

ELECTRONIC SUPPORTING INFORMATION

On the Ir–Si Bond Shortening in Ir–NSiN complexes

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Table of Contents

Table S1. Ir-Si bond length (Å). CCDCrefcode: reference code of the structure in the Cambridge Structural Database; Coordination: coordination mode of the Si-containing ligand; L: NSiN ligand NSiN ^{OPy} =bis(pyridine-2-yloxy)methylsilyl, NSiN ^{4MeOPy} =bis(4-methyl-pyridine-2-yloxy)methylsilyl and NSiN ^Q =bis(8-quinolyl)methylsilyl ligands; and compound number according to Figure 4, respectively. Compounds exhibiting a κ^3 -N,Si,N coordination have been highlighted.	2
Figure S1. Laplacian distribution in complex 8	10
Figure S2. Plot of the computed Si-Ir bond distances vs the NBO charge at the silicon atom.....	11
Figure S3. Plot of the computed Si–Ir bond distances vs the p-backdonation energies ($\Delta E(\rho_4)$).	11
Cartesian coordinates (in Å) and total energies (in a. u., ZPVE included) of all the stationary points discussed in the text. All calculations have been performed at the BP86-D3/def2-SVP level.....	12

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CCDC refcode	Coordination	L	compound	Ir-Si
XEZNOH	κ^3 -N,Si,N	NSiN ^{OPy}	6	2.219
LEFCEH	κ^3 -N,Si,N	NSiN ^{4MeOPy}		2.222
TAHKEV	κ^3 -N,Si,N	NSiN ^{OPy}	8	2.223
DITREG	κ^3 -N,Si,N	NSiN ^{OPy}	7	2.224
XEZNOH	κ^3 -N,Si,N	NSiN ^{OPy}	6	2.228
NADWEW	κ^1 -Si			2.233
VIRFUX	κ^1 -Si			2.233
TEYKEQ	κ^3 -S,Si,S			2.235
DITRAC	κ^3 -N,Si,N	NSiN ^{OPy}	5	2.236
FAPWAW	κ^3 -P,Si,N			2.236
VIRFUX	κ^1 -Si			2.237
ZODFOQ	κ^2 -Si,N			2.250
ZODFOQ	κ^2 -Si,N			2.251
JIWZEV	κ^3 -N,Si,N	NSiN ^Q	4	2.252
UYIDOW	κ^3 -P,Si,P			2.253
ZODFIK	κ^2 -Si,N			2.255
IHONOL	κ^2 -Si,N			2.257
ZODFOQ	κ^2 -Si,N			2.257
QEBKUG	κ^2 -Si,C			2.260
UYIDOW	κ^3 -P,Si,P			2.260
IHONOL	κ^2 -Si,N			2.262
OBOPOK	κ^3 -N,Si,N	NSiN ^Q		2.262
ZODFIK	κ^2 -Si,N			2.263
YIPNAM	κ^2 -Si,C			2.264
ZODFOQ	κ^2 -Si,N			2.264
RITSEU	κ^1 -Si			2.265
MORRIW	μ -Si (bridge Ir, Ru)			2.266
UYIDOW	κ^3 -P,Si,P			2.266
DODZEE	κ^4 -Si,P,P,P			2.267
LAFYOI	κ^2 -Si,Si			2.267
OVELOR	κ^3 -P,Si,P			2.267
REBZIK	κ^3 -P,Si,P			2.267
OBOPOK	κ^3 -N,Si,N	NSiN ^Q		2.268
RECBAB	κ^3 -P,Si,P			2.270
ZODFIK	κ^2 -Si,N			2.270
LEWSAI	κ^1 -Si			2.272
NOKBAR	κ^3 -P,Si,P			2.274
OBOPEA	κ^3 -N,Si,N	NSiN ^Q	1	2.275
ZODFIK	κ^2 -Si,N			2.275

POTKUF	$\kappa^4\text{-Si,P,P,P}$			2.276
YOHNEP	$\kappa^1\text{-Si}$			2.277
OBOPIE	$\kappa^3\text{-N,Si,N}$	NSiN ^Q	2	2.278
VILNAI	$\kappa^1\text{-Si}$			2.278
LEWSAI	$\kappa^1\text{-Si}$			2.279
QEBLAN	$\kappa^2\text{-Si,C}$			2.279
RECBAF	$\kappa^3\text{-P,Si,P}$			2.279
XAMTOW	$\kappa^3\text{-P,Si,P}$			2.279
LAFYIC	$\kappa^2\text{-Si,C}$			2.281
XAMTEM	$\kappa^3\text{-P,Si,P}$			2.283
VIVCIP	$\kappa^2\text{-Si,N}$			2.285
PAYMUX	$\kappa^1\text{-Si}$			2.287
VILQOZ	$\kappa^1\text{-Si}$			2.288
JIWZEV	$\kappa^1\text{-Si}$			2.289
MAKQAT	$\kappa^2\text{-Si,P}$			2.292
LAVVEM	$\kappa^3\text{-Si,P,Si}$			2.293
ANECUS	$\kappa^3\text{-P,Si,P}$			2.294
LAFYEY	$\mu\text{-Si (bridge Ir, Ir)}$			2.294
SIVLUH	$\kappa^3\text{-Si,N,N}$			2.294
KULKEH	$\kappa^2\text{-Si,N}$			2.295
ANEBIF	$\kappa^3\text{-P,Si,P}$			2.296
ANEBOL	$\kappa^3\text{-P,Si,P}$			2.296
LAVVEM	$\kappa^3\text{-Si,P,Si}$			2.296
JAZDET	$\kappa^1\text{-Si}$			2.297
POQJUD	$\kappa^3\text{-Si,P,Si}$			2.298
SIVLOB	$\kappa^3\text{-Si,N,N}$			2.299
UGIMEC	$\kappa^1\text{-Si}$			2.299
ANECIG	$\kappa^3\text{-P,Si,P}$			2.300
SIVLOB	$\kappa^3\text{-Si,N,N}$			2.300
ANECOM	$\kappa^3\text{-P,Si,P}$			2.301
DEJGUU10	$\kappa^2\text{-Si,P}$			2.301
NEMHAQ	$\kappa^2\text{-Si,C}$			2.301
KULKEH	$\kappa^2\text{-Si,N}$			2.302
ANEBUR	$\kappa^3\text{-P,Si,P}$			2.303
JIWZIZ	$\kappa^3\text{-N,Si,N}$	NSiN ^Q	3	2.303
MIZXEB	$\kappa^2\text{-Si,P}$			2.303
MIZXEB	$\kappa^2\text{-Si,P}$			2.303
MORRUI	$\mu\text{-Si (bridge Ir, Ru)}$			2.303
POQJUD	$\kappa^3\text{-Si,P,Si}$			2.303
SIVJOZ	$\kappa^3\text{-Si,N,N}$			2.303
UYIDUC	$\kappa^3\text{-Si,P,P}$			2.303
UYIDUC	$\kappa^3\text{-Si,P,P}$			2.303
POTLEQ	$\kappa^4\text{-Si,P,P,P}$			2.304
UGIMIG	$\kappa^2\text{-Si,S}$			2.304
NEMHAQ	$\kappa^2\text{-Si,C}$			2.305

