Electronic Supplementary Information

Electrostatic repulsion-controlled regioselectivity in nitrene-mediated allylic C-H amidations

Fang Huang,*[a] Xiaoxiao Tian,[a] Fangao Hou,[a] Yaping Xu,[a] and Gang Lu*[b]

[a] College of Chemistry, Chemical Engineering and Materials Science, Shandong Normal University, Jinan, Shandong 250014, China

[b] School of Chemistry and Chemical Engineering, Key Laboratory of Colloid and Interface Chemistry, Ministry of Education, Shandong University, Jinan, Shandong 250100, China

Corresponding Author: fanghuang@sdnu.edu.cn; ganglu@sdu.edu.cn

Table of Contents

EDA Results along IRC

The EDA results along IRC for the regioselectivity-determining nitrene insertion step are shown in Tables S1-S16 and Fig. S1-S7. As described in the bar charts of the main text, the difference of electrostatic interactions between the two regioselective transition states is the decisive factor for the b/l selectivity.

Table S1. EDA energy terms of TS3a along IRC

Energy terms (in kcal/mol) / **TS3a** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.50	3.43	360.13	-151.67	-147.15	-117.22	-13.81
2.45	3.28	360.40	-150.72	-147.33	-116.37	-14.53
2.40	3.32	360.94	-150.07	-147.22	-115.93	-15.34
2.35	3.45	361.52	-150.00	-147.07	-115.98	-15.78
2.30 (TS)	3.94	363.74	-150.58	-146.95	-116.73	-16.54
2.24	4.66	367.13	-151.97	-147.12	-118.16	-17.19
2.23	4.90	368.26	-153.71	-147.63	-118.66	-17.35
2.20	5.46	371.08	-156.32	-147.95	-119.87	-17.66
2.16	6.49	376.04	-159.89	-148.49	-122.23	-18.16
2.10	7.74	382.49	-151.67	-147.15	-125.29	-18.66

Table S2. EDA energy terms of TS4a along IRC

Energy terms (in kcal/mol) / **TS4a** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.50	3.57	345.93	-143.44	-142.34	-117.11	-12.78
2.45	3.09	346.03	-141.71	-142.61	-115.70	-13.61
2.40	2.97	347.44	-141.37	-142.97	-115.26	-14.26
2.35	3.10	350.54	-141.78	-143.56	-115.39	-15.13
2.30	3.47	353.95	-142.81	-143.99	-116.13	-15.84
2.25	4.12	358.47	-144.56	-144.50	-117.51	-16.59
2.22	4.57	361.21	-145.76	-144.81	-118.48	-16.97
2.21 (TS)	4.82	362.74	-146.47	-144.97	-119.04	-17.16
2.15	6.02	369.62	-149.93	-145.71	-121.75	-17.94
2.10	7.13	375.78	-153.34	-146.31	-124.34	-18.54

Table S3. EDA energy terms of TS3a1 along IRC

Energy terms (in kcal/mol) / **TS3a1** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.50	8.89	305.01	-134.28	-124.50	-91.47	-13.70
2.45	8.68	304.57	-133.04	-124.20	-91.05	-14.46
2.40	8.59	304.58	-131.93	-123.83	-90.97	-15.41
2.35	8.68	305.10	-131.45	-123.55	-91.29	-16.12
2.30 (TS)	8.99	306.38	-131.46	-123.21	-92.15	-16.90
2.25	9.52	308.66	-132.02	-122.96	-93.60	-17.72
2.20	10.42	312.68	-133.47	-123.07	-95.99	-18.56
2.16	11.01	315.19	-134.68	-122.95	-97.57	-19.03
2.13	11.72	318.25	-136.24	-122.89	-99.43	-19.50
2.09	12.52	321.93	-138.20	-122.92	-101.58	-20.00

Table S4. EDA energy terms of TS4a1 along IRC

Energy terms (in kcal/mol) / **TS4a1** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.50	8.75	293.42	-127.27	-121.69	-90.00	-12.28
2.45	8.51	293.09	-125.98	-121.35	-89.56	-13.02
2.40	8.80	294.53	-125.49	-121.33	-89.77	-13.94
2.35	8.64	296.31	-125.65	-121.47	-90.30	-14.57
2.30	9.01	299.77	-126.46	-121.77	-91.56	-15.49
2.26	9.46	303.14	-127.56	-122.05	-92.98	-16.21
2.23 (TS)	9.85	305.79	-128.56	-122.23	-94.19	-16.71
2.20	10.30	308.68	-129.74	-122.42	-95.56	-17.21
2.15	11.47	315.42	-132.90	-122.76	-98.99	-18.23
2.10	12.55	321.35	-136.01	-123.03	-102.12	-19.01

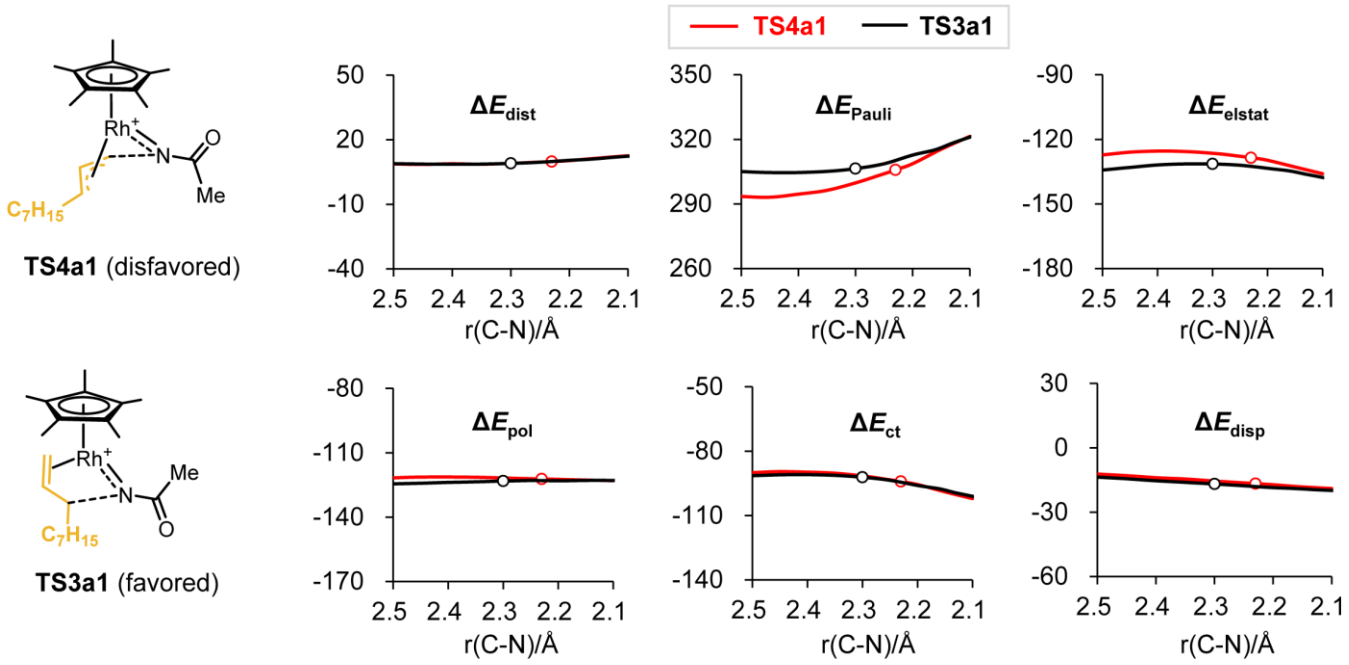

Fig. S1 EDA results along IRC of Rh=N insertion (**TS3a1** vs **TS4a1**). Energies are shown in kcal/mol.

Table S5. EDA energy terms of TS3b along IRC

Energy terms (in kcal/mol) / **TS3b** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.50	10.42	323.98	-137.10	-133.81	-102.32	-13.14
2.46	10.45	324.91	-136.91	-133.94	-102.37	-13.59
2.40	10.63	331.31	-138.26	-134.93	-103.92	-15.02
2.37	10.81	329.70	-137.91	-134.53	-103.70	-14.78
2.34 (TS)	11.03	331.89	-138.64	-134.81	-104.48	-15.15
2.31	11.36	334.66	-139.65	-135.19	-105.52	-15.54
2.24	12.35	341.07	-142.81	-135.11	-108.50	-16.39
2.17	13.94	351.89	-147.67	-136.65	-113.24	-17.27
2.13	14.97	358.77	-150.96	-137.63	-116.37	-17.68
2.08	16.16	366.71	-154.91	-138.80	-120.03	-18.06

Table S6. EDA energy terms of TS4b along IRC

Energy terms (in kcal/mol) / **TS4b** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.51	10.48	305.60	-126.49	-124.85	-104.78	-12.93
2.46	10.00	303.11	-123.83	-124.20	-102.90	-13.68
2.40	9.84	303.81	-122.64	-124.36	-102.08	-14.54
2.35	10.04	306.93	-122.63	-125.74	-102.37	-15.18
2.33	10.26	308.79	-123.04	-126.13	-102.81	-15.53
2.25	11.40	316.76	-125.57	-127.71	-105.33	-16.65
2.22	11.98	320.26	-126.92	-128.34	-106.65	-17.05
2.19 (TS)	12.68	324.24	-128.58	-129.03	-108.25	-17.47
2.16	13.43	328.46	-130.41	-129.76	-109.99	-17.90
2.10	15.23	338.26	-135.08	-131.35	-114.25	-18.78

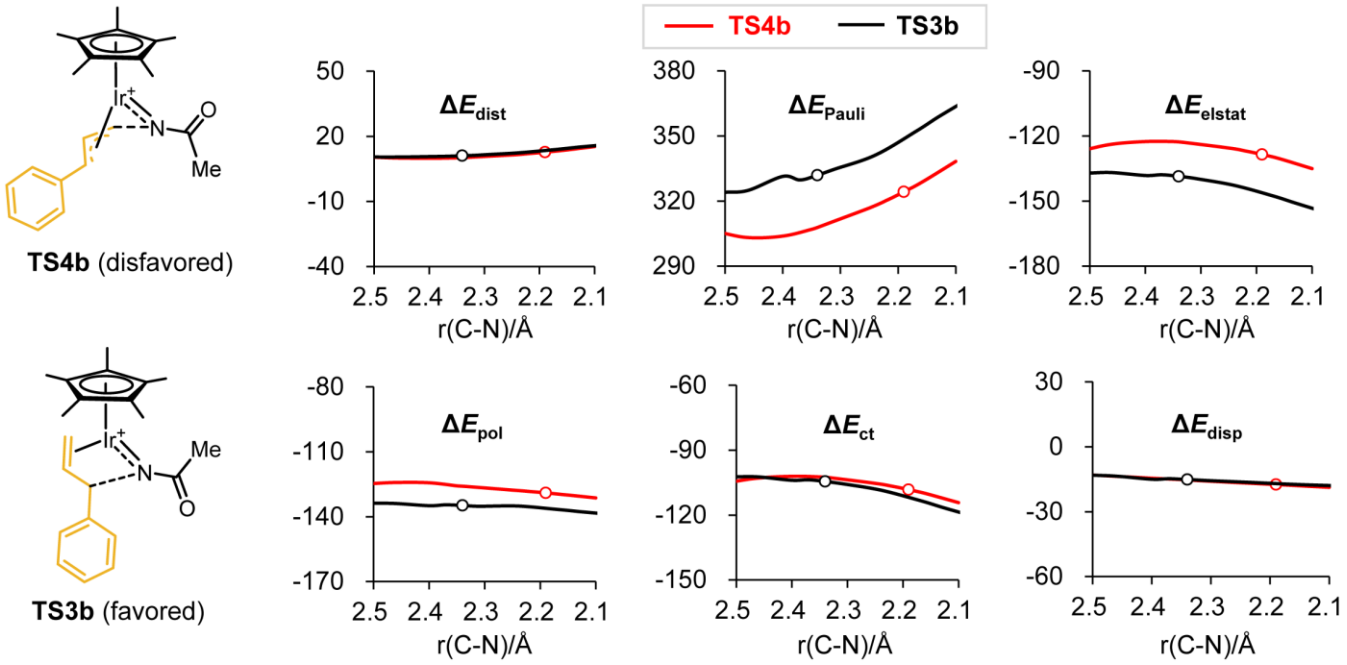

Fig. S2 EDA results along IRC of Ir=N insertion with Ph-substituted allyl substrate (**TS3b** vs **TS4b**). Energies are shown in kcal/mol.

Table S7. EDA energy terms of TS3c along IRC

Energy terms (in kcal/mol) / **TS3c** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.50	11.44	315.23	-140.76	-131.50	-96.40	-12.95
2.48	11.50	316.13	-140.84	-131.62	-96.58	-13.24
2.45	11.58	317.49	-141.10	-131.81	-96.90	-13.58
2.41	17.77	319.29	-141.53	-132.05	-97.41	-13.97
2.37	17.93	322.22	-142.45	-132.45	-98.31	-14.44
2.33 (TS)	12.11	326.62	-144.00	-133.08	-99.79	-14.99
2.28	12.53	331.74	-145.98	-133.79	-101.67	-15.52
2.23	13.16	338.28	-148.76	-134.63	-104.32	-16.03
2.17	14.07	346.82	-152.69	-135.63	-108.06	-16.48
2.11	15.33	357.72	-157.82	-136.88	-113.14	-16.97

Table S8. EDA energy terms of TS4c along IRC

Energy terms (in kcal/mol) / **TS4c** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.50	8.98	282.54	-121.79	-118.66	-91.59	-12.46
2.45	8.41	277.70	-118.14	-117.19	-89.40	-12.99
2.42	8.27	276.63	-116.64	-116.74	-88.65	-13.45
2.35	8.42	278.60	-115.97	-116.92	-88.80	-14.31
2.33	8.60	280.24	-116.20	-117.20	-89.24	-14.65
2.28	9.19	285.01	-117.37	-118.07	-90.82	-15.39
2.25	9.62	288.14	-118.32	-118.62	-91.99	-15.79
2.22	10.13	291.71	-119.52	-119.26	-93.38	-16.21
2.16 (TS)	11.52	300.48	-122.87	-120.74	-97.12	-17.10
2.10	13.22	310.96	-127.29	-122.51	-101.82	-18.02

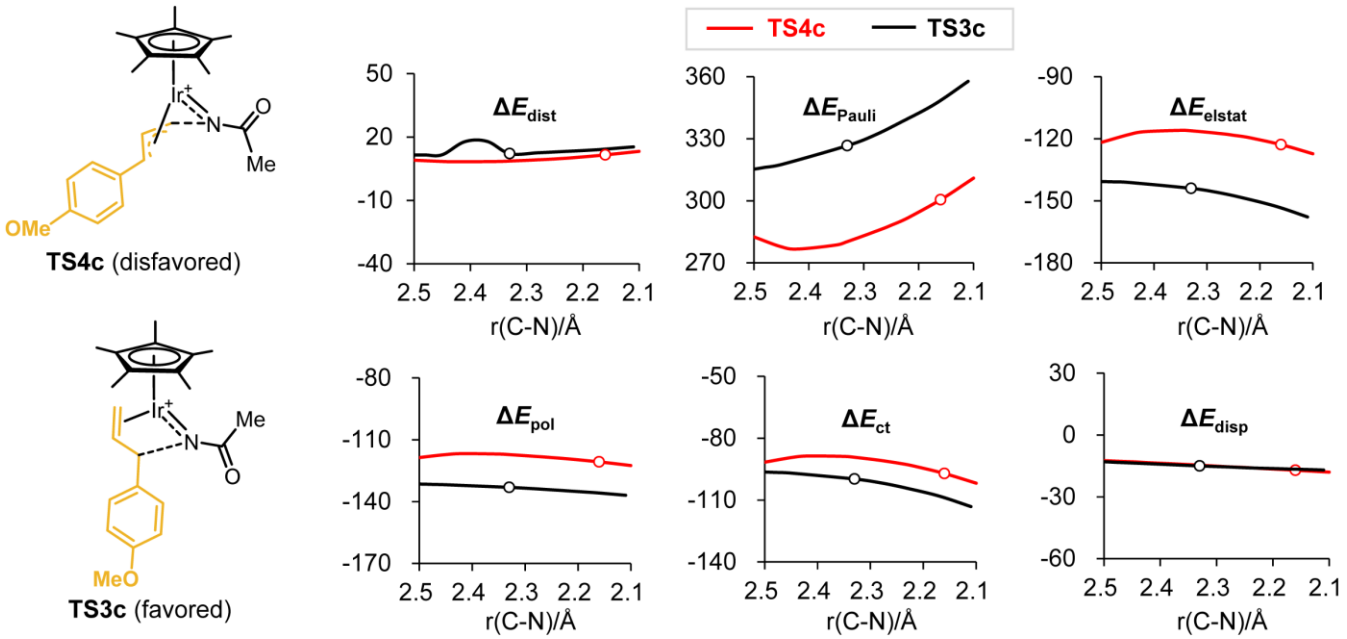

Fig. S3 EDA results along IRC of Ir=N insertion with Ph-4-OMe-substituted allyl substrate (**TS3c** vs **TS4c**). Energies are shown in kcal/mol.

