Supporting information

Thermal decompositions of isolated and crystalline 4,10-dinitro-2,6,8,12- tetraoxa-4,10- diazaisowutrzitane from ab initio molecular dynamics simulations

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Table S1. Calculated relative energies and entropies of the TEX, intermediates, and transition states.

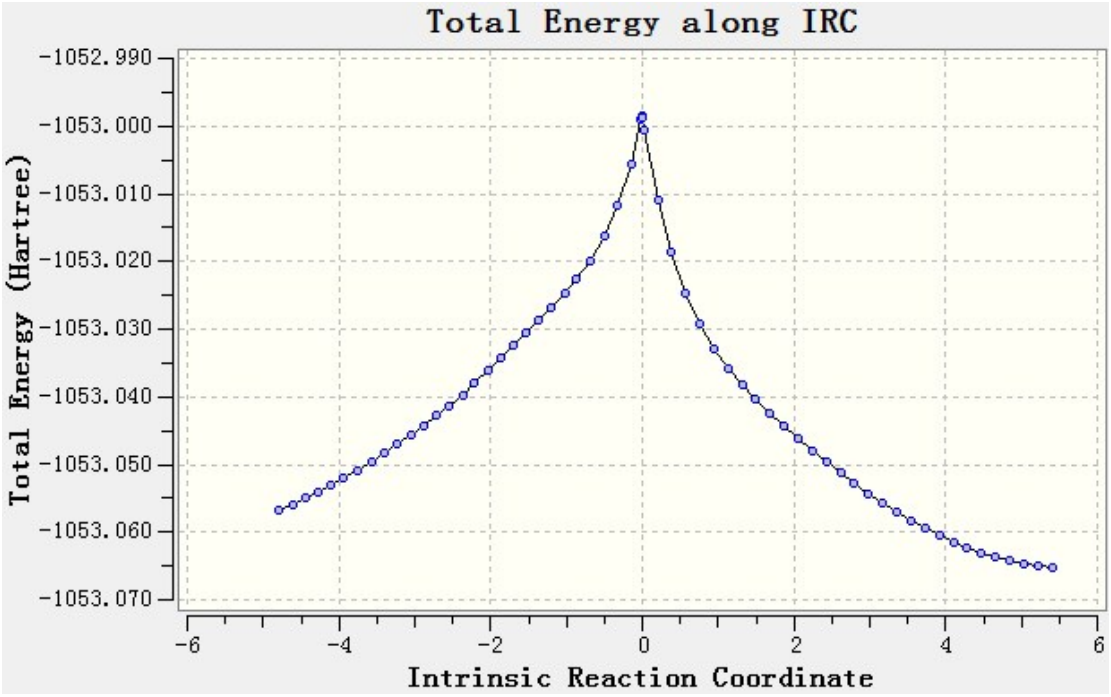
	TEX	TS1	Int1	TS2	Int2	TS3	Int3	TS4	Int4	TS5	TS6	Int5
ΔE (kcal/mol)	0	51.5	-22.79	-17.79	-47.72	-42.72	-68.45	137.05	78.89	321.6	413.7	10.67
ΔS ($Cal \cdot mol^{-1} \cdot K^{-1}$)	0	8.77	0.51	-14.63	-11.45	-19.21	-11.45	-23.79	0.52	-3.07	-10.64	-11.45

Table S2. Calculated frequencies of the transition states. [a]