POQKUE	κ^3 -Si,P,Si			2.305
KULKEH	κ^2 -Si,N			2.306
LAFYEY	μ -Si (bridge Ir, Ir)			2.306
POQKUE	κ^3 -Si,P,Si			2.306
LAFYUO	κ^2 -Si,Si			2.307
ZUJNAT	κ^1 -Si			2.307
ANECOM	κ^3 -Si, P,P			2.308
MORRUI	μ -Si (bridge Ir, Ru)			2.309
DOCPAO	κ^1 -Si			2.311
LAVVEM	κ^3 -Si,Si,P			2.311
QEBLER	κ^2 -Si,C			2.312
REBZEG	κ^3 -Si,P,P			2.312
YUVNOS	κ^1 -Si			2.312
DEJGUU10	κ^2 -Si,P			2.314
REBZEG	κ^3 -Si,P,P			2.314
JEPCIR	κ^1 -Si			2.315
LAVVEM	κ^3 -Si,Si,P			2.315
UGIMAY	κ^1 -Si			2.315
KOBWIJ	κ^2 -Si,Si			2.316
MIZLEP	κ^3 -Si,P,P			2.316
TEYKAM	κ^3 -Si,S,S			2.316
KEVLEC	κ^2 -Si,C			2.317
KOBWIJ	κ^2 -Si,Si			2.317
UGIMAY	κ^1 -Si			2.317
YIMDOP	κ^1 -Si			2.317
KEWQIM	κ^1 -Si			2.318
LEMSOM	κ^1 -Si			2.318
LUFSEL	κ^2 -Si,N			2.318
QEBLER	κ^2 -Si,C			2.319
GUNQIS	κ^2 -Si, Si			2.320
MIZKUE	κ^2 -Si,P			2.320
MORROC	μ -Si (bridge Ir, Ru)			2.320
UYIDIQ	κ^3 -Si,P,P			2.320
LAFZID	κ^1 -Si			2.321
EJOFOZ	κ^1 -Si			2.322
RIJJIF	κ^1 -Si			2.322
YOHNIT	κ^1 -Si			2.322
IMESUP	κ^2 -Si,P			2.323
KOBWAB	κ^2 -Si,Si			2.323
LUFROU	κ^1 -Si			2.323
POQKEO	κ^3 -Si,P,Si			2.323
POQKIS	κ^3 -Si,P,Si			2.323
AKIKAH	κ^4 -Si,N,N,N			2.324
JEPCAJ	κ^1 -Si			2.326
MAKDAG	κ^3 -P,Si,P			2.326

REBZOQ	$\kappa^3\text{-P,Si,P}$			2.327
PERDOI	$\kappa^1\text{-Si}$			2.328
REBZOQ	$\kappa^3\text{-P,Si,P}$			2.328
ANECEC	$\kappa^3\text{-P,Si,P}$			2.329
MIZLAL	$\kappa^2\text{-Si,P}$			2.329
MUJPOX	$\kappa^1\text{-Si}$			2.329
NADWAS	$\kappa^1\text{-Si}$			2.329
DOCPEs	$\kappa^1\text{-Si}$			2.330
LAFZEZ	$\kappa^1\text{-Si}$			2.331
LEWSEM	$\kappa^1\text{-Si}$			2.331
KOBWAB	$\kappa^2\text{-Si,Si}$			2.332
DOCPEs	$\kappa^1\text{-Si}$			2.334
GUNQIS	$\kappa^2\text{-Si, Si}$			2.334
MIZLEP	$\kappa^3\text{-P,Si,P}$			2.334
YOHNIT	$\kappa^1\text{-Si}$			2.334
POQKUE	$\kappa^3\text{-Si,P,Si}$			2.335
LAFYOI	$\kappa^2\text{-Si,Si}$			2.336
MUJPOX	$\kappa^1\text{-Si}$			2.336
NOYMUL	$\kappa^1\text{-Si}$			2.336
POQLAL	$\kappa^3\text{-Si,P,Si}$			2.336
REBZUW	$\kappa^3\text{-P,Si,P}$			2.336
TAKFEQ	$\kappa^1\text{-Si}$			2.336
PACXID	$\kappa^3\text{-Si,N,N}$			2.337
QUDXOD	$\kappa^1\text{-Si}$			2.337
EWUCIJ	$\mu\text{-Si (bridge Rh, Ir)}$			2.338
JEPCAJ	$\kappa^1\text{-Si}$			2.338
BUJHAS	$\kappa^1\text{-Si}$			2.339
REBZUW	$\kappa^3\text{-P,Si,P}$			2.339
MIZLAL	$\kappa^2\text{-Si,P}$			2.340
POQKUE	$\kappa^3\text{-Si,P,Si}$			2.340
RITRUJ	$\kappa^1\text{-Si}$			2.340
RUKNUI	$\kappa^1\text{-Si}$			2.340
UYICIP	$\kappa^3\text{-P,Si,P}$			2.341
REBZUW	$\kappa^3\text{-P,Si,P}$			2.342
VIPLEM	$\kappa^1\text{-Si}$			2.342
FAFKEF	$\kappa^1\text{-Si}$			2.343
JUTWEC	$\kappa^2\text{-Si,N}$			2.343
YIMDEF	$\kappa^1\text{-Si}$			2.343
YUVNUY	$\kappa^2\text{-Si,O}$			2.343
KOBWEF	$\kappa^2\text{-Si,Si}$			2.344
QUDXOD	$\kappa^1\text{-Si}$			2.344
SIFSEF	$\mu\text{-Si (bridge Ir, Ir)}$			2.344
DEKLOW	$\mu\text{-Si (bridge Rh, Ir)}$			2.345
POQLAL	$\kappa^3\text{-Si,P,Si}$			2.345
HATFAL	$\kappa^4\text{-Si,P,P,P}$			2.346