Table S9. EDA energy terms of TS3d along IRC

Energy terms (in kcal/mol) / **TS3d** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.51	10.93	-135.24	-13.57	-132.42	325.48	-105.39
2.45	10.84	-134.64	-14.31	-132.47	326.34	-105.15
2.41	10.91	-134.69	-14.92	-132.54	327.85	-105.43
2.36	11.18	-135.47	-15.64	-132.79	330.84	-106.40
2.33 (TS)	11.42	-136.18	-16.03	-133.02	332.97	-107.19
2.26	12.25	-138.51	-16.88	-133.75	338.98	-109.62
2.23	12.84	-140.17	-17.33	-134.29	342.94	-111.31
2.19	13.61	-142.36	-17.78	-134.94	347.83	-113.50
2.12	15.69	360.61	-148.48	-136.76	-119.37	-18.68
2.07	16.98	368.64	-152.54	-137.99	-123.08	-19.08

Table S8. EDA energy terms of TS4d along IRC

Energy terms (in kcal/mol) / **TS4d** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.51	11.80	315.23	-128.88	-126.59	-110.04	-13.11
2.46	11.18	312.14	-126.02	-125.73	-107.93	-13.86
2.40	10.94	312.19	-124.63	-125.70	-106.88	-14.71
2.36	11.09	314.21	-124.68	-126.13	-106.98	-15.35
2.34	11.28	315.79	-125.00	-126.47	-107.30	-15.69
2.26	12.32	322.70	-127.18	-127.87	-109.38	-16.80
2.23	12.86	325.73	-128.35	-128.42	-110.49	-17.18
2.20 (TS)	13.51	329.21	-129.83	-128.95	-111.94	-17.58
2.14	15.02	337.07	-133.40	-130.30	-115.20	-18.39
2.11	15.93	341.64	-135.67	-131.03	-117.19	-18.80

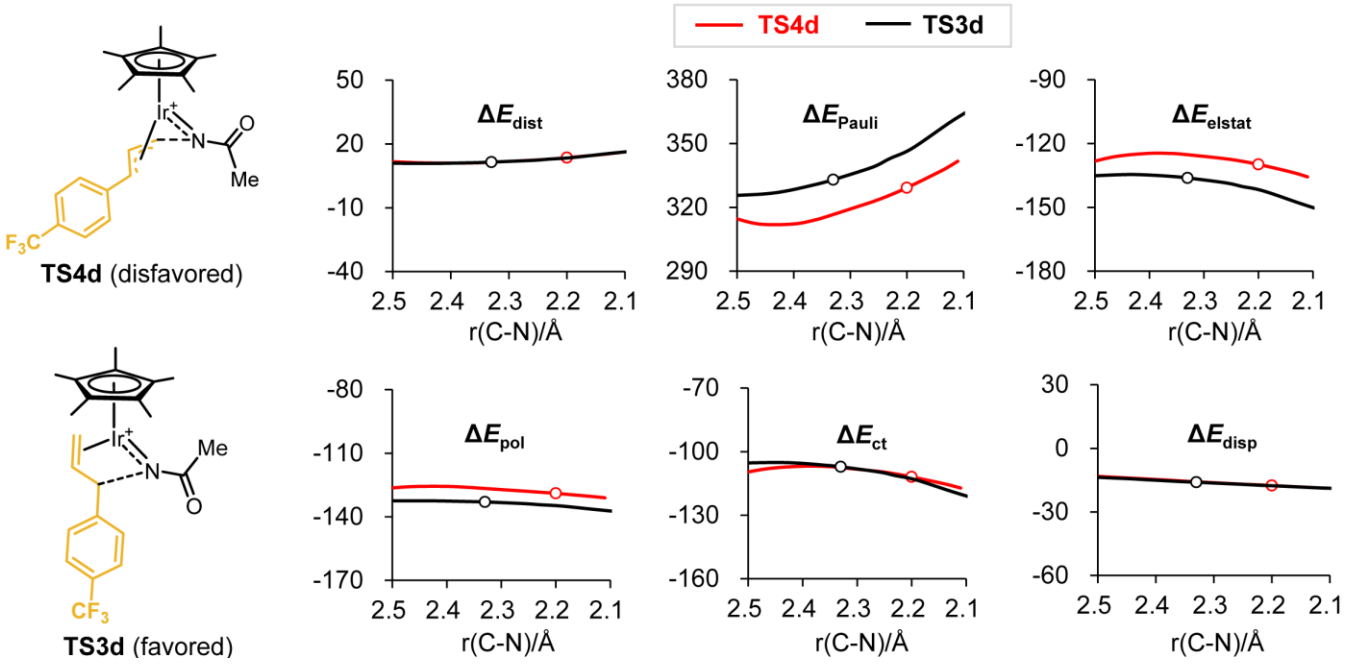

Fig. S4 EDA results along IRC of Ir=N insertion with Ph-4-CF_3-substituted allyl substrate (**TS3d** vs **TS4d**). Energies are shown in kcal/mol.

Table S9. EDA energy terms of TS3e along IRC

Energy terms (in kcal/mol) **TS3e** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.52	4.54	363.69	-148.77	-149.23	-120.39	-14.12
2.45	4.31	364.63	-147.64	-149.80	-119.33	-15.10
2.42	4.26	362.42	-146.53	-147.96	-118.98	-15.57
2.35	4.39	366.21	-146.85	-149.60	-118.98	-16.56
2.30 (TS)	4.73	367.84	-147.29	-149.25	-119.69	-17.24
2.28	5.00	369.13	-147.75	-149.20	-120.26	-17.60
2.25	5.34	370.86	-148.47	-149.21	-121.06	-17.97
2.22	5.79	373.10	-149.49	-149.27	-122.13	-18.35
2.15	7.04	379.30	-152.63	-149.60	-125.17	-19.13
2.12	7.85	383.38	-154.84	-149.90	-127.17	-19.52

Table S10. EDA energy terms of TS4e along IRC

Energy terms (in kcal/mol) **TS4e** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.52	4.77	350.34	-141.94	-143.92	-121.64	-12.85
2.45	4.10	351.06	-139.84	-144.38	-119.77	-14.21
2.41	4.02	352.94	-139.67	-144.99	-119.40	-14.89
2.36	4.15	352.90	-139.47	-143.73	-119.49	-15.48
2.31	4.52	358.93	-141.07	-146.14	-120.09	-16.27
2.28	4.80	360.85	-141.81	-146.35	-120.60	-16.62
2.23	5.58	365.53	-143.87	-146.84	-122.10	-17.33
2.21 (TS)	6.10	368.39	-145.29	-147.14	-123.13	-17.68
2.15	7.33	374.94	-148.75	-147.84	-125.64	-18.42
2.12	8.07	378.71	-150.96	-148.18	-127.19	-18.78

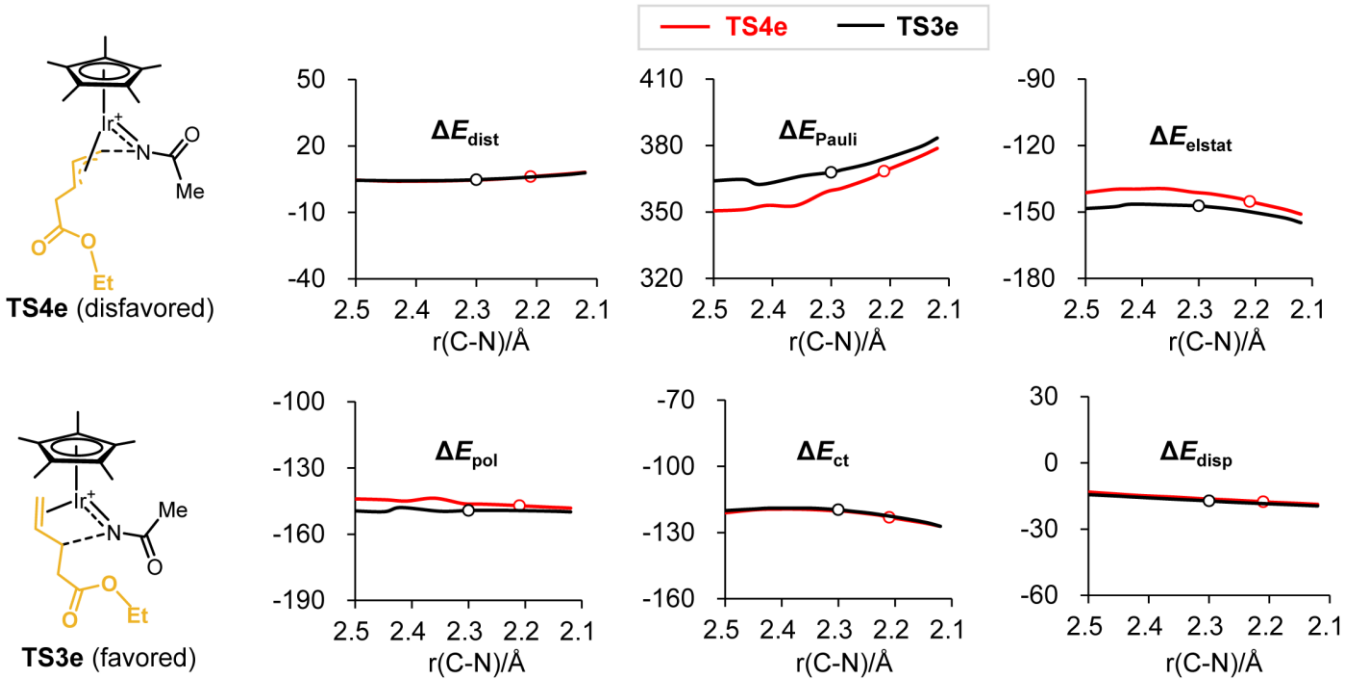

Fig. S5 EDA results along IRC of Ir=N insertion with CH_2CO_2Et-substituted allyl substrate (**TS3e** vs **TS4e**). Energies are shown in kcal/mol.

Table S11. EDA energy terms of TS3f along IRC

Energy terms (in kcal/mol) / **TS3f** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.50	12.55	353.71	-151.82	-144.11	-115.76	-12.21
2.46	12.38	351.32	-150.74	-142.96	-114.30	-12.55
2.39 (TS)	12.52	349.28	-150.06	-141.42	-113.43	-12.96
2.34	12.99	348.78	-150.18	-140.36	-113.56	-13.32
2.30	13.38	349.14	-150.61	-139.81	-114.09	-13.54
2.27	13.89	350.16	-151.42	-139.32	-115.04	-13.80
2.23	14.55	352.03	-152.70	-138.91	-116.51	-14.12
2.18	15.40	354.98	-154.58	-138.64	-118.60	-14.49
2.14	16.51	359.29	-157.22	-138.58	-121.41	-14.93
2.09	17.92	365.26	-160.76	-138.82	-124.99	-15.45

Table S12. EDA energy terms of TS4f along IRC

Energy terms (in kcal/mol) / **TS4f** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.50	10.02	334.69	-139.31	-136.78	-112.99	-10.04
2.46	9.95	333.13	-138.38	-135.84	-112.03	-10.26
2.39	10.33	333.23	-138.43	-134.96	-111.67	-10.68
2.35	10.79	334.35	-139.13	-134.70	-111.97	-10.95
2.30	11.46	336.27	-140.36	-134.52	-112.72	-11.28
2.25 (TS)	12.46	339.27	-142.35	-134.42	-114.09	-11.68
2.19	13.72	343.27	-145.03	-134.42	-116.05	-12.15
2.17	14.51	348.28	-147.10	-136.40	-117.34	-12.55
2.13	15.40	351.24	-149.11	-136.50	-118.83	-12.85
2.10	16.38	354.63	-151.43	-136.65	-120.54	-13.18

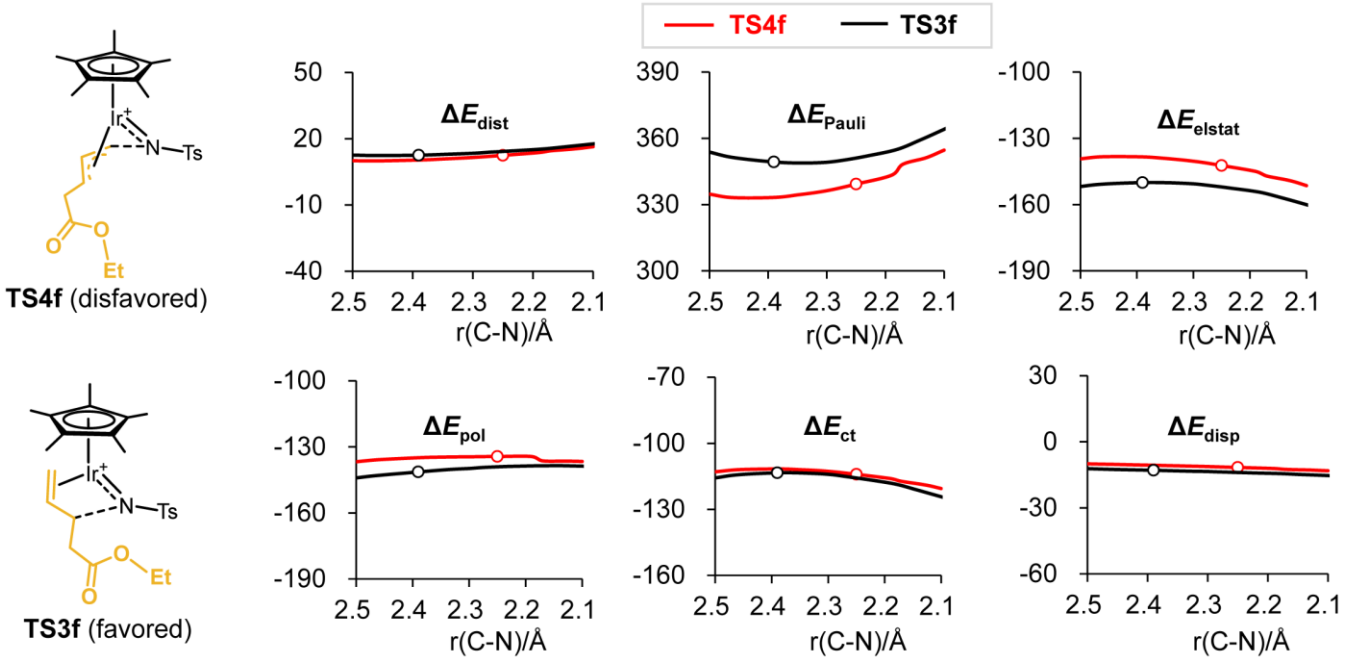

Fig. S6 EDA results along IRC of Ir=N-Ts insertion with CH_2CO_2Et-substituted allyl substrate (**TS3f** vs **TS4f**). Energies are shown in kcal/mol.

