128	0. 576778
1. 101640	1. 119160	0. 124304
0. 922196	0. 283466	1. 657960
-0. 251161	-0. 562183	0. 049665
-0. 330743	-1. 562510	0. 493724
-0. 154811	-0. 715729	-1. 032390
-1. 534170	0. 225179	0. 339448
-1. 451430	1. 227590	-0. 100122
-1. 629910	0. 375203	1. 422590
-2. 801670	-0. 455233	-0. 190553
-2. 882190	-1. 459500	0. 245278
-2. 707200	-0. 601582	-1. 274290
-4. 086280	0. 327366	0. 103487
-4. 182240	0. 472381	1. 187570
-4. 005900	1. 332660	-0. 330575
-5. 354580	-0. 350128	-0. 427915
-5. 259310	-0. 494269	-1. 511060
-5. 435390	-1. 354380	0. 005723
-6. 632890	0. 438535	-0. 129302
-6. 597600	1. 434950	-0. 581237
-7. 517830	-0. 071476	-0. 519970

-6.774240	0.569924	0.948249
TS22		
Cartesian Coordinates (Å)		
X	Y	Z
1.343780	-0.857750	0.021713
1.140130	0.624985	-0.156732
-0.270521	1.060490	0.307009
-1.238220	0.268164	-0.368939
-1.135400	-1.049570	0.133709
0.001490	-1.253740	0.005783
1.872670	1.198570	0.427021
1.257290	0.905682	-1.205770
-0.390415	0.943548	1.388940
-0.487654	2.090780	0.016993
1.812120	-1.401610	-0.794583
1.643130	-1.198300	1.011520

TS23		
Cartesian Coordinates (Å)		
X	Y	Z
1.066150	0.033400	0.476857
0.205693	1.173880	-0.026374
-1.298100	0.862816	0.118774
-1.573830	-0.376481	-0.524866
-0.960790	-1.396170	0.242401
0.141278	-0.970537	0.344146
0.417645	2.099170	0.527175
0.416958	1.365930	-1.082470
-1.598570	0.803962	1.170250
-1.913850	1.600330	-0.400905

2. 310370	-0. 321994	-0. 296411
1. 183380	0. 010388	1. 562690
2. 789080	-1. 220570	0. 099555
2. 088180	-0. 487999	-1. 354490
3. 048180	0. 491951	-0. 243296

TS24

Cartesian Coordinates (Å)

X	Y	Z
-0. 350137	1. 422220	-0. 071234
-0. 815491	0. 019099	-0. 381545
0. 204657	-1. 015200	0. 165222
1. 503000	-0. 708936	-0. 321025
1. 923790	0. 486340	0. 308173
1. 016520	1. 176650	0. 097442
-0. 836008	-0. 112461	-1. 467800
0. 211016	-1. 020780	1. 261150
-0. 012362	-2. 018410	-0. 209669
-0. 406244	2. 158430	-0. 869640
-0. 611105	1. 813590	0. 912121
-2. 216110	-0. 282920	0. 186051
-2. 958760	0. 401349	-0. 229803
-2. 525230	-1. 304210	-0. 056415
-2. 229650	-0. 172594	1. 274450

TS25

Cartesian Coordinates (Å)

X	Y	Z
0. 538347	-0. 162137	0. 505844
-0. 151882	1. 089600	0. 004161
-1. 686820	0. 976788	0. 116445

-2.111400	-0.206291	-0.550185
-1.655410	-1.307940	0.213279
-0.509624	-1.032640	0.342339
0.163405	1.973940	0.574448
0.103506	1.264570	-1.045380
-2.012540	0.945325	1.161550
-2.189200	1.795980	-0.402986
1.739670	-0.685485	-0.247135
0.633264	-0.211238	1.594100
1.977180	-1.695980	0.100588
1.494180	-0.768278	-1.311740
2.986800	0.206283	-0.079812
3.834930	-0.212044	-0.628819
2.808490	1.216550	-0.458329
3.274210	0.287412	0.972470

TS26

Cartesian Coordinates (Å)

X	Y	Z
0.908060	0.014524	-0.028767
-0.053426	1.013480	-0.663037
-1.482750	0.882411	-0.097867
-1.907680	-0.469947	-0.226551
-1.132760	-1.239940	0.672900
-0.022063	-0.878250	0.373741
0.291235	2.042760	-0.492042
-0.101591	0.856292	-1.743740
-1.534020	1.181770	0.954117
-2.198970	1.466410	-0.680267
1.822820	-0.717486	-0.987376

2.388490	-1.503880	-0.480929
1.263560	-1.170480	-1.809870
2.552410	-0.022107	-1.428880
1.553850	0.464357	1.266580
2.055170	-0.363997	1.774090
2.312940	1.234250	1.066450
0.824960	0.892602	1.959360

TS27

Cartesian Coordinates (Å)

X	Y	Z
-2.640860	-0.425437	-0.407209
-1.432910	-0.222296	0.471564
-0.176453	-1.007630	0.161200
1.110320	-0.161903	0.324165
1.228610	0.138118	1.371990
0.946124	1.028090	-0.458169
-0.050753	1.821860	0.153776
-0.925965	1.033880	0.263928
-0.092270	-1.880160	0.823560
-0.207895	-1.377340	-0.868967
2.362690	-0.852609	-0.188928
-1.655990	-0.141089	1.537770
-3.446290	0.267922	-0.153882
-2.391190	-0.291760	-1.463750
-3.039500	-1.444340	-0.294186
3.235200	-0.209750	-0.059334
2.531560	-1.780480	0.363167
2.263980	-1.095380	-1.249900