PEMKOK	κ^1 -Si			2.347
REBZUW	κ^3 -P,Si,P			2.347
XUCYAV	κ^1 -Si			2.347
JISCET	κ^1 -Si			2.348
CEPYUT	μ -Si (bridge Rh, Ir)			2.349
PEMKOK	κ^1 -Si			2.349
SIFSEF	μ -Si (bridge Ir, Ir)			2.350
GUNQOY	κ^2 -Si, Ge			2.352
TEDNUL	κ^2 -Si,P			2.352
TEDNUL01	κ^2 -Si,P			2.352
EWUCEF	μ -Si (bridge Rh, Ir)			2.353
PEMKOK	κ^1 -Si			2.353
RUKBIK	κ^1 -Si			2.353
NUBMOO	κ^1 -Si			2.354
RUKNUI	κ^1 -Si			2.354
CAQYOL	κ^4 -Si,P, P,P			2.355
ERELES	κ^2 -Si,Si			2.355
EWUBOO	μ -Si (bridge Rh, Ir)			2.355
PEMLOL	κ^1 -Si			2.355
KAXBIW	κ^4 -Si,P,P,P			2.356
DOCNUG	κ^1 -Si			2.357
TIVYUU	κ^3 -Si,N,N			2.357
UYICUB	κ^3 -P,Si,P			2.357
DEKMIR	μ -Si (bridge Rh, Ir)			2.358
IKUYES	κ^1 -Si			2.358
PEMMOM	κ^1 -Si			2.358
ERELES	κ^2 -Si,Si			2.359
EWUBII	μ -Si (bridge Rh, Ir)			2.359
KAXCET	κ^4 -Si,P,P,P			2.359
YARWAS	κ^1 -Si			2.359
DEKMAJ	μ -Si (bridge Rh, Ir)			2.360
IFOMAS	κ^1 -Si			2.361
KAWZOZ	κ^4 -Si,P,P,P			2.361
YUTWAL	κ^1 -Si			2.361
EWUCEF	μ -Si (bridge Rh, Ir)			2.362
PEMLOL	κ^1 -Si			2.362
EWUBUU	μ -Si (bridge Rh, Ir)			2.363
UYICEL	κ^3 -P,Si,P			2.363
LUFSEL	κ^2 -Si,N			2.365
MALDIP	κ^3 -P,Si,P			2.365
TOMCUT	κ^2 -Si,P			2.365
EWUBII	μ -Si (bridge Rh, Ir)			2.366
QUDYOE	κ^1 -Si			2.366
UYICEL	κ^3 -P,Si,P			2.366
DEKLOW	μ -Si (bridge Rh, Ir)			2.367

EWUBUU	μ -Si (bridge Rh, Ir)			2.367
EWUCAB	μ -Si (bridge Rh, Ir)			2.367
PEMKOK	κ^1 -Si			2.367
POQKIS	κ^3 -Si,P,Si			2.367
CAQZEC	κ^4 -Si,P, P,P			2.368
SIFSAB	μ -Si (bridge Ir, Ir)			2.368
UYIDAI	κ^3 -P,Si,P			2.368
YUTWAL	κ^1 -Si			2.368
DEKMEN	μ -Si (bridge Rh, Ir)			2.369
EWUCAB	μ -Si (bridge Rh, Ir)			2.369
JIWZIZ	κ^1 -Si			2.369
IFOMEW	κ^1 -Si			2.370
PEMKOK	κ^1 -Si			2.370
POQKEO	κ^3 -Si,P,Si			2.370
QUDXUJ	κ^1 -Si			2.371
UYICEL	κ^3 -P,Si,P			2.371
JISCET	κ^1 -Si			2.372
KOBWEF	κ^2 -Si,Si			2.372
TUKVUS	κ^1 -Si			2.373
UYICOV	κ^3 -P,Si,P			2.374
PEMKOK	κ^1 -Si			2.375
SIFSAB	μ -Si (bridge Ir, Ir)			2.375
UYICOV	κ^3 -P,Si,P			2.375
XOLXON	κ^2 -Si,P			2.376
VIPLAI	κ^2 -Si,C			2.377
DEKLEM	μ -Si (bridge Rh, Ir)			2.378
ERELIW	κ^2 -Si,Si			2.378
DEKMAJ	μ -Si (bridge Rh, Ir)			2.380
ERELAO	Si. B			2.380
XEWQOH	κ^3 -P,Si,P			2.381
XIKFED	κ^1 -Si			2.381
ZAGJAS	κ^1 -Si			2.381
QUDYEU	κ^1 -Si			2.382
YUTVUE	κ^1 -Si			2.383
TUKVUS	κ^1 -Si			2.384
RECBEJ	κ^3 -P,Si,P			2.385
TOMCON	κ^2 -Si,P			2.385
POQKAK	κ^3 -Si,P,Si			2.386
XEWQUN	κ^3 -P,Si,P			2.386
CEPYON	μ -Si (bridge Rh, Ir)			2.387
XETLEP	κ^3 -P,Si,P			2.387
ERELIW	κ^2 -Si,Si			2.388
JIWZOF	κ^2 -Si,N			2.388
YELDIF	κ^1 -Si			2.388
CIWJAT10	κ^1 -Si			2.390