Table S13. EDA energy terms of TS3g along IRC

Energy terms (in kcal/mol) / **TS3g** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.52	8.87	302.15	-135.79	-122.23	-96.82	-8.98
2.46	8.89	302.72	-135.55	-121.88	-96.87	-9.44
2.43	9.07	303.55	-135.79	-121.82	-97.22	-9.68
2.40 (TS)	9.42	305.13	-136.40	-121.87	-97.93	-10.00
2.36	9.88	307.01	-137.16	-121.96	-98.82	-10.34
2.32	10.52	309.74	-138.33	-122.18	-100.16	-10.74
2.28	11.40	315.24	-140.40	-123.76	-102.05	-11.27
2.23	12.57	320.57	-142.81	-124.38	-104.70	-11.90
2.18	14.03	327.79	-146.12	-125.32	-108.26	-12.66
2.13	15.80	337.40	-150.58	-126.75	-112.90	-13.56

Table S14. EDA energy terms of TS4g along IRC

Energy terms (in kcal/mol) / **TS4g** *r*(C-N) (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.52	7.49	290.69	-124.22	-116.98	-97.87	-10.76
2.46	6.92	283.72	-120.42	-114.60	-94.86	-10.84
2.39	7.09	282.23	-119.41	-113.61	-93.99	-11.11
2.36	7.50	283.24	-119.79	-113.49	-94.32	-11.35
2.29	8.64	287.03	-121.58	-113.70	-95.97	-11.87
2.26	9.21	288.97	-122.56	-113.86	-96.91	-12.08
2.24 (TS)	9.91	291.32	-123.79	-114.08	-98.08	-12.32
2.21	10.66	293.82	-125.11	-114.32	-99.36	-12.58
2.15	12.52	300.09	-128.55	-114.97	-102.64	-13.16
2.12	13.63	303.84	-130.68	-115.39	-104.63	-13.49

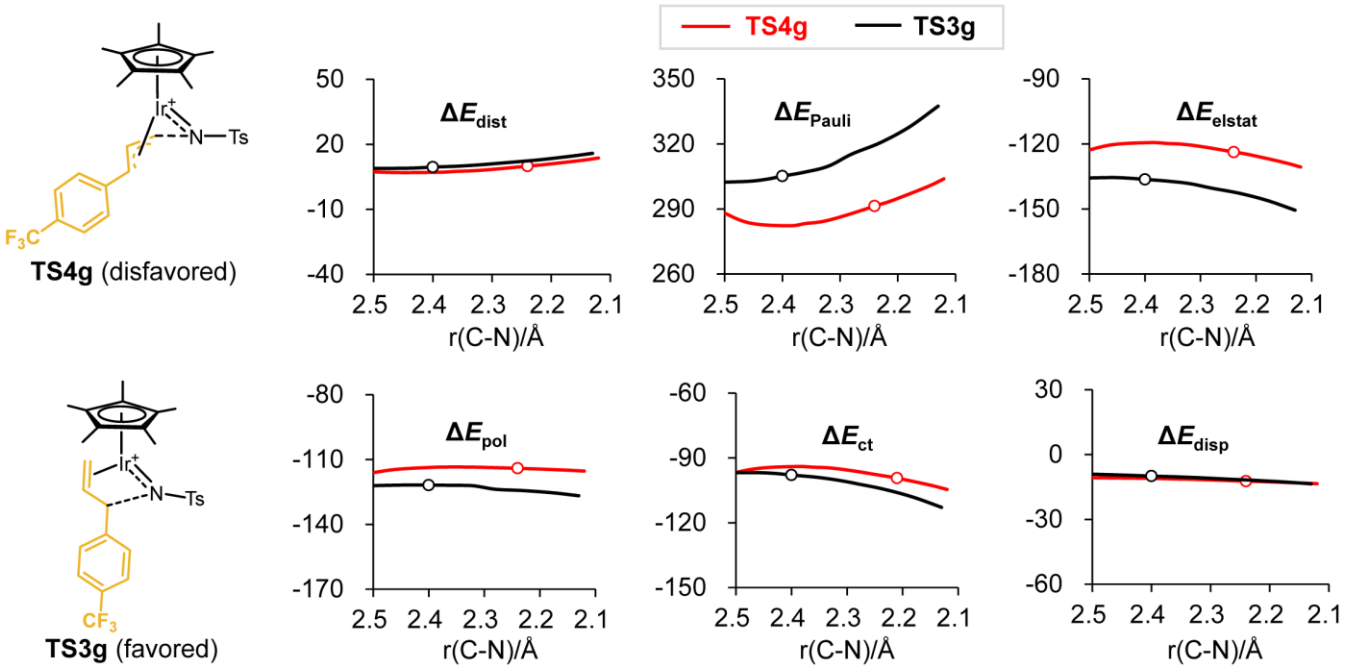

Fig. S7 EDA results along IRC of Ir=N-Ts insertion with Ph-4-CF_3-substituted allyl substrate (**TS3g** vs **TS4g**). Energies are shown in kcal/mol.

Cartesian Coordinates (Å) and Energies of the Optimized Structures

M1

B3LYP SCF energy: -1115.20587500 a.u.
B3LYP enthalpy: -1114.617875 a.u.
B3LYP free energy: -1114.718132 a.u.
B3LYP-D3BJ SCF energy in solution: -1116.54687038 a.u.
B3LYP-D3BJ enthalpy in solution: -1115.958870 a.u.
B3LYP-D3BJ free energy in solution: -1116.059127 a.u.
Three lowest frequencies (cm-1): 18.7963 21.6864 31.6920

Cartesian coordinates

ATOM	X	Y	Z
C	1.519717	0.012404	-0.105482
C	0.375826	-0.504485	-0.933561
C	-0.316654	0.227524	-1.900399
H	0.321928	-1.595525	-1.003949
H	-0.062488	1.277351	-2.072306
H	-0.811080	-0.276473	-2.734795
C	-1.420081	2.671798	-0.052264
O	-2.248418	2.128539	-0.852011
O	-0.746136	1.867186	0.669650
C	-1.223513	4.150551	0.009616
H	-2.119376	4.672812	-0.350183
H	-0.376848	4.424685	-0.641437
H	-0.973918	4.458968	1.033909
H	1.468568	1.107011	-0.021965
H	1.445558	-0.386642	0.920379
C	-3.608822	-0.932077	-0.482731
C	-3.684910	-0.247850	0.812172
C	-2.681538	-0.809293	1.664554
C	-1.939125	-1.795764	0.904635
C	-2.553601	-1.902319	-0.412490
C	-4.707730	0.783702	1.174093
H	-5.676096	0.297187	1.381129
H	-4.863466	1.499974	0.355113
H	-4.421025	1.348368	2.071161
C	-4.550592	-0.707615	-1.622822
H	-5.493031	-1.251579	-1.436765
H	-4.138990	-1.068705	-2.574402
H	-4.798750	0.356768	-1.737857
C	-2.226842	-2.921505	-1.459524
H	-2.834082	-3.827163	-1.290751
H	-1.173124	-3.230226	-1.430263
H	-2.452074	-2.558876	-2.471665
C	-0.889968	-2.703874	1.468252
H	-1.370017	-3.554969	1.981523
H	-0.256858	-2.189428	2.204540
H	-0.238774	-3.120096	0.688195
C	-2.409250	-0.433296	3.084281
H	-2.927711	-1.138215	3.757374
H	-2.767723	0.577520	3.317797

H	-1.336952	-0.480798	3.318185
C	2.875807	-0.412624	-0.708526
C	4.067038	0.072987	0.124229
H	2.955316	-0.019455	-1.737367
H	2.913750	-1.513336	-0.799709
H	4.021800	1.173591	0.215260
H	3.973622	-0.317536	1.154372
Ir	-1.728142	0.128822	-0.173942
C	5.425730	-0.335124	-0.453285
C	6.615731	0.148476	0.381463
H	5.517516	0.056397	-1.483192
H	5.467147	-1.436183	-0.546152
C	7.977652	-0.260192	-0.187115
H	6.573170	1.249765	0.472258
H	6.518869	-0.240306	1.412300
C	9.166918	0.221627	0.649967
H	8.019210	-1.361639	-0.279422
H	8.075503	0.129696	-1.217577
H	9.123173	1.322307	0.741114
H	9.066280	-0.167677	1.679599
C	10.523868	-0.190375	0.078130
H	10.672356	0.215779	-0.936458
H	11.353127	0.172906	0.705246
H	10.614858	-1.287389	0.010045

TS1

B3LYP SCF energy: -1115.17125277 a.u.
B3LYP enthalpy: -1114.589775 a.u.
B3LYP free energy: -1114.688471 a.u.
B3LYP-D3BJ SCF energy in solution: -1116.51787315 a.u.
B3LYP-D3BJ enthalpy in solution: -1115.936395 a.u.
B3LYP-D3BJ free energy in solution: -1116.035091 a.u.
Three lowest frequencies (cm-1): -1086.8156 12.5088 18.0455
Imaginary frequency: -1086.8156 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.799475	0.714268	-0.630085
C	0.299968	-0.273261	-1.589144
C	-0.777930	0.063715	-2.437279
H	0.727818	-1.281180	-1.592436
H	-0.953283	1.103471	-2.724703
H	-1.179665	-0.693418	-3.115114
C	-1.509880	2.851467	0.098183
O	-2.069022	1.955051	-0.644253
O	-0.531221	2.591546	0.832099
C	-2.057685	4.250998	0.011469
H	-1.387958	4.846073	-0.630862
H	-2.052087	4.714983	1.007292

H	-3.064483	4.261002	-0.422940
H	0.883569	1.714953	-1.083381
H	-0.100537	1.308883	0.265106
C	-3.360877	-0.965199	0.023330
C	-2.960100	-0.353857	1.293409
C	-1.770463	-0.995557	1.749679
C	-1.394427	-1.994957	0.763222
C	-2.407797	-2.011340	-0.270053
C	-3.722768	0.719286	2.004338
H	-4.525704	0.265038	2.609943
H	-4.196492	1.413131	1.296784
H	-3.080798	1.298896	2.681179
C	-4.626597	-0.669072	-0.720572
H	-5.473618	-1.209012	-0.263497
H	-4.559391	-0.977800	-1.772309
H	-4.862128	0.403843	-0.701096
C	-2.494226	-2.994054	-1.395676
H	-3.019682	-3.901093	-1.050525
H	-1.501722	-3.306325	-1.749301
H	-3.056156	-2.592573	-2.249433
C	-0.280668	-2.985593	0.916169
H	-0.631358	-3.852973	1.501681
H	0.578896	-2.558114	1.450400
H	0.070875	-3.367373	-0.052171
C	-1.037903	-0.708968	3.021936
H	-1.395470	-1.383543	3.819176
H	-1.197266	0.323250	3.361083
H	0.043547	-0.870609	2.915365
Ir	-1.417425	-0.037485	-0.321879
C	1.992965	0.354436	0.242456
C	3.323196	0.446159	-0.522739
H	1.860971	-0.665007	0.643936
H	2.024435	1.032496	1.111116
H	3.286976	-0.221137	-1.403464
H	3.437495	1.468707	-0.925087
C	4.544104	0.096004	0.333498
C	5.869327	0.191023	-0.429183
H	4.426134	-0.926503	0.738096
H	4.576622	0.765655	1.212386
C	7.096557	-0.158653	0.417457
H	5.831202	-0.476112	-1.310406
H	5.983354	1.213872	-0.832989
C	8.420916	-0.063567	-0.347041
H	7.134824	0.509465	1.298038
H	6.981946	-1.181484	0.822745
H	8.380434	-0.732090	-1.226371
H	8.531578	0.958257	-0.753286
C	9.643128	-0.410817	0.503562
H	9.581600	-1.440354	0.894188
H	10.574543	-0.332070	-0.078583
H	9.734736	0.265605	1.369723

2a

B3LYP SCF energy: -396.21558782 a.u.
B3LYP enthalpy: -396.142418 a.u.
B3LYP free energy: -396.178749 a.u.
B3LYP-D3BJ SCF energy in solution: -396.69900251 a.u.
B3LYP-D3BJ enthalpy in solution: -396.625833 a.u.
B3LYP-D3BJ free energy in solution: -396.662164 a.u.
Three lowest frequencies (cm-1): 163.2176 178.0284 300.5262

Cartesian coordinates

ATOM	X	Y	Z
C	0.980421	0.012957	0.000084
C	-1.201260	-0.181249	0.000383
O	-0.018652	-0.902935	-0.000037
O	-0.838730	1.125131	-0.000043
O	-2.296103	-0.631836	-0.000170
N	0.567248	1.228793	-0.000057
C	2.390701	-0.439621	-0.000032
H	2.592510	-1.056186	0.889828
H	2.592467	-1.055818	-0.890162
H	3.052991	0.435048	0.000117

M2

B3LYP SCF energy: -1282.50189188 a.u.
B3LYP enthalpy: -1281.907773 a.u.
B3LYP free energy: -1282.010399 a.u.
B3LYP-D3BJ SCF energy in solution: -1284.04858384 a.u.
B3LYP-D3BJ enthalpy in solution: -1283.454465 a.u.
B3LYP-D3BJ free energy in solution: -1283.557091 a.u.
Three lowest frequencies (cm-1): 14.8870 22.1984 25.1070

Cartesian coordinates

ATOM	X	Y	Z
C	0.907787	0.261257	-0.817661
C	0.315335	-0.551955	-1.817449
C	-0.901811	-0.127046	-2.435369
H	0.673357	-1.577597	-1.957432
H	-1.008788	0.927592	-2.707124
H	-1.409223	-0.820654	-3.111870
H	0.807729	1.345562	-0.935667
C	-3.095219	-1.115034	0.712073
C	-2.091220	-0.866451	1.756843
C	-0.997743	-1.751529	1.547904
C	-1.265115	-2.499896	0.325936
C	-2.601344	-2.154324	-0.133939
C	-2.276133	0.048574	2.929839

H	-2.823407	-0.475500	3.732410
H	-2.862297	0.941466	2.671317
H	-1.316192	0.382664	3.345892
C	-4.468851	-0.514047	0.684424
H	-5.138069	-1.059070	1.372387
H	-4.919592	-0.561766	-0.316464
H	-4.464700	0.536025	1.010912
C	-3.337373	-2.823509	-1.254321
H	-3.845724	-3.729137	-0.880526
H	-2.660675	-3.140355	-2.060170
H	-4.105120	-2.170566	-1.691467
C	-0.444370	-3.648037	-0.182783
H	-0.735572	-4.577209	0.336449
H	0.629072	-3.497450	-0.003526
H	-0.591043	-3.816372	-1.258823
C	0.177716	-1.938120	2.454414
H	-0.064682	-2.687332	3.228196
H	0.450735	-1.007189	2.969780
H	1.062630	-2.300967	1.915829
C	-2.465359	2.541869	-0.710257
C	-1.307958	3.760278	0.721505
O	-2.337166	3.780929	-0.215333
O	-0.858871	2.469676	0.738260
O	-0.917711	4.665792	1.360745
N	-1.615230	1.712673	-0.187007
C	-3.502250	2.276140	-1.730170
H	-3.299685	2.883061	-2.627178
H	-4.484318	2.585331	-1.339369
H	-3.517911	1.213072	-1.993168
C	2.120200	-0.171537	-0.035227
C	3.439913	0.299492	-0.675348
H	2.131093	-1.270682	0.061483
H	2.056191	0.232317	0.989367
C	4.679604	-0.120271	0.120744
H	3.507085	-0.097126	-1.704412
H	3.421619	1.399634	-0.776201
C	5.998003	0.346571	-0.503744
H	4.601596	0.275015	1.150459
H	4.692827	-1.221550	0.221709
H	6.072713	-0.046604	-1.534562
H	5.983596	1.447647	-0.603390
C	7.238436	-0.074085	0.290081
C	8.558747	0.393317	-0.330638
H	7.252342	-1.175721	0.389225
H	7.161668	0.317869	1.321580
C	9.791843	-0.030094	0.468382
H	8.633476	0.001085	-1.361271
H	8.542558	1.493940	-0.429975
H	9.766344	0.378354	1.492512
H	9.858158	-1.127747	0.552962
H	10.720797	0.322574	-0.006359