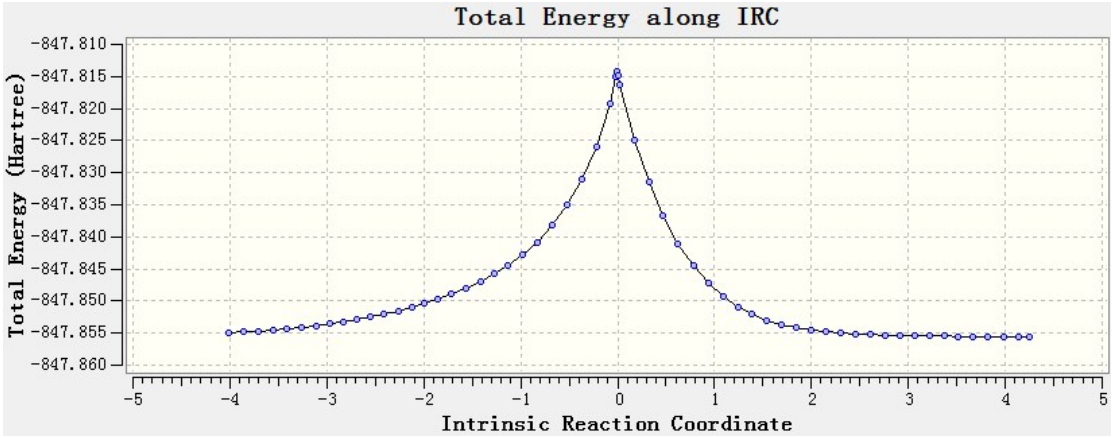
TS1								
-53.02	80.52	84.62	95.13	212.40	224.89	293.43	302.35	357.35
387.04	391.52	397.75	411.70	503.48	569.97	594.73	627.56	642.50
664.03	730.02	732.30	776.37	792.31	802.61	819.48	846.96	854.01
864.12	903.61	943.59	969.21	983.94	1003.74	1009.69	1011.80	1032.42
1052.83	1054.40	1078.39	1135.61	1142.99	1181.51	1221.44	1270.01	1276.58
1277.29	1317.46	1317.65	1334.07	1342.63	1360.46	1363.54	1373.58	1374.34
1377.55	1392.60	1432.92	1433.38	1736.91	1737.33	3139.84	3151.52	3202.69
3203.25	3208.25	3209.27						
TS2								
-114.17	103.88	164.80	267.25	318.56	341.20	351.89	403.14	412.32
443.19	457.65	483.09	624.24	652.64	654.47	713.98	737.37	760.18
783.64	808.11	811.22	812.21	835.39	852.12	905.50	928.55	931.78
962.32	968.67	982.31	1001.71	1023.57	1095.11	1100.59	1132.38	1147.67
1206.87	1252.84	1268.18	1270.76	1274.89	1326.49	1330.74	1337.85	1346.64
1350.51	1366.53	1377.85	1385.03	1420.49	1653.46	3121.68	3122.37	3123.32
3130.11	3130.94	3136.14						
TS3								
-317.85	47.02	57.10	69.40	88.81	119.63	219.87	244.76	270.91
305.3	337.81	369.31	422.29	427.01	475.29	517.39	556.76	571.26
606.43	661.87	678.51	704.81	719.57	751.87	762.38	767.29	794.07
801.68	807.94	831.72	862.65	888.67	928.00	939.97	943.21	978.89
987.92	1003.99	1048.70	1064.85	1089.41	1133.81	1200.20	1216.39	1244.76
1254.65	1259.75	1280.85	1282.35	1291.84	1314.60	1317.75	1340.25	1344.37
1357.70	1357.79	1411.72	1428.14	1536.56	1652.95	3090.99	3114.49	3118.45
3185.12	3194.46	3262.75						
TS4								
-442.72	233.93	245.97	290.24	352.90	359.16	366.58	426.94	475.47
560.61	581.72	663.12	673.57	716.97	723.22	748.89	824.45	855.92