YUTWEP	κ^1 -Si			2.391
HAYWOW	κ^1 -Si			2.394
JISCAP	κ^1 -Si			2.394
DEKMIR	μ -Si (bridge Rh, Ir)			2.395
YIYSIJ	κ^1 -Si			2.396
EJEWUN	κ^1 -Si			2.398
HAYWIQ	κ^1 -Si			2.398
HTSIXI10	κ^2 -Si,Si			2.398
HOCPUN	κ^1 -Si			2.399
MAMNOE	κ^2 -Si,P			2.399
YELDEB	κ^1 -Si			2.400
VIPLIQ	κ^1 -Si, η^2 -C-C			2.401
BUJHAS	κ^1 -Si			2.404
DEKLUC	μ -Si (bridge Rh, Ir)			2.404
HAZJUN	κ^2 -Si,C			2.405
VIPKUB	κ^1 -Si			2.406
HUNGUS	κ^1 -Si			2.407
QAXYOF	κ^1 -Si			2.408
UYIDEM	κ^3 -Si,P,P			2.408
QAXYOF	μ -Si (bridge Ir, Ir)			2.410
LUWNAS	κ^1 -Si			2.411
TOMCON	κ^2 -Si,P			2.411
KOSVEV	κ^2 -Si,H			2.412
DEKMEN	μ -Si (bridge Rh, Ir)			2.413
IYAJUN	κ^1 -Si			2.413
TIVYOO	κ^3 -Si,N,N			2.413
YELDEB	κ^1 -Si			2.413
FICMUZ	κ^1 -Si			2.414
GILJEQ	κ^1 -Si			2.414
JEPCEN	κ^1 -Si			2.416
DEKLIQ	μ -Si (bridge Rh, Ir)			2.417
HTSIXI10	κ^2 -Si,Si			2.417
IFOMIA	κ^1 -Si			2.417
JISCAP	κ^1 -Si			2.418
PAHVIG	κ^1 -Si			2.418
PAYNAE	κ^3 -Si,P,P			2.418
LOMBIB	κ^1 -Si			2.422
ZAGHUK	κ^1 -Si			2.424
RIJJOL	μ -Si (bridge Ir, Ir)			2.425
PAHVIG	κ^1 -Si			2.426
HUNGUS	κ^1 -Si			2.427
JIWZUL	κ^1 -Si			2.427
PAHVOM	κ^1 -Si			2.427
RIJJOL	μ -Si (bridge Ir, Ir)			2.427
ZACMIZ	κ^2 -Si,Si			2.430

ANECAY	$\kappa^3\text{-P,Si,P}$			2.434
KOSVIZ	$\kappa^2\text{-Si,H}$			2.434
YIZBER	$\kappa^1\text{-Si}$			2.436
HUNHED	$\kappa^1\text{-Si}$			2.437
ZACMIZ	$\kappa^2\text{-Si,Si}$			2.437
UBOYEP	$\kappa^2\text{-Si,C}$			2.440
LAFYUO	$\kappa^2\text{-Si,Si}$			2.441
ZIXGIW	$\kappa^2\text{-Si,C}$			2.441
TOHMEI	$\kappa^1\text{-Si}$			2.442
QAXYOF	$\mu\text{-Si (bridge Ir, Ir)}$			2.444
TECKOB	$\kappa^2\text{-Si,P}$			2.444
HUNHED	$\kappa^1\text{-Si}$			2.446
TECKOB	$\kappa^2\text{-Si,P}$			2.446
UGIMEC	$\kappa^1\text{-Si}$			2.446
TESMOT	$\kappa^2\text{-Si,P}$			2.447
POQKOY	$\kappa^3\text{-Si,P,Si}$			2.448
POQKOY	$\kappa^3\text{-Si,P,Si}$			2.453
YIZBAN	$\kappa^1\text{-Si}$			2.453
CURXIW	$\kappa^2\text{-Si,P}$			2.454
POQKAK	$\kappa^3\text{-Si,P,Si}$			2.456
UBOYEP	$\kappa^2\text{-Si,C}$			2.457
QECNUH	$\kappa^2\text{-Si,C}$			2.480
UVAWIZ	$\kappa^1\text{-Si}$			2.501
NENNOM	$\kappa^2\text{-Si,H}$			2.566
NENNIG	$\kappa^2\text{-Si,H}$			2.574

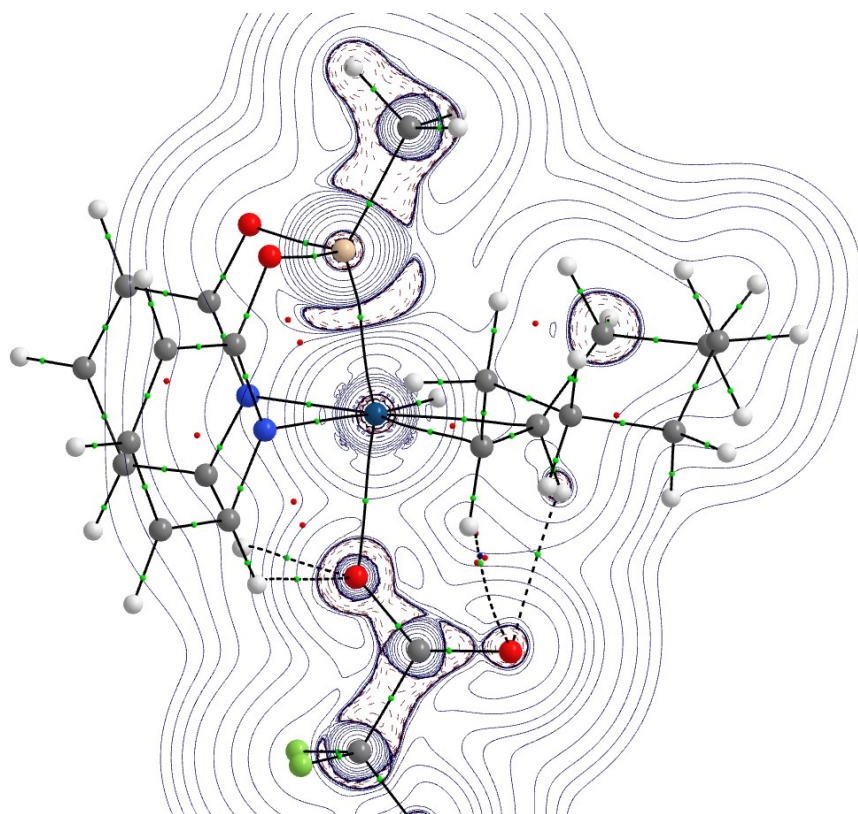


Figure S1. Contour line diagrams $\nabla^2\rho(r)$ for complex **8** in the O–Ir–Si plane. The solid lines connecting the atomic nuclei are the bond paths while the small green and red spheres indicate the corresponding bond critical points and ring critical points, respectively.