Ir -1.212974 -0.375219 -0.279679

TS2
B3LYP SCF energy: -1282.47431105 a.u.
B3LYP enthalpy: -1281.882905 a.u.
B3LYP free energy: -1281.988178 a.u.
B3LYP-D3BJ SCF energy in solution: -1284.03898077 a.u.
B3LYP-D3BJ enthalpy in solution: -1283.447575 a.u.
B3LYP-D3BJ free energy in solution: -1283.552848 a.u.
Three lowest frequencies (cm-1): -283.1984 14.2626 18.6004
Imaginary frequency: -283.1984 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.862277	-0.028696	-0.998907
C	0.130687	-0.909551	-1.824404
C	-1.046352	-0.457397	-2.491039
H	0.367404	-1.978549	-1.800359
H	-1.082729	0.562112	-2.881797
H	-1.654881	-1.185372	-3.033474
H	0.794771	1.042806	-1.203342
C	-3.291518	-0.845919	0.772150
C	-2.268696	-0.556642	1.761078
C	-1.223683	-1.539456	1.623555
C	-1.589285	-2.430360	0.541382
C	-2.871763	-2.009097	0.027103
C	-2.317620	0.512783	2.806758
H	-2.637676	0.077327	3.768964
H	-3.030241	1.306676	2.548698
H	-1.333337	0.978065	2.953031
C	-4.613334	-0.153112	0.649871
H	-5.350548	-0.642367	1.309905
H	-5.008371	-0.196846	-0.374226
H	-4.554137	0.900830	0.952768
C	-3.685879	-2.726600	-1.005453
H	-4.321571	-3.483588	-0.514277
H	-3.056862	-3.255238	-1.734730
H	-4.350459	-2.044920	-1.553363
C	-0.863258	-3.686172	0.159259
H	-1.205340	-4.521121	0.794286
H	0.222831	-3.595721	0.299447
H	-1.053252	-3.974187	-0.884089
C	-0.047250	-1.678980	2.537379
H	-0.348375	-2.232448	3.443931
H	0.336205	-0.701251	2.860543
H	0.775702	-2.235710	2.071596
C	-1.908101	2.750824	-0.728629
C	-0.181457	3.645313	0.818898
O	-1.450501	3.843723	-0.255192

O	0.010287	2.425649	0.877597
O	0.196912	4.681007	1.235915
N	-1.477725	1.558608	-0.448813
C	-3.059677	2.872463	-1.711126
H	-2.718937	3.490862	-2.555215
H	-3.876643	3.411659	-1.208558
H	-3.413975	1.900605	-2.073109
C	2.028439	-0.439792	-0.155815
C	3.369682	-0.037747	-0.809570
H	2.014902	-1.527293	0.027340
H	1.953356	0.064162	0.821510
C	4.580520	-0.419467	0.048603
H	3.451107	-0.512524	-1.803379
H	3.371126	1.051864	-0.987287
C	5.919836	-0.007279	-0.570017
H	4.478149	0.046062	1.045918
H	4.576948	-1.511617	0.221827
H	6.018799	-0.469467	-1.569608
H	5.919680	1.084665	-0.742072
C	7.132098	-0.385419	0.286554
C	8.473947	0.033375	-0.322703
H	7.133588	-1.478564	0.455710
H	7.027802	0.072482	1.287923
C	9.678844	-0.345556	0.539094
H	8.576276	-0.424396	-1.323514
H	8.469292	1.125437	-0.492060
H	9.626661	0.128954	1.533258
H	9.733525	-1.435789	0.696386
H	10.624169	-0.030304	0.070540
Ir	-1.369288	-0.328126	-0.310105

M3

B3LYP SCF energy: -1094.05860155 a.u.
B3LYP enthalpy: -1093.483451 a.u.
B3LYP free energy: -1093.583819 a.u.
B3LYP-D3BJ SCF energy in solution: -1095.38768262 a.u.
B3LYP-D3BJ enthalpy in solution: -1094.812532 a.u.
B3LYP-D3BJ free energy in solution: -1094.912900 a.u.
Three lowest frequencies (cm-1): 9.3633 21.1553 25.5529

Cartesian coordinates

ATOM	X	Y	Z
C	-1.493420	-2.207658	-0.216856
C	-1.329549	-1.759839	1.153131
C	-2.504006	-1.003580	1.519025
C	-3.381368	-0.971722	0.370165
C	-2.748912	-1.715281	-0.701789
C	-0.587011	-3.159336	-0.938559
H	-0.666019	-3.061319	-2.030175

H	0.466220	-3.028947	-0.655169
C	-0.227455	-2.163048	2.081637
H	0.704290	-2.383898	1.545621
H	-0.519298	-3.079167	2.624247
H	-0.017724	-1.388077	2.831324
C	-2.818896	-0.420310	2.859824
H	-1.930037	-0.371598	3.502008
H	-3.576377	-1.035181	3.373949
H	-3.218557	0.599887	2.763192
C	-4.759709	-0.391442	0.343593
H	-4.857707	0.457302	1.032987
H	-5.486474	-1.161418	0.657723
H	-5.048847	-0.057972	-0.662328
C	-3.371134	-2.027671	-2.028542
H	-4.054566	-1.233868	-2.359590
H	-3.960070	-2.958341	-1.955477
H	-2.617682	-2.181758	-2.813479
Ir	-1.454206	0.130736	-0.158662
H	-0.863612	-4.197545	-0.686370
C	-1.084009	1.011966	-2.135166
C	0.076840	0.293190	-1.724454
H	-1.677277	0.620785	-2.965527
H	-1.110152	2.098610	-2.022224
H	0.320979	-0.668587	-2.188103
C	0.786477	0.703510	-0.571217
H	0.728518	1.754961	-0.266772
C	1.939889	-0.060387	0.002663
H	1.893303	-1.123752	-0.284889
H	1.894608	-0.013408	1.103289
N	-1.765418	1.805990	0.602198
C	-1.368600	3.102024	0.404026
O	-0.226940	3.446054	0.687577
C	-2.453105	4.060571	-0.035422
H	-2.000533	4.835666	-0.671014
H	-2.869114	4.554000	0.858052
H	-3.274991	3.557415	-0.565605
C	3.289920	0.537871	-0.455669
C	4.490819	-0.198254	0.148176
H	3.327364	1.605131	-0.176819
H	3.347767	0.505470	-1.558015
C	5.842291	0.362264	-0.305321
H	4.425931	-0.153956	1.250841
H	4.432986	-1.270675	-0.115667
H	5.904456	0.317098	-1.408307
H	5.898296	1.434952	-0.044459
C	7.042050	-0.371982	0.301219
H	6.979722	-1.446503	0.045775
H	6.980280	-0.322496	1.404422
C	8.398035	0.176960	-0.153857
C	9.589372	-0.562130	0.456548
H	8.458238	1.250497	0.101397

H	8.457320	0.127510	-1.256396
H	10.545697	-0.142237	0.107723
H	9.580493	-0.498041	1.557485
H	9.578729	-1.631895	0.188380

TS3a

B3LYP SCF energy: -1094.05063902 a.u.
B3LYP enthalpy: -1093.476521 a.u.
B3LYP free energy: -1093.573865 a.u.
B3LYP-D3BJ SCF energy in solution: -1095.37707224 a.u.
B3LYP-D3BJ enthalpy in solution: -1094.802954 a.u.
B3LYP-D3BJ free energy in solution: -1094.900298 a.u.
Three lowest frequencies (cm-1): -187.6282 14.3079 24.1531
Imaginary frequency: -187.6282 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.104053	-0.623468	-2.503224
C	0.042752	-0.862470	-1.712182
C	0.937771	0.190204	-1.321252
H	0.268461	-1.870373	-1.346999
C	-0.586592	2.716858	-0.029437
C	-1.320795	3.976270	-0.444821
H	-1.550158	4.567282	0.453117
H	-0.652572	4.575997	-1.084642
H	-2.235879	3.765299	-1.016583
C	-1.770706	-0.528271	1.825932
C	-2.826539	0.329150	1.367986
C	-3.570085	-0.404912	0.340058
C	-2.990314	-1.726087	0.219813
C	-1.867388	-1.787950	1.100841
C	-3.191476	1.660141	1.950733
H	-3.872506	1.520442	2.807705
H	-2.303502	2.196232	2.313050
H	-3.707285	2.300046	1.221822
C	-0.786718	-0.187987	2.900083
H	-1.273566	-0.255728	3.888497
H	0.069645	-0.874934	2.906463
H	-0.404997	0.836290	2.777047
C	-0.988516	-2.979720	1.326486
H	-1.369838	-3.565582	2.180545
H	-0.968168	-3.650021	0.456238
H	0.044359	-2.691932	1.567646
C	-3.513217	-2.836596	-0.640086
H	-4.244922	-3.438787	-0.074775
H	-4.025457	-2.455491	-1.534164
H	-2.715231	-3.517570	-0.967736
C	-4.824569	0.067508	-0.325344
H	-5.696882	-0.193772	0.299287

H	-4.828894	1.157585	-0.460359
H	-4.968984	-0.399716	-1.308884
H	-1.175957	0.287391	-3.100036
O	0.198206	2.674998	0.911236
N	-0.783348	1.637468	-0.861712
Ir	-1.531481	-0.046049	-0.373947
H	-1.700969	-1.471759	-2.844601
H	1.042364	1.035594	-2.001586
C	2.008301	0.035539	-0.302932
C	3.409796	-0.004127	-0.961053
H	1.841367	-0.866613	0.307949
H	1.958670	0.908085	0.371446
H	3.464978	-0.847568	-1.671385
H	3.554706	0.913335	-1.557746
C	4.531816	-0.125782	0.076142
C	5.932285	-0.133481	-0.544370
H	4.385783	-1.049134	0.666141
H	4.450286	0.709751	0.794625
C	7.057036	-0.254036	0.488659
H	6.008116	-0.965986	-1.267981
H	6.074194	0.791300	-1.133157
C	8.461256	-0.248134	-0.124199
H	6.973541	0.574295	1.216632
H	6.917798	-1.182386	1.073591
H	8.542501	-1.075382	-0.852594
H	8.597036	0.679966	-0.708584
C	9.578386	-0.367211	0.913096
H	9.494350	-1.304222	1.488586
H	10.571651	-0.357797	0.437860
H	9.547220	0.466750	1.633998

TS4a

B3LYP SCF energy: -1094.04309306 a.u.
B3LYP enthalpy: -1093.468764 a.u.
B3LYP free energy: -1093.565707 a.u.
B3LYP-D3BJ SCF energy in solution: -1095.37261924 a.u.
B3LYP-D3BJ enthalpy in solution: -1094.798290 a.u.
B3LYP-D3BJ free energy in solution: -1094.895233 a.u.
Three lowest frequencies (cm-1): -277.7040 17.1125 27.5642
Imaginary frequency: -277.7040 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.958268	0.896654	-0.303683
C	0.275850	0.714543	-1.514660
C	-0.815035	1.561638	-1.921314
H	0.512561	-0.150346	-2.144863
C	-2.891435	2.521425	0.191646
C	-3.077160	3.348627	1.450949

H	-4.124762	3.269810	1.774169
H	-2.875579	4.403866	1.203743
H	-2.396367	3.052434	2.261510
C	-2.978364	-1.305674	-0.589226
C	-3.040321	-0.940797	0.801444
C	-1.820238	-1.437874	1.433630
C	-1.052774	-2.155140	0.439206
C	-1.739932	-2.041329	-0.809691
C	-4.211376	-0.314049	1.493195
H	-4.921456	-1.098337	1.806921
H	-4.747415	0.378985	0.830300
H	-3.908391	0.235024	2.395279
C	-4.041378	-1.025351	-1.603582
H	-4.865756	-1.750260	-1.486633
H	-3.664048	-1.118487	-2.630760
H	-4.453381	-0.013751	-1.478013
C	-1.326970	-2.664110	-2.108673
H	-1.803576	-3.653362	-2.217877
H	-0.240634	-2.817424	-2.166362
H	-1.636760	-2.059549	-2.972778
C	0.196702	-2.934485	0.707266
H	-0.068271	-3.935793	1.088514
H	0.829054	-2.453480	1.465930
H	0.798193	-3.079024	-0.199914
C	-1.504812	-1.368721	2.895186
H	-1.924143	-2.251706	3.408732
H	-1.938267	-0.475678	3.365323
H	-0.421854	-1.361630	3.079131
H	0.825772	1.851816	0.210973
O	-3.733150	2.427621	-0.687875
N	-1.633895	1.959922	0.088949
H	-0.758858	2.639419	-1.784730
H	-1.471849	1.229158	-2.729021
Ir	-1.299823	0.079150	-0.071507
C	2.143697	0.073832	0.105467
C	3.472449	0.783569	-0.236435
H	2.115033	-0.912912	-0.384555
H	2.110938	-0.105568	1.193505
H	3.508362	0.979570	-1.322706
H	3.491574	1.773598	0.252358
C	4.706204	-0.022031	0.183732
C	6.029162	0.674586	-0.150334
H	4.679775	-1.012902	-0.306310
H	4.659569	-0.220709	1.270290
C	7.267984	-0.129601	0.255481
H	6.067446	0.882039	-1.235664
H	6.055160	1.662457	0.345168
C	8.591602	0.567590	-0.075725
H	7.228054	-0.339748	1.340634
H	7.241674	-1.117101	-0.242096
H	8.627282	0.780147	-1.159731

H	8.616248	1.553164	0.423543
C	9.824541	-0.241860	0.327719
H	9.848478	-1.218750	-0.183519
H	10.755445	0.288449	0.073293
H	9.839620	-0.437056	1.413022

M4

B3LYP SCF energy: -1094.12196957 a.u.
B3LYP enthalpy: -1093.544694 a.u.
B3LYP free energy: -1093.640528 a.u.
B3LYP-D3BJ SCF energy in solution: -1095.43842147 a.u.
B3LYP-D3BJ enthalpy in solution: -1094.861146 a.u.
B3LYP-D3BJ free energy in solution: -1094.956980 a.u.
Three lowest frequencies (cm-1): 19.9783 24.2115 39.9785

Cartesian coordinates

ATOM	X	Y	Z
C	-0.377239	-1.153591	-1.914483
C	0.556382	-0.761015	-0.969922
C	1.060056	0.686565	-0.889111
H	1.013006	-1.504164	-0.308854
C	-0.361684	2.651592	-0.042591
C	0.642828	3.661041	-0.558049
H	0.109178	4.602461	-0.743246
H	1.396245	3.859516	0.221437
H	1.166107	3.341951	-1.469472
C	-2.955004	0.093888	1.479303
C	-3.597001	0.434286	0.252878
C	-3.563715	-0.753380	-0.607795
C	-2.971583	-1.835448	0.130161
C	-2.535783	-1.310939	1.393074
C	-4.237006	1.742863	-0.072392
H	-5.205759	1.822098	0.451039
H	-3.601622	2.578440	0.254178
H	-4.428869	1.848340	-1.148399
C	-2.809372	0.978976	2.674910
H	-3.732468	0.935136	3.279456
H	-1.977227	0.660747	3.317552
H	-2.634114	2.019933	2.375246
C	-1.903742	-2.088199	2.502594
H	-2.687094	-2.450547	3.191820
H	-1.357974	-2.966088	2.131529
H	-1.210574	-1.471195	3.090825
C	-2.852580	-3.261330	-0.317358
H	-3.702536	-3.848166	0.070140
H	-2.867086	-3.354021	-1.411956
H	-1.933319	-3.735473	0.054948
C	-4.189669	-0.841611	-1.962958
H	-5.272771	-1.029824	-1.860927