TS28

Cartesian Coordinates (Å)

X	Y	Z
-0.123387	-0.175357	-0.348770
0.580406	1.060060	0.174141
2.092370	1.026820	-0.133833
2.637530	-0.187369	0.369190
2.127430	-1.240990	-0.426618
0.963407	-1.007070	-0.389578
0.165985	1.974140	-0.272830
0.452751	1.135930	1.258150
2.285770	1.097250	-1.209470
2.627340	1.821660	0.390883
-1.192890	-0.819684	0.503280
-0.342618	-0.141325	-1.418280
-1.455690	-1.797060	0.083127
-0.787065	-1.005860	1.504110
-2.486530	0.019706	0.646370
-3.135180	-0.486922	1.369390
-2.240280	0.992236	1.087560
-3.251890	0.224234	-0.663899
-3.515260	-0.735112	-1.120660
-4.180530	0.775050	-0.491833
-2.666810	0.789332	-1.394880

TS29

Cartesian Coordinates (Å)

X	Y	Z
-0.257212	-0.145048	0.481269
0.694507	-1.245080	0.059176
2.167960	-0.798526	0.169329

2.339850	0.410485	-0.560794
1.647210	1.427940	0.139910
0.587173	0.919827	0.280776
0.567152	-2.141490	0.680969
0.501290	-1.532080	-0.978768
2.464750	-0.641887	1.211750
2.841450	-1.517660	-0.302511
-1.529430	0.078014	-0.312068
-0.388846	-0.058727	1.564310
-1.257390	0.118242	-1.374780
-2.504280	-1.105680	-0.123661
-3.405480	-0.957043	-0.725920
-2.052990	-2.054670	-0.424594
-2.810630	-1.193150	0.923848
-2.205050	1.404150	0.063809
-3.116380	1.557000	-0.520895
-2.484040	1.413640	1.122900
-1.541560	2.253610	-0.117133

TS30

Cartesian Coordinates (Å)

X	Y	Z
0.154535	1.390250	0.467525
0.707782	0.049769	0.024500
-0.384800	-0.672754	-0.825781
-1.591120	-0.778520	-0.085753
-2.136610	0.522336	0.032819
-1.212630	1.113680	0.414164
-0.572565	-0.133888	-1.760600
-0.090923	-1.703190	-1.042280

0.344600	1.693980	1.494950
0.214691	2.205150	-0.253211
1.948780	0.239597	-0.876823
2.754240	0.726568	-0.321485
2.321340	-0.726916	-1.231360
1.718780	0.857456	-1.749300
1.057060	-0.818589	1.245780
1.448970	-1.791860	0.935520
1.819390	-0.329738	1.858710
0.175875	-0.991377	1.867130

TS31

Cartesian Coordinates (Å)

X	Y	Z
-0.621369	-0.145986	0.623294
-1.236420	1.101650	0.022551
-2.777360	1.020620	-0.007564
-3.163270	-0.177544	-0.670987
-2.803590	-1.259430	0.168553
-1.666900	-1.000860	0.392050
-0.957450	1.997660	0.593608
-0.880503	1.239550	-1.002940
-3.201180	1.032770	1.002170
-3.210610	1.829870	-0.599816
0.629983	-0.717272	-0.000339
-0.626746	-0.161521	1.716530
0.804777	-1.727070	0.387399
0.486728	-0.816049	-1.082930
1.888230	0.137596	0.267345
1.732800	1.149960	-0.124856

2.026310	0.244589	1.350530
3.158320	-0.457466	-0.351895
3.307870	-1.471210	0.038420
3.014980	-0.565705	-1.433590
4.409500	0.383719	-0.083100
4.598570	0.480735	0.990606
5.296470	-0.067250	-0.536441
4.304450	1.393180	-0.493024

TS32

Cartesian Coordinates (Å)

X	Y	Z
0.299295	-0.041545	0.142640
-0.735725	-0.766100	0.998717
-2.122480	-0.812969	0.320557
-2.498640	0.503494	-0.065888
-1.643170	0.887183	-1.126050
-0.567213	0.635158	-0.636876
-0.424307	-1.799250	1.201460
-0.847556	-0.263048	1.962940
-2.121810	-1.463480	-0.560196
-2.896660	-1.141700	1.017800
1.094300	1.032820	0.871953
0.391931	1.646720	1.445740
1.738590	0.545990	1.621460
1.948740	1.941690	-0.017894
1.335030	2.437400	-0.775324
2.430220	2.718720	0.581221
2.738880	1.390130	-0.533727
1.047280	-0.916979	-0.855604

1. 479760	-0. 294049	-1. 644630
0. 330634	-1. 578270	-1. 354020
2. 165960	-1. 768670	-0. 224671
2. 633370	-2. 404150	-0. 981521
2. 948400	-1. 143500	0. 212958
1. 781000	-2. 421540	0. 564003

TS33

Cartesian Coordinates (Å)