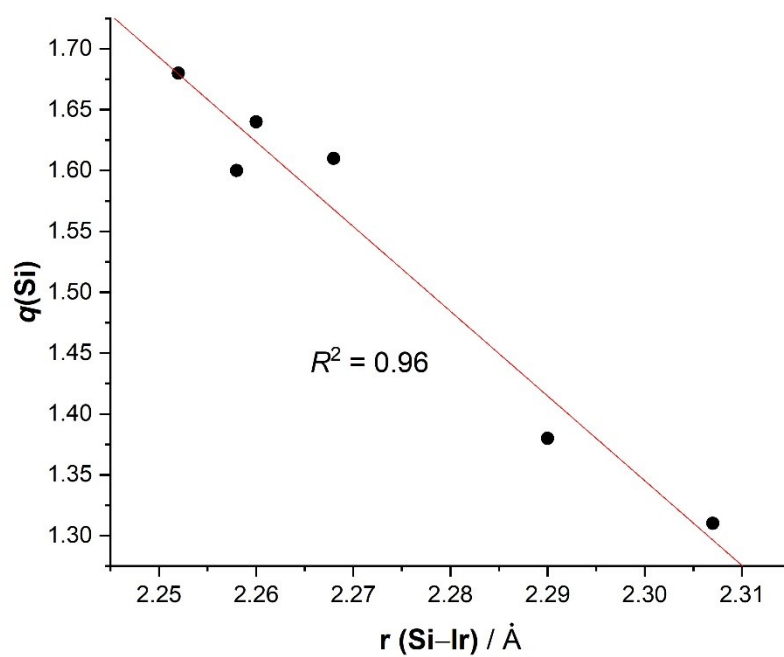


Figure S2. Plot of the computed Si-Ir bond distances vs the computed NBO charge at the silicon atom.

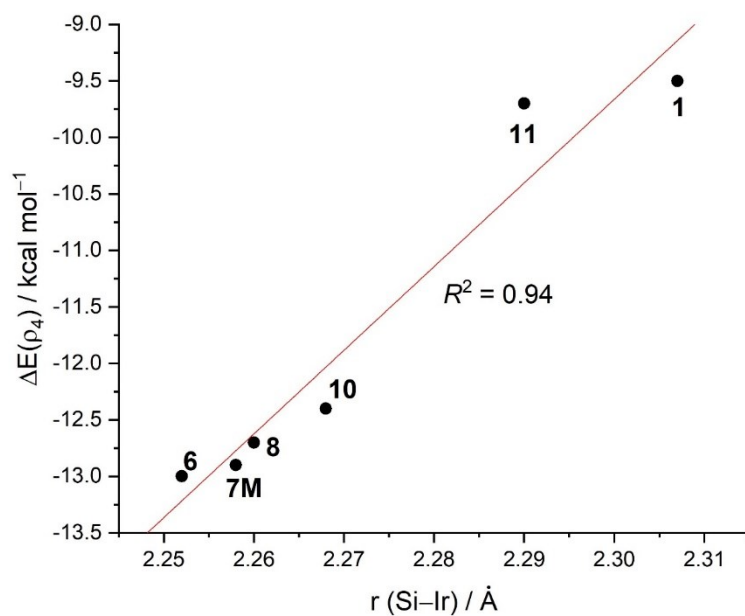


Figure S3. Plot of the computed Si-Ir bond distances vs the p-backdonation energies ($\Delta E(p_4)$).

Cartesian coordinates (in Å) and total energies (in a. u., ZPVE included) of all the stationary points discussed in the text. All calculations have been performed at the BP86-D3/def2-SVP level.

1: E= -2009.414756

Ir	0.278505000	-0.879346000	0.318078000
Cl	0.669860000	-2.041561000	2.583869000
Si	-0.329448000	0.319628000	-1.557195000
N	-1.856099000	-1.217311000	0.453066000
N	-0.123164000	1.081615000	1.352429000
C	0.402121000	0.444738000	-3.306235000
H	0.509569000	-0.565228000	-3.751711000
H	1.400036000	0.928940000	-3.298490000
H	-0.255697000	1.044427000	-3.972112000
C	-2.357482000	-1.824670000	1.535919000
H	-1.612066000	-2.078563000	2.314128000
C	-3.730060000	-2.151687000	1.667595000
H	-4.068726000	-2.652774000	2.586378000
C	-4.109263000	-1.203011000	-0.531456000
C	-4.604182000	-1.854105000	0.634356000
H	-5.673770000	-2.113923000	0.697309000
C	-4.943921000	-0.870649000	-1.640917000
H	-6.012693000	-1.135301000	-1.597340000
C	-4.412534000	-0.229029000	-2.751231000
H	-5.060033000	0.020829000	-3.606828000
C	-3.033293000	0.119809000	-2.781608000
H	-2.643086000	0.653238000	-3.664723000
C	-2.706946000	-0.870561000	-0.593177000
C	-2.171786000	-0.181693000	-1.725902000
C	-0.057222000	1.167741000	2.682604000
H	0.178640000	0.215384000	3.198266000
C	-0.254058000	2.386462000	3.382432000
H	-0.188203000	2.390329000	4.480637000
C	-0.580247000	3.488748000	1.241723000
C	-0.507510000	3.544992000	2.664156000
H	-0.648877000	4.512323000	3.174104000
C	-0.815569000	4.642482000	0.434887000
H	-0.952817000	5.617638000	0.929555000
C	-0.863997000	4.531125000	-0.947998000
H	-1.038647000	5.425301000	-1.567558000
C	-0.697054000	3.261601000	-1.569857000
H	-0.754775000	3.203000000	-2.670097000
C	-0.396183000	2.211453000	0.595471000
C	-0.473117000	2.097757000	-0.832270000
C	2.351609000	-0.206094000	0.512670000
H	2.534674000	-0.236215000	1.603870000
C	2.776500000	1.093276000	-0.147528000
H	2.302567000	1.939019000	0.393336000
H	2.392592000	1.152380000	-1.187434000
C	4.304823000	1.316453000	-0.165378000
H	4.487285000	2.385822000	-0.414199000
H	4.706362000	1.173457000	0.864406000
C	5.119849000	0.448314000	-1.147354000
H	6.146458000	0.873483000	-1.183784000
H	4.713150000	0.581381000	-2.177012000
C	5.220577000	-1.063111000	-0.812980000
H	6.265100000	-1.405050000	-0.979285000