H	-4.071580	0.093296	-2.528336
H	-3.767637	-1.662191	-2.558286
H	-0.631223	-0.505033	-2.759692
O	-1.347681	2.999108	0.579365
N	-0.158765	1.290171	-0.325858
Ir	-1.465055	-0.164642	-0.162125
H	-0.656031	-2.204963	-2.012921
H	1.276380	1.086442	-1.898464
C	2.316603	0.809511	-0.015163
C	3.560896	0.179560	-0.652406
H	2.108162	0.345075	0.965092
H	2.517014	1.872405	0.185594
H	3.368662	-0.883533	-0.888018
H	3.760765	0.669214	-1.622840
C	4.807097	0.279486	0.233983
C	6.062536	-0.329513	-0.397429
H	4.605646	-0.215954	1.201659
H	4.996808	1.341514	0.475312
C	7.304246	-0.241759	0.494859
H	5.867390	-1.388685	-0.648982
H	6.267224	0.174181	-1.360200
C	8.563333	-0.846074	-0.134875
H	7.496496	0.817126	0.749712
H	7.098676	-0.747951	1.456603
H	8.367360	-1.902521	-0.394305
H	8.769587	-0.335961	-1.093395
C	9.796379	-0.760812	0.765444
H	9.636744	-1.295120	1.716895
H	10.680659	-1.203279	0.280746
H	10.041933	0.285588	1.012215

M5

B3LYP SCF energy: -1094.12494996 a.u.
B3LYP enthalpy: -1093.547276 a.u.
B3LYP free energy: -1093.644034 a.u.
B3LYP-D3BJ SCF energy in solution: -1095.44198876 a.u.
B3LYP-D3BJ enthalpy in solution: -1094.864315 a.u.
B3LYP-D3BJ free energy in solution: -1094.961073 a.u.
Three lowest frequencies (cm-1): 15.9245 22.6644 34.8380

Cartesian coordinates

ATOM	X	Y	Z
C	0.901433	0.936196	0.224577
C	0.232913	1.546943	-0.817968
C	-0.762073	2.672708	-0.558561
H	0.515387	1.319165	-1.851597
C	-3.154565	2.466096	0.221038
C	-1.857842	-1.833272	-1.144104
C	-3.030147	-1.354816	-0.403466

C	-2.700477	-1.372405	0.987336
C	-1.322823	-1.860626	1.109335
C	-0.842471	-2.203226	-0.198379
C	-4.359769	-1.012351	-0.993573
H	-5.029239	-1.887233	-0.919082
H	-4.277166	-0.747675	-2.056405
H	-4.823126	-0.171640	-0.461120
C	-1.801311	-2.045126	-2.622705
H	-2.242821	-3.025833	-2.874271
H	-0.769203	-2.041046	-2.998008
H	-2.371627	-1.279728	-3.166912
C	0.438456	-2.906822	-0.527851
H	0.243029	-3.987569	-0.635205
H	1.193105	-2.789774	0.259325
H	0.873985	-2.559280	-1.475009
C	-0.617420	-2.099293	2.406414
H	-0.923198	-3.075873	2.821088
H	-0.868115	-1.334035	3.154235
H	0.473761	-2.120481	2.285167
C	-3.618698	-1.036883	2.115719
H	-4.294361	-1.889117	2.306776
H	-4.229075	-0.156947	1.872566
H	-3.067816	-0.834105	3.043756
H	0.746464	1.341977	1.233796
N	-1.905954	1.905635	-0.081343
H	-0.390815	3.404849	0.181670
H	-0.979590	3.220330	-1.490590
Ir	-1.340248	0.025002	-0.083451
C	2.095784	0.043348	0.058158
C	3.411936	0.846563	0.155732
H	2.053220	-0.473143	-0.913480
H	2.099147	-0.729693	0.842698
H	3.430367	1.605023	-0.646405
H	3.432662	1.407122	1.107206
C	4.654689	-0.044598	0.057384
C	5.972591	0.734591	0.108042
H	4.611067	-0.628912	-0.880254
H	4.635563	-0.786545	0.876829
C	7.214485	-0.158743	0.029508
H	5.994826	1.466725	-0.720033
H	6.008736	1.331227	1.038113
C	8.536475	0.614818	0.064869
H	7.194425	-0.884736	0.863656
H	7.171123	-0.764003	-0.895297
H	8.556354	1.336151	-0.772194
H	8.575116	1.223989	0.986209
C	9.770313	-0.285669	-0.005676
H	9.780569	-0.881159	-0.933887
H	10.700593	0.302843	0.021007
H	9.800147	-0.992647	0.840166
O	-4.079685	1.758744	0.572720

C	-3.279292	3.969431	0.097176
H	-4.285136	4.265712	0.417348
H	-2.530689	4.486890	0.717861
H	-3.122509	4.293469	-0.944395

TS5

B3LYP SCF energy: -1323.05168354 a.u.
B3LYP enthalpy: -1322.409217 a.u.
B3LYP free energy: -1322.514932 a.u.
B3LYP-D3BJ SCF energy in solution: -1324.64841339 a.u.
B3LYP-D3BJ enthalpy in solution: -1324.005947 a.u.
B3LYP-D3BJ free energy in solution: -1324.111662 a.u.
Three lowest frequencies (cm-1): -754.6750 17.2708 22.4369
Imaginary frequency: -754.6750 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.778170	-2.258465	0.524567
C	-1.344127	-1.550971	1.646680
C	-2.693111	-1.186367	1.308739
C	-3.003301	-1.786489	0.007228
C	-1.828944	-2.433725	-0.477081
C	0.553141	-2.945759	0.503236
H	0.936709	-3.076192	-0.518197
H	1.308836	-2.404961	1.088906
C	-0.671073	-1.296771	2.955634
H	0.423508	-1.292562	2.863612
H	-0.939739	-2.106911	3.656559
H	-0.989017	-0.342644	3.392242
C	-3.674409	-0.492572	2.201119
H	-3.173522	0.245359	2.840343
H	-4.187482	-1.226069	2.846931
H	-4.441872	0.030699	1.615234
C	-4.342883	-1.730647	-0.652051
H	-4.726973	-0.700917	-0.674695
H	-5.059710	-2.347378	-0.084253
H	-4.311600	-2.109235	-1.681805
C	-1.704492	-3.249237	-1.727181
H	-2.438610	-2.950627	-2.487267
H	-1.877355	-4.314454	-1.496720
H	-0.701729	-3.174074	-2.171016
H	0.455494	-3.953853	0.942294
C	-0.527916	0.182318	-2.284339
C	0.522641	0.063594	-1.377306
H	-0.748984	-0.634905	-2.974734
H	-0.897304	1.166110	-2.580948
H	1.131962	-0.843692	-1.366470
C	1.004994	1.242329	-0.525729
H	1.248523	2.113105	-1.162269

C	2.242795	0.864921	0.295724
H	2.030761	-0.060453	0.860521
H	2.447364	1.642975	1.043745
N	-0.244020	1.506275	0.258893
C	-0.266351	2.108581	1.553134
O	-1.104352	1.772980	2.358275
C	0.661817	3.278511	1.811124
H	1.371376	3.015110	2.610979
H	0.045159	4.105614	2.193260
H	1.217439	3.617307	0.927936
Ir	-1.394689	-0.252880	-0.241159
C	-2.881085	2.345105	-1.074810
O	-2.954534	1.093665	-0.860051
O	-1.808963	3.007672	-0.959882
C	-4.139762	3.069457	-1.466651
H	-3.903592	3.852947	-2.199700
H	-4.545891	3.567712	-0.570752
H	-4.893267	2.377200	-1.861018
H	-0.959393	2.299450	-0.380781
C	3.497062	0.687447	-0.570213
C	4.747780	0.319129	0.235125
H	3.684393	1.625487	-1.123490
H	3.326264	-0.083512	-1.343509
C	6.008981	0.190032	-0.624414
H	4.914245	1.082478	1.017254
H	4.571000	-0.629643	0.775302
H	5.840855	-0.572038	-1.408136
H	6.177924	1.140427	-1.163512
C	7.267195	-0.169980	0.170823
C	8.529376	-0.281975	-0.690452
H	7.102788	-1.125131	0.704052
H	7.429770	0.588468	0.959162
C	9.783561	-0.639086	0.107949
H	8.364211	-1.038996	-1.478778
H	8.689722	0.673346	-1.222510
H	9.998399	0.120140	0.878316
H	9.670305	-1.608091	0.622249
H	10.668711	-0.710558	-0.543185

TS6

B3LYP SCF energy: -1323.05624031 a.u.
B3LYP enthalpy: -1322.412643 a.u.
B3LYP free energy: -1322.524908 a.u.
B3LYP-D3BJ SCF energy in solution: -1324.64401797 a.u.
B3LYP-D3BJ enthalpy in solution: -1324.000421 a.u.
B3LYP-D3BJ free energy in solution: -1324.112686 a.u.
Three lowest frequencies (cm-1): -95.0642 9.7258 17.8209
Imaginary frequency: -95.0642 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.805133	2.128546	-0.379784
C	3.250515	-1.816292	-1.025101
C	1.828916	-1.893168	-1.199594
C	1.207582	-2.098679	0.114072
C	2.246819	-2.106960	1.093458
C	3.523460	-1.885526	0.405622
C	1.094096	-1.859501	-2.501773
H	0.933581	-2.889428	-2.865189
H	1.655956	-1.315720	-3.272639
H	0.107121	-1.387291	-2.401034
C	4.287652	-1.656140	-2.089920
H	4.808297	-2.615153	-2.250309
H	5.036731	-0.905170	-1.802350
H	3.846508	-1.346939	-3.046334
C	4.876678	-1.893713	1.040082
H	5.264354	-2.926848	1.080791
H	4.844948	-1.506703	2.067732
H	5.592118	-1.287891	0.468080
C	2.088605	-2.313597	2.565003
H	2.298067	-3.368194	2.814381
H	1.069225	-2.085113	2.902636
H	2.788735	-1.690870	3.139156
C	-0.242377	-2.377737	0.359941
H	-0.410026	-3.468273	0.388739
H	-0.877603	-1.970632	-0.437195
H	-0.585947	-1.963457	1.317567
Ir	2.311257	-0.190484	0.060064
H	-1.045835	3.141249	-0.012207
N	0.524232	1.703712	0.113210
C	0.863553	1.739910	1.432164
C	0.052696	2.430303	2.479029
H	-0.105454	3.485727	2.205626
H	0.562223	2.364687	3.447497
H	-0.942024	1.961366	2.545025
O	1.927143	1.142485	1.736674
O	3.678436	1.220223	-0.638626
C	3.467247	2.410521	-1.089231
O	2.339444	2.931486	-1.178897
C	4.696167	3.180701	-1.502941
H	5.391329	2.533854	-2.055656
H	4.412935	4.052702	-2.104744
H	5.217657	3.526139	-0.595337
H	1.334444	2.186650	-0.502295
C	-1.914766	1.170425	-0.048764
C	-3.068583	1.506568	0.544887
H	-1.758865	0.131518	-0.362589
H	-3.223638	2.555358	0.836716
H	-0.692329	2.215864	-1.472873
C	-4.211582	0.572616	0.817557

C	-5.497495	0.933686	0.051156
H	-4.434795	0.587679	1.900853
H	-3.914327	-0.462286	0.574275
C	-6.665002	-0.007974	0.361335
H	-5.787199	1.972887	0.290833
H	-5.286372	0.920879	-1.032993
H	-6.362799	-1.048049	0.137058
H	-6.872768	0.015439	1.447158
C	-7.947523	0.321399	-0.408232
C	-9.110001	-0.627087	-0.100065
H	-7.736869	0.300781	-1.493651
H	-8.252438	1.359915	-0.182254
C	-10.394138	-0.307826	-0.872076
H	-8.801452	-1.666141	-0.321503
H	-9.322044	-0.603823	0.985264
C	-11.547021	-1.262581	-0.559461
H	-10.702647	0.729735	-0.649072
H	-10.179994	-0.329531	-1.956242
H	-12.452153	-1.003964	-1.131132
H	-11.284004	-2.304637	-0.807547
H	-11.811448	-1.235966	0.510938

1a

B3LYP SCF energy: -392.81982119 a.u.
B3LYP enthalpy: -392.527676 a.u.
B3LYP free energy: -392.583341 a.u.
B3LYP-D3BJ SCF energy in solution: -393.30265399 a.u.
B3LYP-D3BJ enthalpy in solution: -393.010509 a.u.
B3LYP-D3BJ free energy in solution: -393.066174 a.u.
Three lowest frequencies (cm-1): 26.9319 40.5096 66.3355

Cartesian coordinates

ATOM	X	Y	Z
C	-3.506958	0.687954	-0.401263
C	-3.998381	-0.718578	-0.188300
C	-5.083332	-1.056918	0.515180
H	-3.405459	-1.518889	-0.649647
H	-5.714563	-0.299760	0.993675
H	-5.386212	-2.100788	0.637833
H	-3.442430	0.886196	-1.488379
C	-2.133823	0.993524	0.230881
C	-0.957347	0.210628	-0.361570
H	-2.190017	0.806401	1.318379
H	-1.934549	2.074355	0.117410
H	-1.120382	-0.873468	-0.225799
H	-0.924027	0.375559	-1.455100
C	0.396458	0.588368	0.247734
C	1.579380	-0.186998	-0.339783
H	0.361072	0.426493	1.341189

H	0.567810	1.672727	0.112626
C	2.933211	0.190181	0.268538
H	1.408067	-1.271262	-0.203935
H	1.613642	-0.025762	-1.433538
C	4.116902	-0.584342	-0.319530
H	3.104875	1.274674	0.133380
H	2.899925	0.028335	1.362371
H	3.944482	-1.667732	-0.183577
H	4.148711	-0.422558	-1.412596
C	5.464937	-0.201144	0.292783
H	6.291882	-0.776723	-0.153203
H	5.684851	0.869052	0.140601
H	5.479045	-0.387167	1.379994
H	-4.253005	1.394269	0.000297

3a

B3LYP SCF energy: -600.67150510 a.u.
B3LYP enthalpy: -600.319533 a.u.
B3LYP free energy: -600.385477 a.u.
B3LYP-D3BJ SCF energy in solution: -601.41704947 a.u.
B3LYP-D3BJ enthalpy in solution: -601.065077 a.u.
B3LYP-D3BJ free energy in solution: -601.131021 a.u.
Three lowest frequencies (cm-1): 29.2187 38.8795 50.5646

Cartesian coordinates

ATOM	X	Y	Z
C	2.129691	0.493530	-0.774549
C	2.504807	1.843522	-0.186321
C	1.925601	2.486188	0.831447
H	3.361459	2.311485	-0.687283
H	2.291907	3.463210	1.158326
H	1.072566	2.077373	1.379813
H	1.865089	0.697991	-1.827842
C	4.108284	-0.963566	0.066602
O	5.067880	-1.636986	-0.268990
C	3.738947	-0.775814	1.528043
H	4.608038	-1.067134	2.130872
H	3.442345	0.255030	1.765167
H	2.898952	-1.439942	1.788225
N	3.309249	-0.377312	-0.889132
C	0.902283	-0.200415	-0.149616
H	0.968597	-0.176027	0.950886
H	0.947619	-1.264720	-0.433951
H	3.629519	-0.595282	-1.827619
C	-0.445727	0.376776	-0.600848
C	-1.646873	-0.310129	0.056124
H	-0.528085	0.280459	-1.699426
H	-0.485266	1.459768	-0.392928
C	-3.001868	0.223661	-0.417840