863.01	881.64	881.84	887.81	950.86	975.48	1013.15	1013.32	1035.70
1049.23	1116.23	1172.19	1230.33	1267.82	1350.82	1355.57	1362.09	1377.47
1387.28	1404.58	1443.41	1448.79	1482.28	1596.48	3122.07	3136.57	3202.32
3203.29	3207.07	3210.70						
TS5								
-95.43	61.14	81.33	114.19	170.82	217.08	264.63	286.64	343.97
370.73	375.42	400.15	438.36	462.81	498.72	597.40	600.36	663.58
701.83	721.48	730.70	758.19	773.67	798.17	810.01	838.91	843.41
844.11	890.22	913.81	938.61	939.12	945.77	970.72	978.21	986.48
999.04	1009.39	1035.14	1102.18	1113.64	1139.53	1170.60	1228.62	1274.51
1280.25	1300.84	1305.60	1316.83	1337.29	1346.63	1347.32	1351.66	1358.56
1371.54	1382.80	1414.42	1421.07	1648.38	1668.89	3128.37	3136.21	3136.44
3140.53	3186.66	3187.79						
TS6								
-424.67	57.31	83.80	212.93	300.57	330.90	352.03	368.14	395.33
431.56	454.98	473.91	535.80	586.51	622.83	628.71	709.01	730.61
748.53	758.38	798.91	812.65	838.01	847.76	866.51	902.14	926.34
938.83	965.86	975.66	1016.53	1024.74	1047.68	1072.63	1125.27	1143.12
1185.88	1229.15	1271.81	1285.66	1296.13	1335.29	1340.40	1346.80	1359.29
1370.86	1379.50	1392.94	1427.07	1458.06	1626.80	3125.63	3132.00	3140.72
3173.80	3191.28	3236.82						

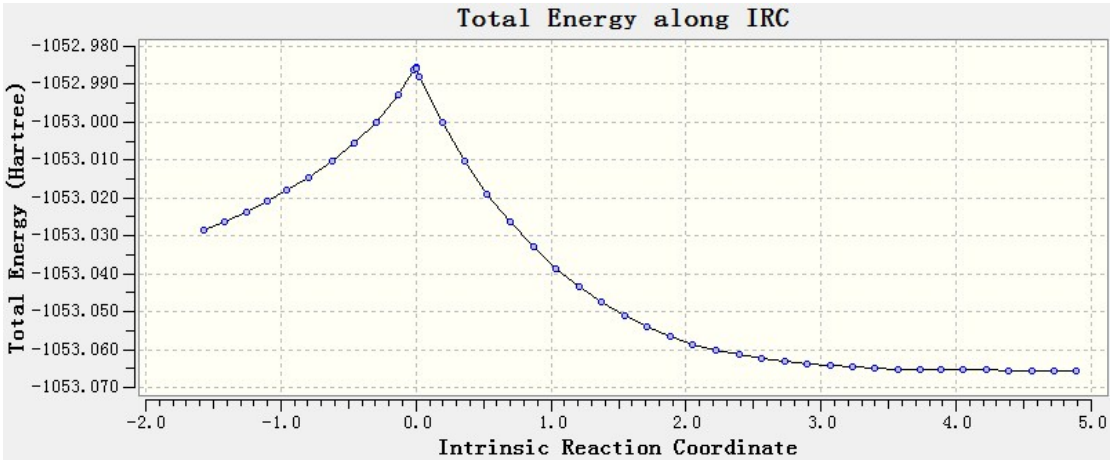
[a] All frequencies are in cm^{-1} and the negative numbers indicate imaginary frequencies.