H	5.034695000	-1.205782000	0.274630000
C	4.297311000	-2.000627000	-1.617510000
H	4.621477000	-2.010380000	-2.683015000
H	4.443982000	-3.039282000	-1.244633000
C	2.791975000	-1.654943000	-1.572335000
H	2.603548000	-0.735746000	-2.161398000
H	2.211780000	-2.462026000	-2.066666000
C	2.323199000	-1.469516000	-0.145566000
H	2.487302000	-2.350978000	0.501669000

11: E= -2510.226455

Ir	0.019812000	0.048483000	-0.579617000
Si	-2.119105000	0.833660000	-0.813614000
N	-0.948706000	-1.862740000	-0.655399000
N	-0.503746000	0.028964000	1.595907000
C	-2.823790000	2.247068000	-1.858983000
H	-2.540234000	2.119545000	-2.923364000
H	-2.453845000	3.233899000	-1.514330000
H	-3.933581000	2.262855000	-1.796473000
C	-0.242683000	-2.964231000	-0.369312000
H	0.803894000	-2.792600000	-0.066368000
C	-0.786794000	-4.268221000	-0.473128000
H	-0.149113000	-5.129385000	-0.225858000
C	-2.880662000	-3.277916000	-1.199265000
C	-2.096197000	-4.428571000	-0.900979000
H	-2.540291000	-5.431229000	-1.012612000
C	-4.235102000	-3.355314000	-1.644025000
H	-4.694398000	-4.348170000	-1.775150000
C	-4.954364000	-2.196905000	-1.905232000
H	-5.997454000	-2.262456000	-2.253238000
C	-4.354513000	-0.920786000	-1.708121000
H	-4.961096000	-0.018456000	-1.894247000
C	-2.278888000	-1.977739000	-1.043724000
C	-3.034523000	-0.786695000	-1.276257000
C	0.348195000	-0.460245000	2.500500000
H	1.307058000	-0.841380000	2.117969000
C	0.079273000	-0.443860000	3.893784000
H	0.831271000	-0.853736000	4.583574000
C	-2.038949000	0.642045000	3.409408000
C	-1.106834000	0.110218000	4.347970000
H	-1.339298000	0.155108000	5.424677000
C	-3.270277000	1.247764000	3.802516000
H	-3.515890000	1.302135000	4.875381000
C	-4.135824000	1.762280000	2.846887000
H	-5.081387000	2.235365000	3.156114000
C	-3.807594000	1.674710000	1.464887000
H	-4.520166000	2.079952000	0.726581000
C	-1.712407000	0.574815000	2.006092000
C	-2.620876000	1.088193000	1.022353000
C	1.065179000	1.880061000	0.012485000
H	1.875182000	1.527066000	0.679548000
C	0.269699000	3.026185000	0.609522000
H	-0.083334000	2.723834000	1.617843000
H	-0.648109000	3.227680000	0.017354000
C	1.084134000	4.331814000	0.744086000
H	0.520133000	5.014263000	1.418357000
H	2.040164000	4.107586000	1.270277000
C	1.394952000	5.091106000	-0.562981000
H	1.798341000	6.085295000	-0.272107000

H	0.439646000	5.310094000	-1.094986000
C	2.396376000	4.415261000	-1.535579000
H	3.102151000	5.181402000	-1.923013000
H	3.028604000	3.695350000	-0.969898000
C	1.779053000	3.703072000	-2.755961000
H	1.310636000	4.457904000	-3.427690000
H	2.602582000	3.238114000	-3.342304000
C	0.722596000	2.623176000	-2.428470000
H	-0.209312000	3.105249000	-2.073283000
H	0.454384000	2.073522000	-3.354915000
C	1.251376000	1.667671000	-1.382758000
H	2.193177000	1.164865000	-1.670131000
H	0.218786000	-0.168196000	-2.145171000
O	1.977530000	-1.144997000	-0.187434000
S	3.377398000	-0.687563000	0.266026000
O	4.128365000	0.075473000	-0.758756000
O	3.389760000	-0.175061000	1.668392000
C	4.213415000	-2.385157000	0.381258000
F	5.423664000	-2.271309000	0.949979000
F	3.457103000	-3.215059000	1.139501000
F	4.352921000	-2.934138000	-0.837354000

6: E= -2353.658331

Ir	-0.393641000	0.089436000	-0.439267000
H	-0.131197000	-0.130271000	-1.994404000
Si	-2.058283000	1.587270000	-0.673529000
C	-2.390826000	3.209509000	-1.530323000
H	-3.457304000	3.487194000	-1.400456000
H	-2.169222000	3.125317000	-2.612971000
H	-1.760118000	4.013028000	-1.100164000
N	-2.013423000	-1.266236000	-0.755810000
C	-3.242552000	-0.761442000	-1.093129000
O	-3.403820000	0.555173000	-1.189956000
C	-4.336520000	-1.624488000	-1.336378000
H	-5.301067000	-1.171058000	-1.602783000
C	-4.154328000	-3.003610000	-1.227504000
H	-4.998225000	-3.686060000	-1.415309000
C	-2.886937000	-3.510716000	-0.875614000
H	-2.698006000	-4.589232000	-0.781929000
C	-1.845043000	-2.612947000	-0.647612000
H	-0.833453000	-2.948022000	-0.375103000
N	-1.085987000	0.190448000	1.669385000
C	-2.032145000	1.125134000	1.976007000
O	-2.513755000	1.909022000	1.010143000
C	-2.494246000	1.275817000	3.305266000
H	-3.254666000	2.041994000	3.510156000
C	-1.968610000	0.450144000	4.301811000
H	-2.317005000	0.556449000	5.341398000
C	-0.995575000	-0.515391000	3.969630000
H	-0.560963000	-1.182120000	4.727868000
C	-0.581776000	-0.611407000	2.639609000
H	0.179168000	-1.331466000	2.293797000
C	1.203291000	1.345495000	0.354331000
H	1.755447000	0.646626000	1.010655000
C	1.416570000	1.180869000	-1.042746000
H	2.107019000	0.372942000	-1.345446000
C	1.297576000	2.301288000	-2.059858000
H	0.444970000	2.970517000	-1.818547000
H	1.062481000	1.847869000	-3.045361000