H	-1.595263	-1.398030	-0.135824
H	-1.574991	-0.198188	1.154160
H	-3.049826	1.313132	-0.233270
H	-3.077177	0.103512	-1.514764
C	-4.201757	-0.455476	0.248502
C	-5.558822	0.070782	-0.229136
H	-4.128840	-0.331101	1.345354
H	-4.150405	-1.545755	0.068516
C	-6.750698	-0.611576	0.443630
H	-5.608193	1.160582	-0.050735
H	-5.631165	-0.055684	-1.324900
H	-7.708662	-0.210374	0.075944
H	-6.750311	-1.698132	0.253523
H	-6.728887	-0.470003	1.537375

4a

B3LYP SCF energy: -600.68194004 a.u.
B3LYP enthalpy: -600.329875 a.u.
B3LYP free energy: -600.397023 a.u.
B3LYP-D3BJ SCF energy in solution: -601.42545405 a.u.
B3LYP-D3BJ enthalpy in solution: -601.073389 a.u.
B3LYP-D3BJ free energy in solution: -601.140537 a.u.
Three lowest frequencies (cm-1): 21.6365 30.4338 41.7643

Cartesian coordinates

ATOM	X	Y	Z
C	5.454717	0.320724	-0.182745
H	5.166235	-1.507918	-0.947878
N	4.792291	-0.882266	-0.240595
C	4.936837	1.336905	0.822607
H	3.880272	1.584000	0.636823
H	5.012648	0.949902	1.852063
H	5.549494	2.241990	0.734130
O	6.421415	0.538968	-0.891602
C	3.553692	-1.261131	0.426058
H	3.536517	-2.364687	0.459507
H	3.572256	-0.928416	1.476194
C	2.299550	-0.759889	-0.249431
C	1.324901	-0.072076	0.358115
H	2.209672	-0.994309	-1.318677
H	1.433460	0.154869	1.428912
C	0.057825	0.411426	-0.288909
H	0.083867	0.190487	-1.369882
H	0.005385	1.513277	-0.198759
C	-1.215524	-0.187694	0.332673
C	-2.508100	0.349626	-0.288187
H	-1.220530	0.013518	1.419942
H	-1.182943	-1.287353	0.230792
C	-3.781518	-0.246041	0.319388

H	-2.532533	1.450194	-0.181470
H	-2.497922	0.155851	-1.376923
H	-3.759036	-1.346080	0.207263
H	-3.788273	-0.057421	1.409195
C	-5.074337	0.298369	-0.295143
C	-6.349616	-0.296965	0.309900
H	-5.067274	0.111678	-1.385446
H	-5.097027	1.398524	-0.181646
C	-7.635556	0.254850	-0.307166
H	-6.326846	-1.396056	0.194183
H	-6.354191	-0.111862	1.399672
H	-8.530946	-0.194746	0.151134
H	-7.707333	1.347559	-0.174494
H	-7.679534	0.052498	-1.390618

TS3a1

B3LYP SCF energy: -1100.24054743 a.u.
B3LYP enthalpy: -1099.666613 a.u.
B3LYP free energy: -1099.763869 a.u.
B3LYP-D3BJ SCF energy in solution: -1101.57600217 a.u.
B3LYP-D3BJ enthalpy in solution: -1101.002068 a.u.
B3LYP-D3BJ free energy in solution: -1101.099324 a.u.
Three lowest frequencies (cm-1): -164.7834 16.5737 21.5108
Imaginary frequency: -164.7834 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.290242	-0.715115	-2.588989
C	-0.168173	-0.908855	-1.772523
C	0.671364	0.175804	-1.349902
H	0.061046	-1.904429	-1.376932
C	-0.886946	2.706442	-0.140134
C	-1.660454	3.948309	-0.545322
H	-2.005909	4.462467	0.363407
H	-0.972770	4.627473	-1.075183
H	-2.507712	3.728067	-1.210281
C	-1.902601	-0.495862	1.751126
C	-2.994563	0.316728	1.308058
C	-3.744724	-0.450266	0.317707
C	-3.123170	-1.746620	0.189117
C	-1.976213	-1.765417	1.043295
C	-3.376807	1.649092	1.872866
H	-4.023576	1.505492	2.755786
H	-2.494004	2.217102	2.196787
H	-3.937632	2.258323	1.151157
C	-0.905244	-0.107641	2.795222
H	-1.372483	-0.149842	3.794492
H	-0.038292	-0.780958	2.807839
H	-0.543339	0.918440	2.631448

C	-1.066705	-2.933164	1.269084
H	-1.422259	-3.517715	2.135454
H	-1.043467	-3.614447	0.407351
H	-0.037352	-2.620205	1.493574
C	-3.635687	-2.885329	-0.639494
H	-4.326684	-3.504310	-0.041630
H	-4.191653	-2.535093	-1.520016
H	-2.827323	-3.544850	-0.985093
C	-5.022467	-0.019012	-0.327961
H	-5.874735	-0.296557	0.317753
H	-5.061283	1.068992	-0.473773
H	-5.176215	-0.502917	-1.302053
H	-1.406640	0.203440	-3.165613
O	-0.092883	2.689630	0.797602
N	-1.071015	1.633968	-0.969112
H	-1.883780	-1.574785	-2.906409
H	0.766550	1.021662	-2.030604
Rh	-1.730322	-0.072676	-0.448549
C	1.737375	0.046882	-0.320174
C	3.141325	0.003832	-0.972407
H	1.574870	-0.848445	0.301996
H	1.678798	0.928680	0.340032
H	3.201329	-0.847445	-1.673186
H	3.284307	0.914617	-1.579654
C	4.262246	-0.102264	0.067554
C	5.663307	-0.110559	-0.551757
H	4.119503	-1.020301	0.666715
H	4.176706	0.740091	0.777554
C	6.788443	-0.221316	0.481845
H	5.741492	-0.947741	-1.269742
H	5.802899	0.810451	-1.146947
C	8.192404	-0.215542	-0.131659
H	6.702982	0.611365	1.204616
H	6.651969	-1.146357	1.072681
H	8.275025	-1.046386	-0.855815
H	8.325806	0.709758	-0.721002
C	9.310521	-0.326806	0.905405
H	10.303424	-0.317457	0.429393
H	9.277984	0.510657	1.622181
H	9.229130	-1.261134	1.485640

TS4a1

B3LYP SCF energy: -1100.23585378 a.u.
B3LYP enthalpy: -1099.661830 a.u.
B3LYP free energy: -1099.759452 a.u.
B3LYP-D3BJ SCF energy in solution: -1101.57285980 a.u.
B3LYP-D3BJ enthalpy in solution: -1100.998836 a.u.
B3LYP-D3BJ free energy in solution: -1101.096458 a.u.
Three lowest frequencies (cm-1): -246.8541 13.6832 24.4124

Imaginary frequency: -246.8541 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.863800	0.789048	-0.431614
C	0.106431	0.540480	-1.572688
C	-0.994259	1.376494	-1.974501
H	0.293775	-0.373666	-2.147283
C	-2.955548	2.581120	0.145659
C	-3.078407	3.466604	1.375615
H	-4.099741	3.375764	1.772944
H	-2.928620	4.512531	1.062255
H	-2.339432	3.228542	2.153632
C	-3.268266	-1.186352	-0.534929
C	-3.272082	-0.808001	0.850766
C	-2.080156	-1.375158	1.465522
C	-1.371005	-2.129033	0.461384
C	-2.080473	-1.990753	-0.775231
C	-4.382095	-0.092191	1.553403
H	-5.146693	-0.822042	1.871503
H	-4.871463	0.637127	0.893304
H	-4.031752	0.430679	2.453715
C	-4.339100	-0.855720	-1.524323
H	-5.216380	-1.503900	-1.353313
H	-4.007497	-1.016824	-2.558784
H	-4.661141	0.190928	-1.423222
C	-1.739724	-2.658527	-2.072039
H	-2.304226	-3.602413	-2.164903
H	-0.672679	-2.910315	-2.141827
H	-2.006331	-2.038650	-2.939878
C	-0.150239	-2.961213	0.702205
H	-0.444745	-3.953732	1.085033
H	0.515611	-2.508523	1.449914
H	0.427400	-3.124205	-0.217277
C	-1.728196	-1.301817	2.917193
H	-2.201805	-2.141473	3.456441
H	-2.084602	-0.371229	3.379360
H	-0.644473	-1.375767	3.080982
H	0.732560	1.753954	0.065708
O	-3.824752	2.500053	-0.713591
N	-1.739675	1.957053	0.050719
H	-0.914747	2.458438	-1.895976
H	-1.675380	1.020288	-2.751469
Rh	-1.496191	0.070610	-0.087379
C	2.042372	-0.030500	-0.009942
C	3.369777	0.700394	-0.319462
H	2.033278	-1.013438	-0.509108
H	1.995553	-0.216643	1.077197
H	3.425480	0.903837	-1.403211
H	3.363376	1.686908	0.176605
C	4.606223	-0.089148	0.122619

C	5.922486	0.637836	-0.171098
H	4.610281	-1.074318	-0.379047
H	4.536325	-0.300604	1.205518
C	7.167934	-0.144710	0.256187
H	5.982907	0.858695	-1.252713
H	5.915780	1.620200	0.335894
C	8.483157	0.586729	-0.031881
H	7.105131	-0.370273	1.337155
H	7.176366	-1.125562	-0.254805
H	8.540770	0.815853	-1.111538
H	8.472907	1.565298	0.481557
C	9.724056	-0.200275	0.391052
H	9.784057	-1.168156	-0.134079
H	10.648288	0.355538	0.168739
H	9.716117	-0.411925	1.473352

TS3b

B3LYP SCF energy: -1049.94547565 a.u.
B3LYP enthalpy: -1049.493037 a.u.
B3LYP free energy: -1049.578454 a.u.
B3LYP-D3BJ SCF energy in solution: -1051.20940772 a.u.
B3LYP-D3BJ enthalpy in solution: -1050.756969 a.u.
B3LYP-D3BJ free energy in solution: -1050.842386 a.u.
Three lowest frequencies (cm-1): -148.7020 23.2999 28.5762
Imaginary frequency: -148.7020 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.376020	-0.571351	-2.507278
C	0.739719	-0.994479	-1.746400
C	1.887462	-0.141673	-1.536848
H	0.803601	-2.030115	-1.401988
C	0.790666	2.494279	0.122750
C	0.396000	3.895398	-0.306084
H	0.307141	4.530989	0.586092
H	1.193907	4.310828	-0.943637
H	-0.537198	3.908223	-0.887696
C	-1.157841	-0.498873	1.751684
C	-1.974057	0.605218	1.326201
C	-2.839755	0.116051	0.250497
C	-2.575809	-1.291928	0.060347
C	-1.522506	-1.660219	0.953369
C	-2.050572	1.949118	1.984539
H	-2.803656	1.931175	2.790977
H	-1.087940	2.233696	2.430497
H	-2.346193	2.735955	1.276617
C	-0.149352	-0.451849	2.856740
H	-0.661649	-0.441858	3.834485
H	0.516558	-1.324678	2.841041

H	0.472626	0.452930	2.785118
C	-0.946128	-3.033163	1.117254
H	-1.468864	-3.564907	1.930949
H	-1.057638	-3.639317	0.207755
H	0.119336	-3.001187	1.385782
C	-3.322125	-2.203446	-0.866526
H	-4.198239	-2.632370	-0.350590
H	-3.694598	-1.671813	-1.753205
H	-2.703286	-3.045059	-1.208652
C	-3.929607	0.899900	-0.410283
H	-4.870395	0.777188	0.154982
H	-3.700709	1.973728	-0.440066
H	-4.113935	0.560060	-1.438560
H	-0.303015	0.328514	-3.121363
O	1.473368	2.262808	1.112280
N	0.414788	1.497132	-0.750403
Ir	-0.731485	0.031081	-0.397081
H	-1.109758	-1.311413	-2.833804
H	2.014089	0.684533	-2.233767
C	3.017751	-0.424096	-0.696133
C	4.110846	0.477272	-0.726373
C	3.100789	-1.564764	0.142613
C	5.245675	0.245721	0.043936
H	4.054329	1.363360	-1.363085
C	4.237022	-1.794657	0.905598
H	2.272630	-2.273684	0.188330
C	5.310234	-0.889583	0.859507
H	6.081660	0.947275	0.012509
H	4.299467	-2.679947	1.542067
H	6.201229	-1.074963	1.464354

TS4b

B3LYP SCF energy: -1049.93747349 a.u.
B3LYP enthalpy: -1049.484907 a.u.
B3LYP free energy: -1049.570174 a.u.
B3LYP-D3BJ SCF energy in solution: -1051.20518768 a.u.
B3LYP-D3BJ enthalpy in solution: -1050.752621 a.u.
B3LYP-D3BJ free energy in solution: -1050.837888 a.u.
Three lowest frequencies (cm-1): -284.9835 19.1162 29.4750
Imaginary frequency: -284.9835 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.589903	-1.367648	-0.771632
C	-0.823742	-0.788974	-1.791082
C	0.457463	-1.309098	-2.192711
H	-1.182031	0.109292	-2.301360
C	2.539652	-2.182325	-0.062218
C	2.799284	-3.172376	1.059399

H	3.795285	-2.978081	1.481304
H	2.802379	-4.188076	0.630605
H	2.030453	-3.138256	1.844263
C	1.882777	1.666467	-0.275449
C	1.929859	1.115501	1.057489
C	0.593607	1.253670	1.626176
C	-0.241114	1.948712	0.669620
C	0.537383	2.175452	-0.508047
C	3.160610	0.636117	1.762470
H	3.687366	1.494179	2.214562
H	3.856199	0.142262	1.069695
H	2.922079	-0.067047	2.572126
C	3.048166	1.756442	-1.208943
H	3.726846	2.562885	-0.881209
H	2.734525	1.985476	-2.236142
H	3.615462	0.814084	-1.221942
C	0.092175	2.902754	-1.740246
H	0.378219	3.966289	-1.671548
H	-0.998158	2.866591	-1.868565
H	0.561426	2.500702	-2.649185
C	-1.654428	2.378189	0.905748
H	-1.666980	3.344545	1.438942
H	-2.206491	1.653696	1.520001
H	-2.207955	2.511295	-0.033027
C	0.195633	0.884727	3.021303
H	0.382484	1.736010	3.699169
H	0.772051	0.028811	3.397551
H	-0.872260	0.635983	3.087761
H	-1.224699	-2.305229	-0.348099
O	3.410933	-1.770576	-0.812567
N	1.203339	-1.859973	-0.208490
H	0.624172	-2.382709	-2.241000
H	1.073304	-0.717594	-2.874086
Ir	0.522807	-0.071262	-0.124926
C	-2.926159	-0.955852	-0.351646
C	-3.669303	0.048865	-1.011078
C	-3.525268	-1.629126	0.735965
C	-4.959865	0.366148	-0.593722
H	-3.250264	0.569148	-1.875272
C	-4.813937	-1.304611	1.156543
H	-2.968942	-2.419054	1.247604
C	-5.534763	-0.305313	0.493365
H	-5.528756	1.133894	-1.123259
H	-5.263081	-1.838311	1.997117
H	-6.548389	-0.055555	0.815437

TS3c

B3LYP SCF energy: -1164.39427881 a.u.