X	Y	Z
-1. 226270	-0. 118138	0. 652353
-1. 834860	1. 099800	-0. 012642
-3. 371240	0. 990108	-0. 108030
-3. 707160	-0. 234163	-0. 750642
-3. 367400	-1. 283760	0. 136849
-2. 246100	-0. 998338	0. 402119
-1. 596490	2. 017300	0. 542452
-1. 435820	1. 213450	-1. 025180
-3. 839790	1. 024730	0. 881232
-3. 791210	1. 773290	-0. 743355
0. 060866	-0. 684692	0. 101537
-1. 279500	-0. 100866	1. 744300
0. 236603	-1. 678330	0. 528504
-0. 033350	-0. 819760	-0. 982484
1. 290690	0. 202662	0. 395842
1. 133090	1. 198560	-0. 035413
1. 377590	0. 346385	1. 479980
2. 596910	-0. 386984	-0. 147827
2. 749110	-1. 385930	0. 280749
2. 505650	-0. 532225	-1. 231920

3.827120	0.480294	0.143951
3.916890	0.626191	1.227290
3.675550	1.478000	-0.285728
5.128480	-0.116579	-0.399865
5.985660	0.524283	-0.175811
5.325730	-1.100170	0.037934
5.082650	-0.242030	-1.486240

TS34

Cartesian Coordinates (Å)

X	Y	Z
-1.820790	-0.129206	0.652383
-2.379450	1.119280	0.000129
-3.918570	1.068910	-0.103347
-4.297810	-0.134077	-0.761656
-4.002890	-1.205850	0.115326
-2.872820	-0.966003	0.388937
-2.109580	2.020010	0.568036
-1.971410	1.230540	-1.009090
-4.389950	1.109810	0.884308
-4.305500	1.874870	-0.731115
-0.556031	-0.740634	0.097859
-1.876690	-0.122670	1.744310
-0.422993	-1.746620	0.511318
-0.651876	-0.856714	-0.988249
0.708571	0.090552	0.408054
0.593322	1.098870	-0.007387
0.799235	0.213176	1.494450
1.990370	-0.544008	-0.143702
2.098530	-1.555680	0.267727

1. 894520	-0. 666218	-1. 230110
3. 254370	0. 266165	0. 165527
3. 350840	0. 387099	1. 252430
3. 145840	1. 279050	-0. 243991
4. 537670	-0. 365033	-0. 386837
4. 646580	-1. 376770	0. 022410
4. 441400	-0. 485681	-1. 472710
5. 795970	0. 449848	-0. 074086
6. 692090	-0. 027668	-0. 479900
5. 732970	1. 455310	-0. 502322
5. 938420	0. 559396	1. 005720

TS35

Cartesian Coordinates (Å)

X	Y	Z
-2. 434050	-0. 112409	0. 647618
-2. 989340	1. 109970	-0. 054783
-4. 525220	1. 041340	-0. 188949
-4. 878900	-0. 183692	-0. 820388
-4. 592360	-1. 227240	0. 092669
-3. 470750	-0. 967917	0. 383933
-2. 739660	2. 030440	0. 490293
-2. 560740	1. 193520	-1. 058140
-5. 017480	1. 105340	0. 787234
-4. 906580	1. 825150	-0. 847413
-1. 149160	-0. 725493	0. 143480
-2. 517420	-0. 074200	1. 737180
-1. 017480	-1. 718640	0. 587340
-1. 214700	-0. 871689	-0. 941230
0. 098521	0. 126687	0. 465086

-0.016944	1.123780	0.023361
0.160393	0.275560	1.550230
1.400380	-0.505980	-0.039736
1.506140	-1.509070	0.392744
1.335420	-0.648505	-1.125920
2.648300	0.321468	0.289524
2.715090	0.458016	1.376670
2.539040	1.327220	-0.136714
3.950600	-0.304424	-0.222055
4.059250	-1.311870	0.200527
3.885730	-0.437790	-1.309850
5.200510	0.518483	0.110469
5.091150	1.525770	-0.309856
5.267520	0.648986	1.197490
6.496040	-0.112130	-0.408226
7.367300	0.498352	-0.155094
6.651650	-1.106870	0.021399
6.473630	-0.223162	-1.496990

TS36

Cartesian Coordinates (Å)

X	Y	Z
1.519370	0.317808	0.309117
0.453864	1.306570	-0.205862
-0.989876	0.996165	0.192246
-1.499290	-0.210287	-0.394463
-1.019510	-1.321930	0.335412
0.085072	-1.408340	0.023377
0.686626	2.306250	0.179077
0.508897	1.371130	-1.298590

-1.109620	0.932343	1.279060
-1.660320	1.769910	-0.192571
2.514500	0.720022	0.068352
1.473980	0.264400	1.402910
1.398910	-1.070350	-0.269819
1.976940	-1.855730	0.214205
1.380710	-1.143420	-1.357500

TS37

Cartesian Coordinates (Å)

X	Y	Z
1.287240	0.023370	-0.413418
0.599241	1.204830	0.237235
-0.873140	1.391200	-0.177988
-1.834440	0.286856	0.265406
-1.584730	-0.976593	-0.365584
-0.492615	-1.606530	0.271533
0.440727	-0.993146	-0.097902
-1.243140	2.330960	0.248696
-0.939856	1.495800	-1.266930
-1.817730	0.143727	1.351280
-2.854880	0.530687	-0.043990
1.154730	2.121130	-0.014151
0.663578	1.104980	1.328010
2.651560	-0.359654	0.097999
1.185270	-0.002085	-1.501880
3.021820	-1.271580	-0.376131
3.379890	0.437713	-0.111373
2.645650	-0.512806	1.181370