C	2.583590000	3.147227000	-2.186995000
H	3.452335000	2.467273000	-2.341652000
H	2.501424000	3.745724000	-3.121248000
C	2.898414000	4.112598000	-1.024525000
H	3.727089000	4.770517000	-1.364662000
H	2.031081000	4.796238000	-0.869377000
C	3.304973000	3.464573000	0.324743000
H	3.697769000	2.440810000	0.135076000
H	4.158527000	4.029019000	0.758174000
C	2.207230000	3.399587000	1.405149000
H	1.951804000	4.430851000	1.738364000
H	2.625578000	2.884404000	2.298846000
C	0.900930000	2.687246000	0.984553000
H	0.251438000	2.568321000	1.877593000
H	0.337358000	3.325931000	0.272362000
S	1.922257000	-2.465347000	-0.541760000
O	0.906164000	-1.602327000	0.254343000
O	1.569621000	-3.903318000	-0.494060000
O	2.334407000	-1.863352000	-1.834157000
C	3.421266000	-2.255386000	0.597721000
F	3.767444000	-0.947846000	0.662601000
F	3.129063000	-2.676965000	1.843514000
F	4.469182000	-2.953110000	0.135646000

10: E= -1852.848686

Ir	0.096551000	-0.500388000	-0.432883000
H	0.002438000	-2.083390000	-0.565899000
Si	0.252028000	-0.424741000	1.828478000
C	-0.636722000	-1.014509000	3.365147000
H	-0.035342000	-0.759094000	4.262284000
H	-0.782156000	-2.112918000	3.330589000
H	-1.629363000	-0.529048000	3.454641000
N	2.204512000	-0.880460000	-0.210467000
C	2.715384000	-1.072338000	1.048098000
O	1.912980000	-0.989937000	2.102652000
C	4.089461000	-1.356032000	1.237025000
H	4.446798000	-1.500452000	2.265852000
C	4.929936000	-1.436522000	0.126991000
H	6.001046000	-1.655655000	0.262375000
C	4.394941000	-1.233103000	-1.161209000
H	5.021300000	-1.287549000	-2.062952000
C	3.033262000	-0.959486000	-1.286987000
H	2.534607000	-0.792669000	-2.258571000
N	0.625790000	1.656731000	-0.151326000
C	0.685286000	2.134677000	1.126629000
O	0.456786000	1.311129000	2.148693000
C	0.977504000	3.497744000	1.376477000
H	1.011957000	3.839418000	2.420271000
C	1.209337000	4.350668000	0.295496000
H	1.437043000	5.413617000	0.474827000
C	1.152821000	3.841981000	-1.018612000
H	1.332140000	4.482634000	-1.893911000
C	0.857593000	2.488577000	-1.195714000
H	0.787966000	2.000974000	-2.186192000
C	-1.904460000	0.337260000	-0.691662000
H	-1.835124000	0.863040000	-1.663149000
C	-1.991073000	-1.083015000	-0.760976000
H	-1.990433000	-1.514746000	-1.778707000
C	-2.681891000	-1.949071000	0.278053000

H	-2.473384000	-1.573550000	1.301400000
H	-2.234751000	-2.964474000	0.233423000
C	-4.209654000	-2.058959000	0.082568000
H	-4.424593000	-2.347830000	-0.972081000
H	-4.568382000	-2.908514000	0.705107000
C	-5.045695000	-0.812077000	0.443076000
H	-6.112091000	-1.125402000	0.450502000
H	-4.823114000	-0.512973000	1.493790000
C	-4.895946000	0.412903000	-0.495379000
H	-4.527165000	0.067152000	-1.486566000
H	-5.899298000	0.848563000	-0.692407000
C	-3.994566000	1.554114000	0.016122000
H	-4.473013000	2.037310000	0.898075000
H	-3.942399000	2.339705000	-0.770814000
C	-2.555939000	1.145247000	0.409106000
H	-1.972421000	2.065611000	0.622255000
H	-2.575718000	0.562199000	1.353887000
Cl	0.306640000	-0.300441000	-2.947556000

7M: E= -2000.859120

Ir	0.221438000	-0.668965000	0.034461000
Cl	0.635794000	-1.591285000	-2.299437000
P	2.480247000	-0.712248000	0.266505000
Si	-0.375722000	0.437494000	1.909998000
O	-0.125851000	2.143601000	1.460510000
O	-2.144092000	0.317011000	1.876902000
N	0.166609000	1.438402000	-0.743196000
N	-1.927574000	-0.749154000	-0.188468000
C	0.002066000	0.460147000	3.742697000
C	0.019610000	2.444887000	0.169058000
C	0.025946000	3.801772000	-0.236630000
C	0.170494000	4.104627000	-1.592594000
C	0.301420000	3.057368000	-2.527903000
C	0.292593000	1.741628000	-2.058871000
C	-2.715075000	-0.230688000	0.805820000
C	-4.126468000	-0.269813000	0.712837000
C	-4.721415000	-0.845432000	-0.410835000
C	-3.903210000	-1.372238000	-1.430471000
C	-2.517370000	-1.302551000	-1.281352000
H	0.204353000	-2.151251000	0.630598000
H	-0.666544000	1.182311000	4.255588000
H	1.053093000	0.759727000	3.926425000
H	-0.160425000	-0.546817000	4.177540000
H	-0.090615000	4.576185000	0.534400000
H	0.174885000	5.155558000	-1.923402000
H	0.408698000	3.254824000	-3.604294000
H	0.398825000	0.860466000	-2.718056000
H	-4.709120000	0.161121000	1.538762000
H	-5.819189000	-0.882988000	-0.494713000
H	-4.329180000	-1.832273000	-2.333584000
H	-1.810922000	-1.684041000	-2.039060000
C	3.198816000	-0.119148000	1.859828000
H	2.789864000	-0.730775000	2.688167000
H	4.306239000	-0.188696000	1.855377000
H	2.895503000	0.935852000	2.015328000
C	3.350640000	0.309406000	-0.996753000
H	4.452811000	0.221696000	-0.909183000
H	3.004703000	-0.054945000	-1.985088000
H	3.043603000	1.367638000	-0.880708000

C	3.211637000	-2.384845000	0.045893000
H	2.856069000	-2.757652000	-0.935538000
H	4.320129000	-2.353458000	0.079104000
H	2.822564000	-3.051922000	0.839774000