B3LYP enthalpy: -1163.906529 a.u.

B3LYP free energy: -1163.996927 a.u.
B3LYP-D3BJ SCF energy in solution: -1165.79252721 a.u.
B3LYP-D3BJ enthalpy in solution: -1165.304777 a.u.
B3LYP-D3BJ free energy in solution: -1165.395175 a.u.
Three lowest frequencies (cm-1): -127.1027 20.6486 31.2230
Imaginary frequency: -127.1027 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.967822	-0.508968	-2.501516
C	0.216861	-0.877371	-1.821940
C	1.363918	0.015991	-1.753388
H	0.367748	-1.914385	-1.510698
C	0.323147	2.484737	0.169078
C	-0.051164	3.899775	-0.234211
H	-0.042396	4.541503	0.657690
H	0.701464	4.283536	-0.942791
H	-1.029756	3.943178	-0.734380
C	-1.532794	-0.614393	1.760031
C	-2.374894	0.509971	1.446459
C	-3.309349	0.075378	0.407545
C	-3.050255	-1.313157	0.116102
C	-1.941906	-1.728459	0.920354
C	-2.410643	1.815265	2.182491
H	-3.106075	1.750768	3.036896
H	-1.419327	2.081366	2.573757
H	-2.754620	2.637319	1.539152
C	-0.465215	-0.627906	2.809776
H	-0.922414	-0.701954	3.811894
H	0.212394	-1.484135	2.692108
H	0.137318	0.291764	2.773214
C	-1.361271	-3.109068	0.972167
H	-1.863224	-3.699436	1.758137
H	-1.494366	-3.649670	0.024754
H	-0.289136	-3.095232	1.214290
C	-3.842484	-2.174632	-0.820935
H	-4.672308	-2.661779	-0.280802
H	-4.284075	-1.589927	-1.639895
H	-3.231492	-2.973619	-1.264615
C	-4.437634	0.891896	-0.139955
H	-5.339149	0.745766	0.481053
H	-4.204553	1.965275	-0.134372
H	-4.693394	0.601771	-1.168311
H	-0.980717	0.395676	-3.113453
O	1.020453	2.232184	1.143831
N	-0.090306	1.504575	-0.705275
Ir	-1.223971	0.034481	-0.368244
H	-1.688469	-1.279283	-2.784516
H	1.387357	0.832196	-2.474477
C	2.572859	-0.226174	-1.050019
C	3.671709	0.649428	-1.261996

C	2.756995	-1.310225	-0.140931
C	4.889911	0.462260	-0.632519
H	3.551093	1.493184	-1.946105
C	3.960903	-1.507773	0.492267
H	1.932706	-1.994968	0.064287
C	5.049777	-0.625142	0.256416
H	5.709773	1.153018	-0.825630
H	4.116877	-2.335097	1.186564
O	6.168233	-0.903167	0.913608
C	7.331206	-0.091911	0.762360
H	7.136790	0.941831	1.090359
H	8.097864	-0.540594	1.404735
H	7.681330	-0.094426	-0.282458

TS4c

B3LYP SCF energy: -1164.38159092 a.u.
B3LYP enthalpy: -1163.894032 a.u.
B3LYP free energy: -1163.986950 a.u.
B3LYP-D3BJ SCF energy in solution: -1165.78543143 a.u.
B3LYP-D3BJ enthalpy in solution: -1165.297873 a.u.
B3LYP-D3BJ free energy in solution: -1165.390791 a.u.
Three lowest frequencies (cm-1): -299.0809 10.0682 22.0947
Imaginary frequency: -299.0809 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.271607	-1.272056	-0.964359
C	-0.348530	-0.671369	-1.828896
C	0.919780	-1.270502	-2.163378
H	-0.601823	0.268123	-2.327740
C	2.762543	-2.413689	0.022877
C	2.841365	-3.418678	1.159408
H	3.848458	-3.380469	1.597500
H	2.688406	-4.428073	0.743224
H	2.075423	-3.250286	1.929783
C	2.499612	1.583662	-0.230804
C	2.509639	1.012355	1.098991
C	1.188128	1.236503	1.666866
C	0.401126	1.993056	0.715939
C	1.197282	2.191710	-0.455535
C	3.703662	0.436804	1.794721
H	4.313665	1.250182	2.224304
H	4.340066	-0.131031	1.101779
H	3.414888	-0.229309	2.619208
C	3.671755	1.613034	-1.160123
H	4.366480	2.415983	-0.857667
H	3.369338	1.812506	-2.197066
H	4.221609	0.661012	-1.137708
C	0.803117	2.963939	-1.678240

H	1.155228	4.006481	-1.596740
H	-0.287139	2.998407	-1.809277
H	1.246558	2.543522	-2.592034
C	-0.989038	2.494399	0.952837
H	-0.958190	3.442921	1.516412
H	-1.584913	1.780527	1.538660
H	-1.524220	2.686485	0.013452
C	0.759408	0.870388	3.053749
H	0.993766	1.696713	3.747477
H	1.279166	-0.026320	3.417334
H	-0.322213	0.686499	3.109899
H	-0.976360	-2.228971	-0.527573
O	3.708905	-2.143204	-0.700094
N	1.495117	-1.900386	-0.173637
H	1.009554	-2.350567	-2.252299
H	1.611468	-0.708977	-2.795774
Ir	1.034068	-0.049448	-0.104464
C	-2.605627	-0.819508	-0.657731
C	-3.208884	0.323457	-1.249113
C	-3.387573	-1.574496	0.247364
C	-4.509144	0.679847	-0.952302
H	-2.652918	0.927964	-1.968848
C	-4.697149	-1.227735	0.556712
H	-2.951359	-2.462273	0.712947
C	-5.275564	-0.090527	-0.043595
H	-4.982845	1.548377	-1.413422
H	-5.264737	-1.843241	1.254104
O	-6.522266	0.333671	0.174309
C	-7.386347	-0.381150	1.048447
H	-6.983115	-0.409940	2.074476
H	-8.338305	0.163227	1.048962
H	-7.555801	-1.409712	0.689097

TS3d

B3LYP SCF energy: -1386.72549893 a.u.
B3LYP enthalpy: -1386.264584 a.u.
B3LYP free energy: -1386.358991 a.u.
B3LYP-D3BJ SCF energy in solution: -1388.40634429 a.u.
B3LYP-D3BJ enthalpy in solution: -1387.945429 a.u.
B3LYP-D3BJ free energy in solution: -1388.039836 a.u.
Three lowest frequencies (cm-1): -161.3632 16.5391 19.2908
Imaginary frequency: -161.3632 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.603745	-0.178677	-2.583041
C	-0.324464	-0.549761	-2.109071
C	0.725466	0.418579	-1.903760
H	-0.081083	-1.606699	-1.971163

C	-0.350962	2.638119	0.257641
C	-1.025800	3.993673	0.163453
H	-1.033398	4.457197	1.160070
H	-0.433254	4.638312	-0.506643
H	-2.044713	3.931632	-0.244841
C	-1.512275	-0.834158	1.709380
C	-2.528576	0.179053	1.629792
C	-3.526240	-0.283161	0.661277
C	-3.134663	-1.596250	0.196740
C	-1.887932	-1.919003	0.813474
C	-2.632868	1.392350	2.502757
H	-3.171969	1.140741	3.432126
H	-1.641070	1.772692	2.782966
H	-3.186213	2.204606	2.011572
C	-0.309870	-0.787626	2.598262
H	-0.591503	-1.063289	3.629543
H	0.469667	-1.487708	2.269056
H	0.126599	0.221528	2.618476
C	-1.130445	-3.200556	0.649898
H	-1.436716	-3.916270	1.432355
H	-1.326034	-3.677613	-0.320321
H	-0.046275	-3.054712	0.755831
C	-3.929828	-2.472693	-0.722902
H	-4.636893	-3.089491	-0.142058
H	-4.521329	-1.885562	-1.439025
H	-3.290249	-3.161600	-1.292348
C	-4.814411	0.408616	0.344473
H	-5.592940	0.087983	1.059154
H	-4.722467	1.500197	0.424105
H	-5.171762	0.166569	-0.665608
H	-1.755326	0.808595	-3.023490
O	0.563614	2.396363	1.034624
N	-0.769050	1.718703	-0.679887
Ir	-1.606133	0.044961	-0.362135
H	-2.296398	-0.957715	-2.908439
H	0.641926	1.354896	-2.451153
C	2.007943	0.167844	-1.291038
C	2.952167	1.219887	-1.269802
C	2.374135	-1.081150	-0.732562
C	4.214843	1.036303	-0.714822
H	2.684299	2.190844	-1.691881
C	3.635567	-1.267374	-0.187249
H	1.670492	-1.914729	-0.737340
C	4.556737	-0.206123	-0.171209
H	4.938178	1.852764	-0.706273
H	3.921427	-2.237740	0.222511
C	5.911989	-0.411020	0.479918
F	6.378694	-1.644453	0.240205
F	5.818264	-0.264831	1.810207
F	6.811167	0.471456	0.031788

TS4d

B3LYP SCF energy: -1386.71921118 a.u.

B3LYP enthalpy: -1386.258178 a.u.

B3LYP free energy: -1386.352070 a.u.

B3LYP-D3BJ SCF energy in solution: -1388.40462293 a.u.

B3LYP-D3BJ enthalpy in solution: -1387.943590 a.u.

B3LYP-D3BJ free energy in solution: -1388.037482 a.u.

Three lowest frequencies (cm-1): -274.1861 19.9391 20.8064

Imaginary frequency: -274.1861 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.598571	-1.425458	-0.971496
C	0.240150	-0.837799	-1.927641
C	1.571573	-1.320467	-2.185129
H	-0.092696	0.041742	-2.486217
C	3.442142	-2.119071	0.156816
C	3.626438	-3.078094	1.318878
H	4.574906	-2.845425	1.822980
H	3.695633	-4.102072	0.916256
H	2.789937	-3.049855	2.031674
C	2.664842	1.712932	-0.193870
C	2.637581	1.168676	1.143042
C	1.260386	1.258953	1.615378
C	0.470150	1.915393	0.595704
C	1.321391	2.168686	-0.525060
C	3.832550	0.743629	1.937956
H	4.280450	1.622766	2.432425
H	4.601217	0.288746	1.298091
H	3.567029	0.023371	2.723874
C	3.889590	1.840741	-1.042842
H	4.516068	2.670152	-0.671658
H	3.642060	2.056845	-2.090624
H	4.487809	0.918183	-1.009538
C	0.936747	2.878183	-1.787795
H	1.173473	3.952357	-1.699607
H	-0.139322	2.798844	-1.993662
H	1.486245	2.498459	-2.660791
C	-0.969583	2.297253	0.728052
H	-1.048643	3.286092	1.211994
H	-1.529696	1.582045	1.345458
H	-1.470047	2.365090	-0.246458
C	0.779913	0.883055	2.981963
H	0.876771	1.748845	3.660272
H	1.367696	0.059908	3.409859
H	-0.276905	0.583796	2.975071
H	-0.257561	-2.356080	-0.514186
O	4.363680	-1.692795	-0.521652
N	2.116001	-1.841431	-0.118376

H	1.776094	-2.388757	-2.197718
H	2.242324	-0.715209	-2.799356
Ir	1.367393	-0.078374	-0.128633
C	-1.980863	-1.041116	-0.681541
C	-2.687015	-0.070966	-1.424543
C	-2.657566	-1.703985	0.364428
C	-4.011621	0.232766	-1.123182
H	-2.212761	0.436372	-2.267265
C	-3.980428	-1.396927	0.672489
H	-2.136016	-2.473845	0.938690
C	-4.659252	-0.420426	-0.066112
H	-4.553890	0.970452	-1.717321
H	-4.493127	-1.923251	1.479574
C	-6.076487	-0.037314	0.305985
F	-6.072712	0.947958	1.221685
F	-6.743078	-1.072620	0.831902
F	-6.760898	0.405299	-0.757374

TS3e

B3LYP SCF energy: -1125.32846202 a.u.
B3LYP enthalpy: -1124.855631 a.u.
B3LYP free energy: -1124.946931 a.u.
B3LYP-D3BJ SCF energy in solution: -1126.69372383 a.u.
B3LYP-D3BJ enthalpy in solution: -1126.220893 a.u.
B3LYP-D3BJ free energy in solution: -1126.312193 a.u.
Three lowest frequencies (cm-1): -165.9816 20.0554 23.5316
Imaginary frequency: -165.9816 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.088509	-0.752677	-2.292252
C	0.843954	-1.196781	-1.183288
C	1.746795	-0.328554	-0.483595
H	0.729651	-2.217105	-0.801010
C	0.496100	2.520377	0.276451
C	0.172928	3.887744	-0.289795
H	1.105018	4.338218	-0.668730
H	-0.546412	3.843800	-1.119975
H	-0.205840	4.527696	0.519921
C	-1.842326	-0.311645	1.630720
C	-2.525093	0.694549	0.868886
C	-3.042632	0.049853	-0.342735
C	-2.714952	-1.358557	-0.279899
C	-1.945434	-1.571158	0.905451
C	-2.788695	2.102754	1.305818
H	-3.711129	2.141028	1.910143
H	-1.968357	2.493598	1.923659
H	-2.927779	2.777297	0.449978
C	-1.190199	-0.105430	2.960861

H	-1.958108	-0.080234	3.753625
H	-0.492079	-0.917119	3.205114
H	-0.636543	0.843890	2.991600
C	-1.415720	-2.885797	1.390120
H	-2.109103	-3.313714	2.134364
H	-1.319216	-3.617324	0.576583
H	-0.438212	-2.783160	1.882561
C	-3.154360	-2.403953	-1.259515
H	-4.113349	-2.843279	-0.935603
H	-3.310099	-1.984958	-2.262962
H	-2.430799	-3.227236	-1.341273
C	-3.917114	0.701362	-1.367926
H	-4.975004	0.616738	-1.063110
H	-3.688585	1.769860	-1.479454
H	-3.816023	0.225778	-2.352940
H	0.403024	0.132843	-2.846887
O	0.973503	2.349088	1.393987
N	0.321661	1.476842	-0.599996
Ir	-0.856805	-0.010422	-0.388561
H	-0.529431	-1.470231	-2.836357
H	2.256052	0.449250	-1.049386
C	2.330311	-0.644867	0.844492
H	1.828855	-1.479439	1.351914
H	2.226106	0.260115	1.473071
C	3.834403	-0.963385	0.798489
O	4.344147	-1.783788	1.510708
O	4.470923	-0.200181	-0.091166
C	5.915290	-0.349505	-0.179636
C	6.421271	0.596116	-1.245138
H	6.137971	-1.402763	-0.409762
H	6.341605	-0.130246	0.811297
H	7.515028	0.505072	-1.327298
H	5.984963	0.361367	-2.228171
H	6.183377	1.641223	-0.995033

TS4e

B3LYP SCF energy: -1125.31971953 a.u.
B3LYP enthalpy: -1124.846638 a.u.
B3LYP free energy: -1124.938745 a.u.
B3LYP-D3BJ SCF energy in solution: -1126.69007633 a.u.
B3LYP-D3BJ enthalpy in solution: -1126.216995 a.u.
B3LYP-D3BJ free energy in solution: -1126.309102 a.u.
Three lowest frequencies (cm-1): -276.4116 14.6592 19.6285
Imaginary frequency: -276.4116 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.677159	0.342215	-0.471319
C	-1.341823	0.505423	0.879664

C	-0.583042	1.635491	1.345310
H	-1.586939	-0.282388	1.600127
C	1.769422	2.723773	-0.372777
C	2.126643	3.388068	-1.689933
H	1.746302	2.840458	-2.563749
H	3.218715	3.499690	-1.745332
H	1.680775	4.396282	-1.698568
C	2.382450	-0.797170	1.129416
C	2.718353	-0.661432	-0.261748
C	1.812314	-1.528182	-1.014090
C	0.973945	-2.236003	-0.070727
C	1.292112	-1.759097	1.239079
C	3.881836	0.103820	-0.811559
H	4.784936	-0.530124	-0.790524
H	4.090832	1.003354	-0.216270
H	3.718526	0.407645	-1.854618
C	3.081462	-0.106169	2.256991
H	4.061687	-0.581700	2.434165
H	2.510800	-0.167765	3.193025
H	3.250982	0.955400	2.024073
C	0.698148	-2.242137	2.527137
H	1.336420	-3.031649	2.959500
H	-0.301909	-2.673488	2.384748
H	0.626044	-1.439849	3.275058
C	0.008071	-3.325654	-0.417140
H	0.543192	-4.289355	-0.472783
H	-0.467199	-3.161324	-1.393673
H	-0.782103	-3.437696	0.337781
C	1.871962	-1.776173	-2.489006
H	2.604937	-2.574216	-2.701592
H	2.188191	-0.881118	-3.041707
H	0.902763	-2.102037	-2.890335
H	-1.601898	1.215394	-1.122921
O	2.348954	2.947566	0.678431
N	0.656104	1.909266	-0.458368
H	-0.803190	2.637027	0.981761
H	-0.117645	1.590721	2.333096
Ir	0.648207	0.043698	-0.010288
C	-2.524209	-0.790598	-0.970579
H	-2.418226	-1.676751	-0.324486
H	-2.249983	-1.079946	-1.993479
C	-4.021943	-0.448693	-1.011957
O	-4.408097	0.172911	0.108385
O	-4.745727	-0.738224	-1.925826
C	-5.815623	0.510836	0.219169
C	-6.026246	1.230860	1.532247
H	-6.399594	-0.420475	0.154743
H	-6.091801	1.130358	-0.647978
H	-7.088848	1.495938	1.641433
H	-5.744339	0.595088	2.385651
H	-5.437194	2.159846	1.576633

TS3f

B3LYP SCF energy: -1791.30805997 a.u.