TS38

Cartesian Coordinates (Å)

X	Y	Z
1.114940	0.063685	-0.314346
0.282535	-1.129270	0.205748
-1.193690	-1.160640	-0.195275
-1.972120	-0.110071	0.392155
-1.761280	1.084970	-0.333713
-0.706056	1.409060	-0.029027
0.733281	-2.056000	-0.170591
0.350655	-1.171710	1.299630
-1.322050	-1.124580	-1.282310
-1.664400	-2.071390	0.186049
0.992874	0.112171	-1.404120
0.656251	1.382950	0.266112
1.033570	2.284080	-0.215932
0.625604	1.447430	1.354840
2.613930	-0.154917	-0.022406
2.967490	-1.077380	-0.493988
3.217310	0.672435	-0.405012
2.795150	-0.234048	1.053940

TS38

Cartesian Coordinates (Å)

X	Y	Z
0.221889	1.435670	-0.226106
1.652780	1.190200	0.290686
2.316640	-0.106456	-0.176071
1.692000	-1.288390	0.342503
0.521735	-1.559850	-0.401279
-0.239934	-0.739271	-0.038937

2. 293020	2. 016630	-0. 039860
1. 658560	1. 210290	1. 386450
2. 346600	-0. 178519	-1. 268690
3. 338130	-0. 165897	0. 210661
-0. 083961	2. 454050	0. 057245
0. 219378	1. 415450	-1. 322960
-0. 806635	0. 454131	0. 295134
-0. 804369	0. 348180	1. 384740
-2. 182110	0. 474960	-0. 325183
-2. 617750	1. 475070	-0. 165223
-2. 093360	0. 366612	-1. 412920
-3. 134220	-0. 587793	0. 232933
-4. 119600	-0. 516325	-0. 234337
-2. 749420	-1. 595120	0. 053260
-3. 267260	-0. 469508	1. 312440

TS40

Cartesian Coordinates (Å)

X	Y	Z
1. 505300	-1. 376800	-0. 266038
0. 088956	-1. 088140	0. 274086
-0. 556749	0. 229052	-0. 174562
0. 169748	1. 373200	0. 336445
1. 316700	1. 610810	-0. 451612
2. 058340	0. 803372	-0. 114321
-0. 564722	-1. 906000	-0. 045191
0. 102078	-1. 105430	1. 370790
-0. 545791	0. 307271	-1. 268670
1. 776160	-2. 406250	0. 012815
1. 491470	-1. 359280	-1. 361850

2.571190	-0.438487	0.239841
3.535140	-0.472925	-0.265079
2.643050	-0.319553	1.321100
-1.984260	0.419801	0.346065
-2.275510	1.449020	0.117777
-1.981070	0.330502	1.437940
-3.006800	-0.547964	-0.259347
-2.811070	-1.586580	0.018785
-4.013110	-0.302741	0.089072
-3.012290	-0.488249	-1.352090

TS41

Cartesian Coordinates (Å)

X	Y	Z
-1.156960	0.021753	0.008103
-0.357026	1.206890	-0.526074
1.054900	1.395490	0.064692
2.052670	0.272488	-0.222822
1.698110	-0.973780	0.394003
0.711536	-1.613210	-0.386220
-0.277227	-0.971779	-0.179298
1.479160	2.317440	-0.350562
0.999430	1.546120	1.147300
2.180710	0.103745	-1.297310
3.025420	0.512292	0.216292
-0.936243	2.125610	-0.345235
-0.274748	1.111100	-1.614820
-2.348880	-0.358233	-0.844493
-1.412320	0.005943	1.500980
-2.815720	-1.282120	-0.493381

-3.114020	0.431558	-0.803856
-2.071060	-0.489039	-1.893760
-1.940800	-0.902040	1.801120
-0.488589	0.062557	2.080200
-2.037740	0.864443	1.788730

TS42

Cartesian Coordinates (Å)

X	Y	Z
0.472533	-1.284110	-0.689884
1.010860	-0.035524	-0.013889
0.082872	1.182900	-0.288256
-1.352840	1.140530	0.240727
-2.167220	0.145115	-0.392878
-1.878600	-1.117260	0.176494
-0.846970	-1.377170	-0.249574
0.556410	2.072240	0.146818
0.038288	1.354200	-1.370070
-1.401960	0.996418	1.323920
-1.858330	2.078420	-0.007335
0.303656	-1.215570	-1.765100
2.396970	0.280390	-0.627613
3.090120	-0.552869	-0.481986
2.320950	0.474857	-1.701150
2.830630	1.167060	-0.152335
1.178720	-0.278097	1.498270
1.899740	-1.081020	1.678560
1.551610	0.621364	1.997730
0.237266	-0.566184	1.969830
0.910477	-2.231070	-0.374352

TS43

Cartesian Coordinates (Å)