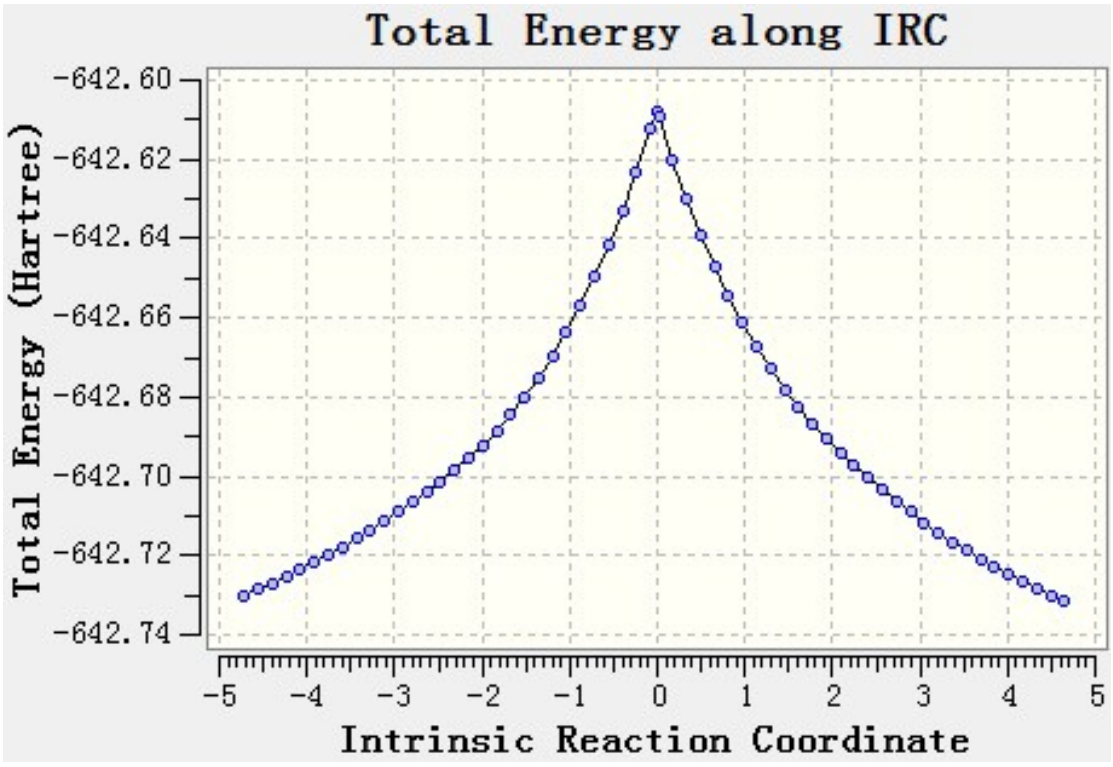
TS2


Total Energy along IRC
Total Energy (Hartree)
-847.810
-847.815
-847.820
-847.825
-847.830
-847.835
-847.840
-847.845
-847.850
-847.855
-847.860
-5
-4
-3
-2
-1
0
1
2
3
4
5
Intrinsic Reaction Coordinate