B3LYP enthalpy: -1790.747714 a.u.

B3LYP free energy: -1790.855508 a.u.

B3LYP-D3BJ SCF energy in solution: -1793.19764722 a.u.

B3LYP-D3BJ enthalpy in solution: -1792.637301 a.u.

B3LYP-D3BJ free energy in solution: -1792.745095 a.u.

Three lowest frequencies (cm-1): -99.0525 9.6166 15.2584

Imaginary frequency: -99.0525 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.944935	0.767242	-2.414931
C	0.816214	1.766328	-1.419898
C	-0.314019	1.809415	-0.548120
H	1.606490	2.509478	-1.269070
C	3.098528	0.423308	1.059153
C	2.617631	-0.908273	1.388301
C	2.867552	-1.743639	0.246063
C	3.524455	-0.932676	-0.775776
C	3.699442	0.390955	-0.253515
C	2.107492	-1.341526	2.725182
H	2.964268	-1.545150	3.391475
H	1.487595	-0.565994	3.195172
H	1.497733	-2.249159	2.649434
C	3.101591	1.581293	2.005712
H	3.982151	1.512994	2.668361
H	3.162216	2.546677	1.484811
H	2.210957	1.581954	2.649154
C	4.440710	1.514575	-0.914888
H	5.511510	1.466370	-0.653766
H	4.373338	1.466919	-2.010770
H	4.076335	2.499953	-0.591335
C	4.052089	-1.453097	-2.076803
H	5.037405	-1.923976	-1.916136
H	3.389993	-2.214456	-2.511301
H	4.187115	-0.652441	-2.816296
C	2.620005	-3.214298	0.154837
H	3.474108	-3.750492	0.605321
H	1.705418	-3.500487	0.688751
H	2.532983	-3.547079	-0.888161
H	0.064275	0.223128	-2.759965
N	-0.388545	-0.574748	-0.394667
H	-1.259698	1.416836	-0.916391
Ir	1.470485	-0.105199	-0.417487
S	-1.075769	-1.383989	0.923173
O	-1.157915	-0.361376	1.989068
O	-0.369221	-2.649860	1.188301

C	-2.724418	-1.775474	0.377412
C	-2.997709	-3.058366	-0.104631
C	-3.726647	-0.800848	0.456652
C	-4.295164	-3.361086	-0.520119
H	-2.207533	-3.809799	-0.138173
C	-5.014556	-1.124458	0.036401
H	-3.503692	0.190198	0.855911
C	-5.323674	-2.406354	-0.457013
H	-4.514296	-4.364343	-0.894270
H	-5.803424	-0.370197	0.101722
C	-6.730755	-2.748693	-0.872174
H	-6.760231	-3.638669	-1.516859
H	-7.206705	-1.914366	-1.409876
H	-7.354716	-2.960360	0.013385
C	-0.381190	2.597311	0.703192
H	-0.740285	1.911491	1.497577
H	0.586622	3.012496	1.010859
C	-1.399078	3.748902	0.655400
O	-1.195506	4.816713	1.162680
O	-2.516093	3.390569	0.016864
C	-3.581697	4.378178	-0.053305
C	-4.681789	3.823454	-0.929454
H	-3.158713	5.313187	-0.450707
H	-3.925977	4.581019	0.972711
H	-5.503330	4.553099	-0.993233
H	-4.318810	3.627980	-1.950101
H	-5.088307	2.887388	-0.516803
H	1.790181	0.811793	-3.104427

TS4f

B3LYP SCF energy: -1791.30065414 a.u.
B3LYP enthalpy: -1790.739852 a.u.
B3LYP free energy: -1790.847427 a.u.
B3LYP-D3BJ SCF energy in solution: -1793.19140405 a.u.
B3LYP-D3BJ enthalpy in solution: -1792.630602 a.u.
B3LYP-D3BJ free energy in solution: -1792.738177 a.u.
Three lowest frequencies (cm-1): -238.4760 11.5480 14.3055
Imaginary frequency: -238.4760 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.454347	1.266812	-0.129543
C	1.128885	0.776006	-1.401329
C	-0.230373	0.657774	-1.842628
H	1.918252	0.405784	-2.063149
C	0.345138	-3.102689	-0.678817
C	0.137461	-2.960746	0.737518
C	1.357986	-2.385902	1.293415
C	2.337253	-2.279673	0.227889

C	1.703439	-2.673685	-0.985893
C	-1.014739	-3.497819	1.525690
H	-0.758850	-4.512130	1.879237
H	-1.925652	-3.558697	0.918589
H	-1.245010	-2.872849	2.397608
C	-0.635849	-3.687342	-1.642343
H	-0.610814	-4.788916	-1.569633
H	-0.400784	-3.420511	-2.681632
H	-1.656274	-3.351666	-1.412417
C	2.339775	-2.741398	-2.340940
H	2.696297	-3.767274	-2.536306
H	3.207720	-2.073298	-2.425245
H	1.630566	-2.489251	-3.142229
C	3.777844	-1.913270	0.405012
H	4.360709	-2.825020	0.622891
H	3.931744	-1.224433	1.246271
H	4.210939	-1.463619	-0.499427
C	1.605864	-2.139599	2.748214
H	1.968441	-3.065734	3.228051
H	0.685374	-1.834539	3.264283
H	2.365006	-1.361831	2.908150
H	0.672880	1.792879	0.421495
N	-1.040996	0.175409	0.198668
H	-0.957894	1.434840	-1.618621
H	-0.451390	0.029298	-2.709486
Ir	0.495529	-0.926158	-0.090143
C	2.867548	1.548397	0.283979
H	3.558140	0.769161	-0.073927
H	2.971956	1.611992	1.375104
C	3.352532	2.858613	-0.356725
O	3.054039	3.197453	-1.475616
O	4.157018	3.527493	0.461976
C	4.741265	4.759291	-0.038430
C	5.585215	5.358632	1.063882
H	3.922788	5.426095	-0.351096
H	5.331656	4.520609	-0.937044
H	6.041682	6.295850	0.710766
H	4.975473	5.586773	1.951268
H	6.393821	4.674427	1.362757
S	-2.569079	-0.484210	0.576704
O	-2.901601	-1.590377	-0.337480
O	-2.476260	-0.709168	2.029009
C	-3.695328	0.857136	0.266489
C	-3.828972	1.870074	1.224289
C	-4.444643	0.868338	-0.913706
C	-4.719200	2.912283	0.978769
H	-3.254409	1.828429	2.151196
C	-5.330814	1.923010	-1.138767
H	-4.347098	0.052656	-1.632054
C	-5.484633	2.959333	-0.202356
H	-4.831312	3.704485	1.723770

H	-5.922806	1.935217	-2.057513
C	-6.467743	4.077010	-0.433264
H	-6.063194	5.044864	-0.099730
H	-6.745720	4.163128	-1.493407
H	-7.394840	3.900180	0.139042

TS3g

B3LYP SCF energy: -2052.70624862 a.u.
B3LYP enthalpy: -2052.157865 a.u.
B3LYP free energy: -2052.267775 a.u.
B3LYP-D3BJ SCF energy in solution: -2054.91211109 a.u.
B3LYP-D3BJ enthalpy in solution: -2054.363727 a.u.
B3LYP-D3BJ free energy in solution: -2054.473637 a.u.
Three lowest frequencies (cm-1): -102.8885 13.4358 16.8543
Imaginary frequency: -102.8885 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.658085	-0.224646	-2.584390
C	-0.556302	-0.991763	-2.138326
C	0.697887	-0.385109	-1.784229
H	-0.613449	-2.083079	-2.156577
C	-3.056256	-2.269828	0.028760
C	-2.293292	-1.880820	1.200874
C	-2.764398	-0.584532	1.649090
C	-3.757206	-0.146098	0.693140
C	-3.947007	-1.205385	-0.289364
C	-1.300899	-2.727256	1.932682
H	-1.808192	-3.281606	2.741990
H	-0.827101	-3.469572	1.276089
H	-0.514311	-2.113634	2.393509
C	-2.956735	-3.586746	-0.680811
H	-3.627334	-4.323119	-0.205693
H	-3.253414	-3.512717	-1.736409
H	-1.941000	-4.004934	-0.637100
C	-4.968919	-1.187385	-1.383577
H	-5.946669	-1.505882	-0.982756
H	-5.102019	-0.181315	-1.805014
H	-4.714227	-1.873997	-2.202470
C	-4.538889	1.124005	0.783978
H	-5.371458	0.991692	1.497689
H	-3.906500	1.947610	1.142858
H	-4.972071	1.408703	-0.184262
C	-2.451762	0.056626	2.963899
H	-3.144143	-0.339412	3.727704
H	-1.423178	-0.151492	3.284128
H	-2.564969	1.146299	2.919393
H	-1.514636	0.822081	-2.858383
N	-0.577862	1.091521	-0.395474

H	0.874990	0.625844	-2.144464
Ir	-1.808685	-0.358564	-0.362747
S	-0.265633	2.004138	0.994894
O	0.449753	1.148566	1.957601
O	-1.535959	2.652558	1.377761
C	0.854786	3.273438	0.432074
C	0.351859	4.378042	-0.265762
C	2.216335	3.160623	0.723573
C	1.236553	5.366199	-0.691440
H	-0.719096	4.466898	-0.456716
C	3.085938	4.165282	0.291790
H	2.578347	2.308214	1.300966
C	2.615953	5.280261	-0.421557
H	0.848593	6.231674	-1.235385
H	4.150707	4.088364	0.527483
C	3.550520	6.378034	-0.859768
H	4.603230	6.067695	-0.796163
H	3.427533	7.270046	-0.221928
H	3.343806	6.692705	-1.894574
H	-2.503064	-0.730726	-3.055106
C	1.841106	-1.054724	-1.218186
C	3.037930	-0.312705	-1.071006
C	1.837071	-2.416333	-0.827265
C	4.185810	-0.904838	-0.556404
H	3.055040	0.739589	-1.363805
C	2.983650	-3.007662	-0.316237
H	0.933179	-3.017733	-0.932595
C	4.158430	-2.251382	-0.173674
H	5.106822	-0.328794	-0.454821
H	2.981108	-4.060715	-0.030223
C	5.392511	-2.886193	0.441308
F	6.512226	-2.318848	-0.022437
F	5.446492	-4.198176	0.177910
F	5.378783	-2.737394	1.774113

TS4g

B3LYP SCF energy: -2052.69859440 a.u.
B3LYP enthalpy: -2052.150170 a.u.
B3LYP free energy: -2052.259381 a.u.
B3LYP-D3BJ SCF energy in solution: -2054.90597624 a.u.
B3LYP-D3BJ enthalpy in solution: -2054.357552 a.u.
B3LYP-D3BJ free energy in solution: -2054.466763 a.u.
Three lowest frequencies (cm-1): -248.3473 15.2445 20.4570
Imaginary frequency: -248.3473 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.916507	1.178880	-0.843823
C	0.364173	0.389247	-1.859809

C	-1.047671	0.315891	-2.105025
H	1.013555	-0.219275	-2.496120
C	-0.638048	-3.181630	-0.392727
C	-0.765144	-2.807776	0.998782
C	0.521729	-2.269509	1.409906
C	1.453566	-2.414902	0.305488
C	0.739139	-2.953181	-0.804230
C	-1.920439	-3.112650	1.896614
H	-1.740928	-4.086122	2.386114
H	-2.861841	-3.169691	1.337690
H	-2.048604	-2.348008	2.672691
C	-1.723853	-3.801134	-1.211930
H	-1.820484	-4.869757	-0.951807
H	-1.513483	-3.740905	-2.288320
H	-2.688357	-3.313695	-1.009947
C	1.310165	-3.307168	-2.143970
H	1.575774	-4.377938	-2.166404
H	2.226009	-2.742121	-2.365272
H	0.591994	-3.137441	-2.958898
C	2.913113	-2.095655	0.362224
H	3.466719	-2.967966	0.750788
H	3.123258	-1.249595	1.030359
H	3.325212	-1.856823	-0.626901
C	0.857877	-1.803237	2.791091
H	1.190938	-2.660836	3.401794
H	-0.016027	-1.358272	3.285828
H	1.669432	-1.062893	2.786429
H	0.228666	1.803742	-0.271528
N	-1.647027	0.330307	0.050015
H	-1.677937	1.193581	-1.983923
H	-1.421147	-0.444054	-2.795947
Ir	-0.296735	-0.997792	-0.174374
S	-3.175492	-0.056680	0.702909
O	-3.744199	-1.220858	0.001498
O	-2.927815	-0.101116	2.154454
C	-4.169018	1.370128	0.325826
C	-4.079609	2.500834	1.147215
C	-5.029410	1.337482	-0.775282
C	-4.855977	3.615647	0.841314
H	-3.423099	2.495346	2.019052
C	-5.798727	2.466445	-1.062899
H	-5.106417	0.434287	-1.382932
C	-5.726483	3.621066	-0.265756
H	-4.793671	4.500537	1.480395
H	-6.477162	2.445688	-1.919609
C	-6.578190	4.827849	-0.561640
H	-7.418299	4.893696	0.150910
H	-6.000789	5.760295	-0.463980
H	-7.004263	4.788349	-1.574147
C	2.339067	1.390555	-0.589012
C	3.354833	0.961900	-1.471675

C	2.716015	2.100450	0.571168
C	4.693327	1.222390	-1.195541
H	3.100477	0.448266	-2.401179
C	4.056151	2.352225	0.855184
H	1.942896	2.458368	1.255700
C	5.049279	1.907305	-0.024942
H	5.468902	0.906457	-1.895799
H	4.334010	2.905210	1.753925
C	6.513089	2.125103	0.297565
F	7.031118	1.037354	0.895080
F	6.688051	3.162908	1.124915
F	7.227902	2.350046	-0.813449