X	Y	Z
0.813310	1.448290	-0.225954
2.250710	1.126580	0.229074
2.815530	-0.214007	-0.243892
2.149470	-1.349100	0.325419
0.931477	-1.563740	-0.357681
0.238459	-0.690999	0.021095
2.921410	1.908650	-0.146031
2.309480	1.163610	1.322840
2.789050	-0.305063	-1.335180
3.849200	-0.326705	0.095808
0.580524	2.486530	0.054703
0.759165	1.414140	-1.321140
-0.245625	0.535693	0.356203
-0.202908	0.448501	1.446560
-1.642010	0.622982	-0.208237
-2.020200	1.646670	-0.044841
-1.605380	0.496904	-1.298100
-2.633000	-0.379454	0.397858
-2.259930	-1.396240	0.234682
-2.667600	-0.236771	1.484350
-4.044080	-0.249764	-0.181580
-4.045140	-0.421086	-1.262590
-4.725900	-0.975787	0.269034
-4.456830	0.748484	-0.003929

TS44

Cartesian Coordinates (Å)

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X	Y	Z
0.060537	0.664393	1.138890
-1.476460	0.784017	1.074680
-2.215220	-0.429990	0.509571
-1.934330	-0.671394	-0.876927
-0.699519	-1.346540	-0.989894
0.112813	-0.503707	-0.739157
-1.849050	0.940993	2.093990
-1.769890	1.669930	0.503401
-1.994010	-1.342960	1.072490
-3.294940	-0.255237	0.529016
0.457644	1.552470	1.655030
0.313887	-0.191315	1.771520
0.778483	0.531707	-0.201640
2.230420	0.075932	-0.135350
2.612350	-0.002478	-1.158940
2.815670	0.882897	0.336630
2.503060	-1.241180	0.602409
3.560360	-1.506430	0.521659
2.265430	-1.176990	1.666930
1.918680	-2.061210	0.176822
0.533795	1.658450	-1.185370
0.918729	2.607090	-0.782125
1.043180	1.471780	-2.133680
-0.527757	1.798660	-1.398220

TS45

Cartesian Coordinates (Å)

X	Y	Z
-1.484750	-1.449490	-0.169238

-2.865690	-0.965697	0.314102
-3.309590	0.404603	-0.200837
-2.514890	1.488780	0.298147
-1.304540	1.550820	-0.428476
-0.688949	0.629228	-0.031429
-3.623920	-1.690400	-0.005443
-2.890140	-0.951321	1.409690
-3.311050	0.447769	-1.295410
-4.314790	0.634955	0.163875
-1.347600	-2.493960	0.148652
-1.464660	-1.464060	-1.266040
-0.320580	-0.626547	0.341684
-0.317127	-0.491969	1.427980
1.039820	-0.880103	-0.259872
1.313920	-1.931720	-0.068583
0.978967	-0.789536	-1.352130
2.148970	0.032891	0.277896
2.210400	-0.077969	1.367970
1.877190	1.078720	0.092349
3.522620	-0.252726	-0.338675
3.791520	-1.300410	-0.155092
3.458340	-0.141575	-1.427910
4.627130	0.659612	0.202234
4.741080	0.544108	1.284750
5.592530	0.433827	-0.258917
4.402160	1.712230	0.004555

TS46

Cartesian Coordinates (Å)

X	Y	Z
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-2.061640	-1.436530	-0.196072
-3.445550	-0.937437	0.262151
-3.856550	0.446047	-0.244922
-3.055520	1.511150	0.284143
-1.828920	1.562160	-0.415632
-1.236250	0.626788	-0.015622
-4.207440	-1.646100	-0.083609
-3.494560	-0.936470	1.357020
-3.834060	0.502475	-1.338680
-4.865510	0.688276	0.101279
-1.947840	-2.487050	0.111011
-2.016550	-1.437310	-1.292230
-0.896965	-0.638748	0.352186
-0.918150	-0.515756	1.439690
0.473439	-0.909665	-0.218075
0.723609	-1.968160	-0.032132
0.442382	-0.805928	-1.310360
1.584760	-0.023267	0.358760
1.609800	-0.142412	1.449270
1.339720	1.028790	0.172026
2.969480	-0.335029	-0.218418
3.212040	-1.390100	-0.034235
2.942630	-0.215904	-1.309420
4.084840	0.545615	0.356332
4.112310	0.426770	1.446380
3.842330	1.599100	0.172193
5.465400	0.229964	-0.226229
5.478930	0.372740	-1.311270
6.236750	0.875475	0.202547

5.752100	-0.807330	-0.026227
TS47		
Cartesian Coordinates (Å)		
X	Y	Z
-2.698840	-1.398650	-0.138726
-4.044700	-0.813017	0.331064
-4.393990	0.573884	-0.212090
-3.523370	1.610380	0.261263
-2.314820	1.572180	-0.469755
-1.761920	0.620628	-0.050707
-4.849940	-1.490920	0.024052
-4.069380	-0.775215	1.426110
-4.396780	0.593876	-1.307340
-5.379270	0.881887	0.149791
-2.633120	-2.443590	0.200049
-2.678190	-1.436490	-1.234900
-1.482620	-0.646276	0.359161
-1.477860	-0.480835	1.441190
-0.138849	-1.013480	-0.220074
0.061950	-2.072380	0.016603
-0.185501	-0.964019	-1.315520
1.025960	-0.156267	0.291881
1.053460	-0.204731	1.387690
0.839826	0.893550	0.037250
2.386040	-0.585633	-0.268975
2.570380	-1.636130	-0.008193
2.354360	-0.545934	-1.365480
3.553110	0.271494	0.233251
3.580710	0.239625	1.330310