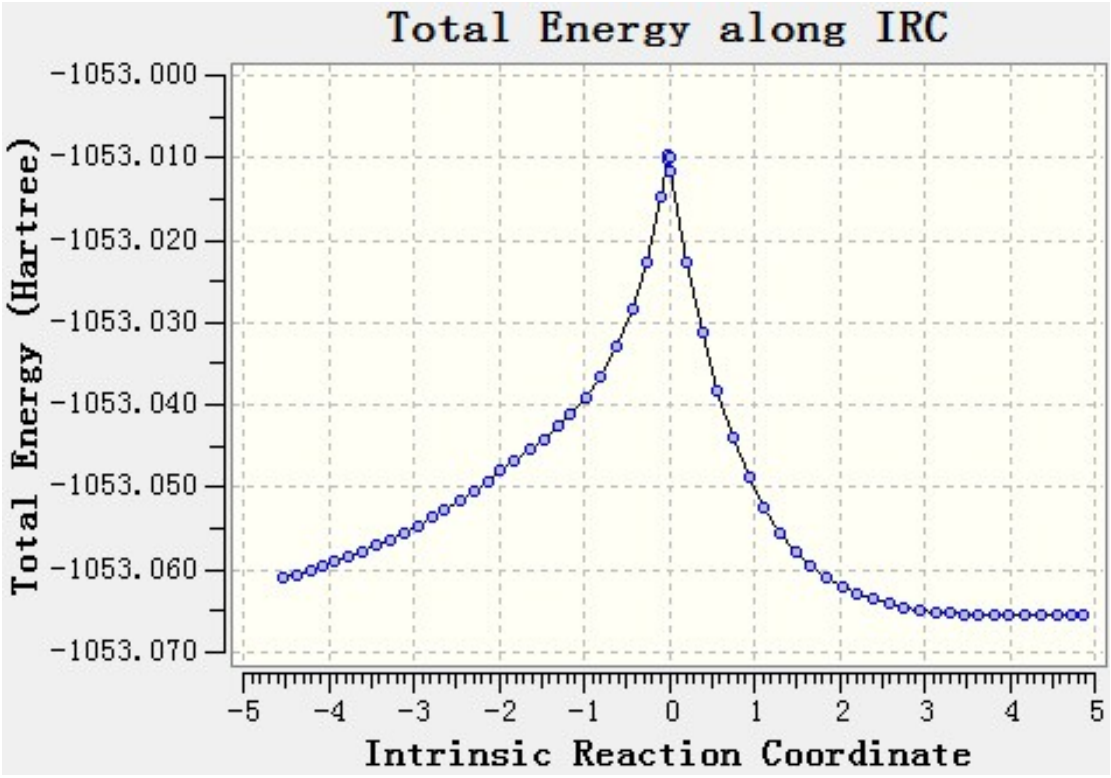
TS3


Total Energy along IRC
Total Energy (Hartree)
-1052.980
-1052.990
-1053.000
-1053.010
-1053.020
-1053.030
-1053.040
-1053.050
-1053.060
-1053.070
-2.0
-1.0
0.0
1.0
2.0
3.0
4.0
5.0
Intrinsic Reaction Coordinate

TS4


Total Energy along IRC
Total Energy (Hartree)
-642.60
-642.62
-642.64
-642.66
-642.68
-642.70
-642.72
-642.74
-5
-4
-3
-2
-1
0
1
2
3
4
5
Intrinsic Reaction Coordinate

TS5



TS6

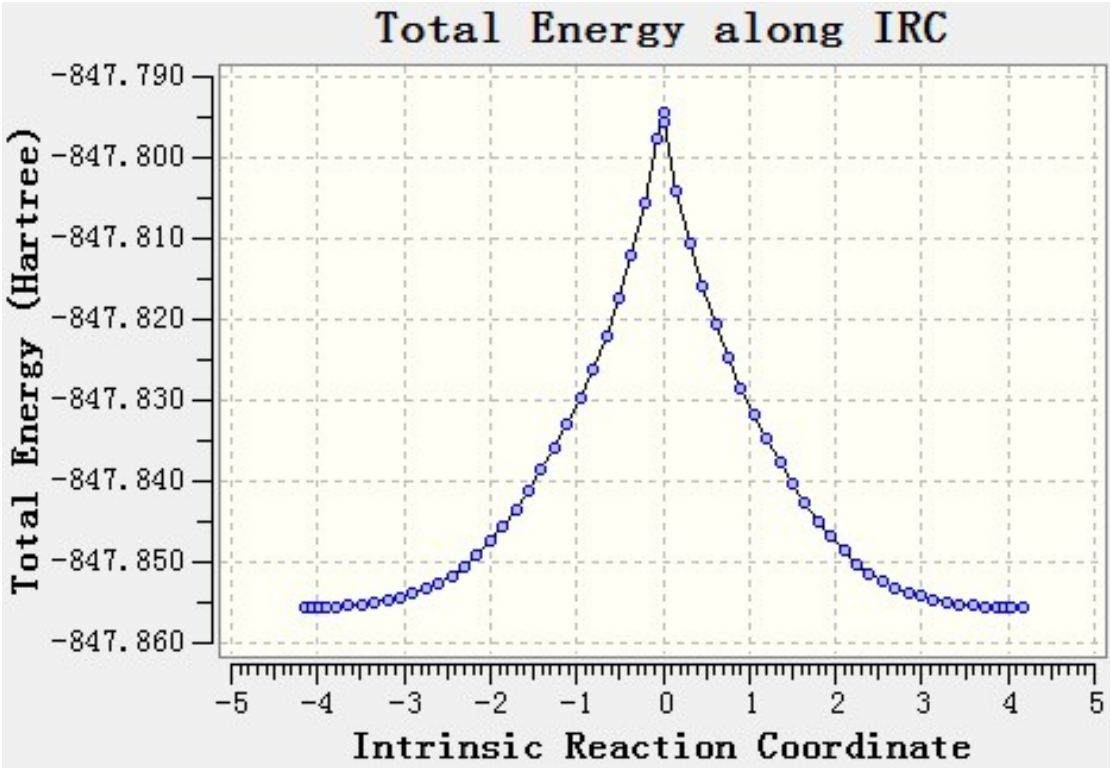


Figure S1. The IRC calculation results of the transition states.