8: E= -1918.529333

Ir	-0.033000000	-0.216198000	-0.514543000
H	-0.117571000	-0.091481000	-2.100808000
Si	-0.714523000	-2.366895000	-0.375755000
C	-2.110192000	-3.481892000	-0.921514000
H	-1.873392000	-4.532123000	-0.652325000
H	-2.252719000	-3.414830000	-2.018689000
H	-3.057966000	-3.193943000	-0.423834000
N	1.834305000	-1.181797000	-0.903445000
C	1.857956000	-2.543032000	-1.063009000
O	0.731686000	-3.235583000	-0.935922000
C	3.069307000	-3.212297000	-1.359225000
H	3.038400000	-4.303797000	-1.480299000
C	4.245700000	-2.471946000	-1.480184000
H	5.194499000	-2.982109000	-1.710051000
C	4.208721000	-1.073466000	-1.302182000
H	5.113750000	-0.455391000	-1.385562000
C	2.986336000	-0.466868000	-1.016003000
H	2.870189000	0.618098000	-0.858328000
N	0.411147000	-0.607434000	1.632140000
C	-0.001434000	-1.799021000	2.155754000
O	-0.625916000	-2.677425000	1.372212000
C	0.221398000	-2.104621000	3.520115000
H	-0.130643000	-3.073257000	3.901076000
C	0.878799000	-1.171452000	4.324633000
H	1.059399000	-1.395253000	5.388039000
C	1.311456000	0.049788000	3.767334000
H	1.836219000	0.806186000	4.367953000
C	1.057145000	0.290741000	2.415734000
H	1.362764000	1.217216000	1.901966000
C	-1.766626000	0.806335000	0.334257000
H	-1.328955000	1.712130000	0.797360000
C	-1.886494000	0.840733000	-1.082642000
H	-1.523195000	1.770618000	-1.557076000
C	-2.942149000	0.088081000	-1.870035000
H	-3.117615000	-0.919561000	-1.439006000
H	-2.552059000	-0.083837000	-2.895244000
C	-4.289606000	0.837681000	-1.959867000
H	-4.105111000	1.881787000	-2.301553000
H	-4.888567000	0.357972000	-2.765431000
C	-5.147647000	0.870963000	-0.677432000
H	-6.151130000	1.250900000	-0.967348000
H	-5.323128000	-0.172635000	-0.325756000
C	-4.610584000	1.736892000	0.491035000
H	-3.917526000	2.507285000	0.085742000
H	-5.451899000	2.308364000	0.939083000
C	-3.917228000	0.975385000	1.638223000
H	-4.667036000	0.352296000	2.176340000
H	-3.549792000	1.718985000	2.380594000
C	-2.740265000	0.062666000	1.223103000
H	-2.237616000	-0.308025000	2.141122000
H	-3.125440000	-0.836363000	0.696574000
O	1.146067000	1.642281000	-0.267992000
C	0.885654000	2.886466000	-0.503447000

O	-0.101679000	3.413492000	-1.010022000
C	2.071229000	3.775953000	0.003082000
F	1.888146000	5.081792000	-0.252270000
F	2.222670000	3.635388000	1.355000000
F	3.248310000	3.398873000	-0.570240000

12: E= -2359.805903

Rh	-0.404919000	0.116397000	-0.541661000
Si	-2.097853000	1.532899000	-0.832032000
S	1.925677000	-2.254473000	0.586413000
N	-1.914374000	-1.282777000	-1.019893000
N	-1.268276000	0.058903000	1.524578000
O	-3.317569000	0.487318000	-1.566115000
O	-2.719100000	1.739402000	0.797188000
O	1.063430000	-1.582692000	-0.490525000
O	1.567024000	-3.676705000	0.799334000
O	2.143039000	-1.406849000	1.798921000
C	-2.371304000	3.184920000	-1.654102000
H	-3.458466000	3.403772000	-1.692636000
H	-1.970145000	3.169903000	-2.687065000
H	-1.866082000	3.993339000	-1.089160000
C	-3.123646000	-0.828335000	-1.463799000
C	-4.158327000	-1.729666000	-1.802185000
C	-3.935031000	-3.100822000	-1.657482000
C	-2.690885000	-3.556372000	-1.176969000
C	-1.704730000	-2.617204000	-0.870969000
C	-2.304657000	0.911936000	1.766259000
C	-2.951033000	0.952233000	3.022863000
C	-2.516512000	0.092026000	4.034265000
C	-1.447862000	-0.788501000	3.779073000
C	-0.853012000	-0.769959000	2.514353000
C	1.100847000	1.398838000	0.407082000
C	1.357368000	1.350606000	-0.981387000
C	1.280619000	2.569987000	-1.873229000
H	0.512961000	3.276848000	-1.497594000
H	0.966880000	2.285742000	-2.899348000
C	2.652853000	3.280283000	-1.937096000
H	3.351626000	2.662056000	-2.543620000
H	2.522993000	4.233709000	-2.497117000
C	3.318845000	3.570921000	-0.576913000
H	3.640282000	2.613904000	-0.109100000
H	4.260357000	4.122903000	-0.785930000
C	2.472591000	4.376354000	0.443200000
H	1.703028000	4.978914000	-0.093892000
H	3.131082000	5.123763000	0.936076000
C	1.794704000	3.566851000	1.568116000
H	1.397654000	4.282504000	2.321799000
H	2.566686000	2.965239000	2.099759000
C	0.634910000	2.633038000	1.154059000
H	0.104343000	2.308221000	2.072771000
H	-0.104491000	3.212381000	0.560264000
C	3.610227000	-2.246444000	-0.278479000
F	3.564842000	-2.951346000	-1.421039000
F	4.548219000	-2.773996000	0.523897000
F	3.963115000	-0.972822000	-0.573499000
H	-0.108912000	0.140238000	-2.071851000
H	-5.111758000	-1.316619000	-2.159194000
H	-4.732182000	-3.816643000	-1.912844000
H	-2.477258000	-4.626079000	-1.042684000

H	-0.705007000	-2.900406000	-0.506637000
H	-3.779346000	1.661029000	3.160380000
H	-3.008490000	0.108188000	5.019738000
H	-1.066478000	-1.477092000	4.546259000
H	0.017217000	-1.401168000	2.284393000
H	1.624029000	0.653449000	1.035339000
H	2.072532000	0.577673000	-1.314931000