3. 373500	1. 320570	-0. 034853
4. 916230	-0. 163484	-0. 317142
4. 888550	-0. 133278	-1. 413200
5. 096510	-1. 211170	-0. 046754
6. 076220	0. 699767	0. 187335
6. 152000	0. 662184	1. 278720
7. 032620	0. 363937	-0. 223126
5. 942350	1. 748000	-0. 097884

TS48

Cartesian Coordinates (Å)

X	Y	Z
1. 518400	-1. 244650	-0. 131789
0. 209573	-1. 448750	0. 305676
-0. 925697	-1. 478430	0. 490521
-1. 429520	-0. 685740	-0. 563282
-1. 638710	0. 652607	-0. 099434
-0. 403839	1. 333120	0. 493118
0. 887583	1. 255860	-0. 353130
1. 896270	0. 190009	0. 122884
2. 080200	-1. 998010	0. 419236
1. 341310	-1. 514110	-1. 173780
2. 097320	0. 340011	1. 189840
2. 855360	0. 376669	-0. 387402
0. 640392	1. 083500	-1. 406780
1. 392730	2. 225330	-0. 312675
-0. 217124	0. 924314	1. 490100
-0. 685033	2. 380970	0. 646368
-1. 973900	1. 163730	-1. 007500
-2. 457340	0. 657998	0. 629109

TS49

Cartesian Coordinates (Å)

X	Y	Z
-1.995060	-0.949023	0.372880
-0.576410	-1.282980	-0.133599
0.523741	-0.270886	0.210864
0.295174	1.000740	-0.441190
-0.663629	1.749440	0.274768
-1.661720	1.254230	-0.002005
-0.280157	-2.246880	0.294848
-0.594710	-1.415210	-1.222050
0.540706	-0.078405	1.290660
-2.643560	-1.815950	0.176282
-1.977240	-0.831496	1.462470
-2.613400	0.274268	-0.255527
-3.514520	0.663693	0.215356
-2.636950	0.303956	-1.345030
1.906030	-0.722440	-0.264839
2.068550	-1.741620	0.101676
1.892480	-0.784003	-1.358950
3.045480	0.189275	0.197927
4.007190	-0.171939	-0.175735
2.901480	1.209170	-0.162577
3.103760	0.223766	1.290200

TS50

Cartesian Coordinates (Å)

X	Y	Z
0.948029	1.394250	-0.022080
-0.412049	1.464650	-0.342674

-1.553330	1.398420	-0.420358
-1.884580	0.543810	0.653946
-1.987630	-0.802737	0.177635
-0.739400	-1.331660	-0.529219
0.601812	-1.136040	0.214801
1.482440	0.014759	-0.324275
1.370930	2.212520	-0.604855
0.833876	1.633510	1.036930
1.546560	-0.100907	-1.413800
0.424080	-0.983721	1.286200
1.185460	-2.057960	0.131677
-0.680021	-0.883437	-1.524950
-0.918917	-2.399930	-0.693420
-2.189210	-1.360980	1.097490
-2.858750	-0.886589	-0.482079
2.920500	-0.101010	0.234922
3.362610	-1.062510	-0.043706
3.563660	0.692826	-0.153148
2.920560	-0.030708	1.326930

TS51

Cartesian Coordinates (Å)

X	Y	Z
1.057970	0.127816	-0.739528
0.316963	-0.872137	-0.171565
-0.477852	-1.666170	0.175985
-1.612230	-1.301640	-0.579737
-2.461370	-0.457075	0.204898
-1.792150	0.800451	0.762689
-0.980884	1.647460	-0.244478

0.544922	1.434100	-0.178802
0.709394	-0.057794	-1.759940
0.874485	1.562070	0.858159
1.029840	2.246450	-0.745447
-1.334580	1.462430	-1.265240
-1.171680	2.705830	-0.043549
-1.155000	0.519343	1.605900
-2.602250	1.404530	1.186400
-3.254690	-0.200153	-0.504372
-2.897520	-1.043400	1.021820
2.511900	-0.242501	-0.531674
2.704900	-1.195140	-1.035330
3.135880	0.501184	-1.054060
2.968380	-0.340344	0.930483
4.014030	-0.653858	0.984598
2.887290	0.617149	1.451180
2.371050	-1.073370	1.479930

TS52

Cartesian Coordinates (Å)

X	Y	Z
-1.393770	0.011011	-0.007007
-0.438861	-0.837833	-0.443605
0.475621	-1.568180	-0.679796
1.345560	-1.330950	0.402664
2.325410	-0.355124	0.029439
1.756400	0.970964	-0.476539
0.652455	1.614480	0.393410
-0.783218	1.400940	-0.130321
-0.814565	1.713440	-1.180470

-1.449480	2.095190	0.407500
0.736569	1.268620	1.428730
0.821420	2.695030	0.425891
1.388490	0.833001	-1.496910
2.611140	1.652290	-0.554069
2.884180	-0.215912	0.960521
2.996940	-0.787960	-0.720911
-1.615090	-0.479522	1.409590
-2.360430	0.152486	1.915090
-1.988990	-1.506030	1.418910
-0.698402	-0.452645	2.001840
-2.553190	-0.246128	-0.948742
-2.884940	-1.286670	-0.901609
-3.413500	0.384073	-0.677765
-2.292980	-0.013788	-1.985060

TS53

Cartesian Coordinates (Å)

X	Y	Z
-0.702446	1.41867	-0.21033
0.592863	1.44921	0.31286
1.71898	1.36042	0.523177
2.16728	0.576714	-0.562449
2.20626	-0.801653	-0.173341
0.893976	-1.34848	0.388588
-0.367079	-1.10262	-0.470408
-1.32306	0.048038	-0.032589
-1.19444	2.23725	0.316253
-0.411204	1.67649	-1.2297
-0.072798	-0.928994	-1.51182

-0.967015	-2.01869	-0.476075
0.757413	-0.957896	1.39792
1.04805	-2.42663	0.508243
2.47798	-1.30139	-1.10864
3.01519	-0.948976	0.55151
-1.79631	-0.14166	1.42141
-2.56538	0.595264	1.67115
-2.22778	-1.13692	1.5654
-0.982118	-0.018671	2.13901
-2.56565	-0.010449	-0.963312
-3.08723	-0.965041	-0.837929
-3.27051	0.792249	-0.73034
-2.2772	0.084581	-2.01374

TS54

Cartesian Coordinates (Å)

X	Y	Z
0.528318	0.599351	-0.383096
0.002483	-0.565977	0.103089
-0.582486	-1.549870	0.373585
-1.639920	-1.536460	-0.560531
-2.804250	-0.960600	0.041757
-2.608070	0.441866	0.619237
-1.918370	1.469270	-0.307162
-0.426036	1.707660	-0.002494
0.462846	0.314668	-1.438590
-0.311328	1.943770	1.062950
-0.108044	2.615300	-0.540989
-2.036460	1.171980	-1.355330
-2.429820	2.430960	-0.204577

-2.056400	0.364189	1.560170
-3.609630	0.797061	0.886483
-3.516390	-0.949438	-0.789628
-3.181140	-1.637090	0.817420
1.941620	0.684436	0.143435
2.388280	1.630420	-0.207759
1.922000	0.762428	1.238510
2.847490	-0.480311	-0.278131
2.411120	-1.421280	0.072493
2.864310	-0.541485	-1.372660
4.277940	-0.344560	0.249964
4.899260	-1.186380	-0.067087
4.751050	0.573203	-0.114023
4.295280	-0.314308	1.344040

TS55

Cartesian Coordinates (Å)

X	Y	Z
-0.099218	0.550254	-1.003790
-0.560034	-0.660586	-0.564092
-1.142830	-1.640000	-0.270813
-2.465700	-1.327940	-0.649537
-3.185730	-0.833017	0.484949
-2.553230	0.375860	1.175950
-2.133530	1.544600	0.255065
-0.624030	1.602520	-0.053266
-0.649786	0.527384	-1.949140
-0.070818	1.576440	0.891887
-0.401240	2.586140	-0.499097
-2.699540	1.509280	-0.682718

-2.405290	2.487180	0.739389
-1.692470	0.039320	1.760540
-3.293770	0.724206	1.904660
-4.157780	-0.576955	0.051358
-3.326690	-1.646690	1.205680
1.397340	0.399954	-1.182470
1.584770	-0.363322	-1.945840
1.794640	1.341030	-1.599080
2.189460	0.046172	0.086078
2.063990	0.832908	0.838699
1.774370	-0.869178	0.524944
3.686340	-0.152044	-0.178861
3.818510	-0.945492	-0.924192
4.098040	0.759846	-0.628706
4.479470	-0.501380	1.083640
5.541340	-0.639710	0.862351
4.397430	0.290831	1.834660
4.111350	-1.426630	1.537670

TS56

Cartesian Coordinates (Å)

X	Y	Z
-0.677462	0.640713	-0.995661
-1.068120	-0.612316	-0.612749
-1.599840	-1.630070	-0.354744
-2.946450	-1.352740	-0.671984
-3.647440	-0.957609	0.512014
-3.044400	0.235429	1.255990
-2.698520	1.472640	0.395745
-1.204350	1.607460	0.040619

-1.267360	0.651118	-1.917230
-0.615726	1.540130	0.962140
-1.033140	2.625980	-0.345773
-3.296430	1.473770	-0.522748
-2.986200	2.372710	0.947178
-2.154800	-0.097068	1.798250
-3.778110	0.510091	2.022100
-4.643380	-0.719190	0.125063
-3.730120	-1.817670	1.186410
0.814884	0.569389	-1.244750
1.000350	-0.129995	-2.067390
1.154110	1.553890	-1.608880
1.675870	0.164482	-0.037699
1.540320	0.884204	0.777405
1.326650	-0.802531	0.343618
3.168120	0.070033	-0.374839
3.311250	-0.656070	-1.185510
3.514070	1.035430	-0.767376
4.041340	-0.330140	0.819758
3.899110	0.395789	1.629760
3.695270	-1.294180	1.211460
5.530780	-0.423834	0.475961
6.124890	-0.710132	1.348270
5.710330	-1.168040	-0.306366
5.914450	0.535191	0.113372

TS57

Cartesian Coordinates (Å)

X	Y	Z
1.555230	0.309962	0.567738

1.148890	1.057370	-0.591315
-1.030490	-1.456560	0.272988
0.370230	2.161890	-0.192617
-1.937280	-0.324352	-0.273203
-1.852900	1.034370	0.374813
0.828447	0.494443	1.361820
-0.852109	-1.301380	1.344240
-2.984760	-0.647520	-0.152491
2.531390	0.669387	0.912628
-1.606920	-2.383760	0.210333
-1.798210	-0.230536	-1.356390
-1.799100	1.045680	1.464120
-2.546490	1.778640	-0.017773
1.591960	-1.164610	0.190715
1.801470	-1.728210	1.108460
2.435470	-1.350160	-0.482443
0.308055	-1.692010	-0.475538
0.232937	-1.264270	-1.478730
0.444078	-2.768700	-0.617522
-0.646538	1.691510	0.030127

TS58

Cartesian Coordinates (Å)

X	Y	Z
2.101290	-0.717752	-0.379184
1.198170	-1.535100	0.395408
-0.022709	1.671230	-0.514433
0.039141	-1.824860	-0.349032
-1.489320	1.328200	-0.186188
-1.861260	-0.130252	-0.383187

1.709540	-0.670769	-1.396010
0.266344	1.145530	-1.430690
-2.154970	1.927620	-0.825256
3.058880	-1.247690	-0.405708
0.058937	2.737540	-0.745686
-1.704770	1.633100	0.844515
-1.979540	-0.395209	-1.437980
2.263380	0.665460	0.258561
2.824950	1.298890	-0.439835
2.882740	0.569713	1.156360
0.932688	1.320120	0.650850
0.427643	0.639270	1.342100
1.143070	2.226300	1.227490
-0.748934	-0.969650	-0.210305
-2.929050	-0.711831	0.508149
-3.088150	-1.774220	0.310438
-2.675360	-0.593073	1.565830
-3.888950	-0.198744	0.346326

TS59

Cartesian Coordinates (Å)

X	Y	Z
1.957330	-1.122240	-0.469138
1.003640	-1.523760	0.529911
0.808911	1.800140	-0.297480
-0.194362	-1.927110	-0.091675
-0.658689	1.420480	0.027552
-1.285000	0.285645	-0.755175
1.406780	-0.842073	-1.369360
1.027810	1.560480	-1.345240

-1.289250	2.303790	-0.170826
2.603960	-1.971240	-0.718880
0.879377	2.889540	-0.233891
-0.756851	1.241660	1.103580
-0.990356	0.279055	-1.808930
2.753560	0.055804	0.077135
3.394410	0.419444	-0.735834
3.427890	-0.291745	0.866877
1.897210	1.206700	0.636527
1.424790	0.870089	1.562880
2.587510	2.005800	0.924266
-0.708287	-0.916004	-0.360138
-2.766760	0.019664	-0.567745
-3.322730	0.868661	-0.998578
-3.046500	-0.850435	-1.171390
-3.220910	-0.197882	0.881241
-3.063550	0.691885	1.496290
-4.287320	-0.435082	0.915702
-2.675840	-1.026810	1.340090

TS60

Cartesian Coordinates (Å)

X	Y	Z
-2.389930	-1.188440	0.402940
-1.330990	-1.586140	-0.486364
-1.377160	1.789820	0.238411
-0.166953	-1.871800	0.253138
0.138506	1.520520	0.065023
0.759074	0.420446	0.900938
-1.938060	-0.851688	1.337800

-1.678660	1.547070	1.264810
0.681249	2.442120	0.335920
-3.022440	-2.055330	0.625672
-1.524900	2.869340	0.145801
0.357990	1.365820	-0.996584
0.390399	0.412082	1.931200
-3.178300	-0.068232	-0.264708
-3.911520	0.296559	0.465558
-3.755050	-0.475882	-1.101570
-2.315790	1.095430	-0.784994
-1.720060	0.733859	-1.627010
-3.000660	1.841660	-1.199540
0.267754	-0.818388	0.498776
2.260850	0.221200	0.822989
2.749290	1.107000	1.263990
2.539380	-0.619270	1.469620
2.832510	-0.015338	-0.582842
2.630080	0.853890	-1.217280
2.310690	-0.862430	-1.040240
4.339810	-0.284905	-0.565793
4.575850	-1.175220	0.025388
4.724460	-0.447065	-1.576260
4.890230	0.556371	-0.132027

TS61

Cartesian Coordinates (Å)

X	Y	Z
-2.793000	-1.231200	0.342152
-1.620010	-1.625750	-0.390890
-1.904040	1.767550	0.025964

-0.542906	-1.811160	0.497626
-0.370394	1.543640	0.039998
0.191423	0.571992	1.057260
-2.469040	-0.796642	1.289980
-2.307960	1.604990	1.032650
0.111886	2.512280	0.254988
-3.398400	-2.116990	0.566169
-2.071570	2.828190	-0.180746
-0.033279	1.279340	-0.967781
-0.305119	0.640518	2.029890
-3.560440	-0.216581	-0.496007
-4.384340	0.160339	0.122752
-4.023910	-0.721829	-1.349870
-2.708820	0.952926	-1.021810
-2.020930	0.567521	-1.778740
-3.387710	1.630220	-1.549230
-0.184295	-0.723108	0.717846
1.698600	0.459200	1.185470
2.081830	1.413780	1.584620
1.931530	-0.292230	1.948980
2.456620	0.117110	-0.105702
2.303210	0.907323	-0.849787
2.035250	-0.799204	-0.534652
3.961620	-0.068948	0.118775
4.119440	-0.863584	0.857996
4.379110	0.844731	0.560025
4.723510	-0.409937	-1.165050
4.615640	0.382878	-1.912160
5.791940	-0.540946	-0.972373

4. 349620 -1. 336830 -1. 610760

TS62