Modeling the Direct Activation of Dihydrogen by a P₂C₂-Cyclic Biradical:
Formation of a Cyclic Bis(P-H λ^5 -phosphorane)

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Supporting Information

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Synthesis and Spectroscopic Data

All manipulations with organolithium reagents were carried out under an argon atmosphere by means of the standard Schlenk techniques, and the employed solvents were dried by appropriate methods. ^1H , $^{13}\text{C}\{^1\text{H}\}$ and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra were recorded on a Bruker AVANCE400 spectrometer in CDCl_3 at 298 K with internal Me_4Si (^1H , ^{13}C) or external 85% H_3PO_4 (^{31}P) standard, respectively. Melting points were measured on a Yanagimoto MP-J3 apparatus without correction. ESI-MS spectra were taken on a Bruker APEX3 spectrometer. Compound **1** was prepared according to our previous reports.

Preparation of 3: To a solution of **1** (85 mg, 0.13 mmol)¹ in THF (3 mL) was added a mixture of LiAlH_4 (10 mg, 0.26 mmol) in THF (1 mL) and the solution was stirred for 20 min. Methanol (1.0 mL, 0.024 mmol) was added to the solution and stirred for 10 min. The solvent was removed in vacuo and the residue was extracted with hexane. The organic layer was concentrated and the residual solid was washed with ethanol to afford 62 mg of **3** as greenish-yellow powder (73% yield). Single crystals for X-ray analysis were obtained by recrystallization from dichloromethane at 0 °C. M.p. 130–132 °C (decomp); ^1H NMR (400 MHz, CDCl_3) δ = 0.37 (9H, d, $^3J_{\text{PH}}$ = 16.2 Hz, *t*-BuP), 1.24 (18H, s, *p*-*t*-Bu), 1.49 (18H, s, *o*-*t*-Bu), 1.54 (18H, s, *o*-*t*-Bu), 1.92 (3H, dd, $^2J_{\text{PH}}$ = 12.0 Hz, $^4J_{\text{PH}}$ = 2.8 Hz, Me), 7.02 (2H, s, *m*-Mes*), 7.19 (2H, s, *m*-Mes*), 7.45 (1H, ddd, $^1J_{\text{PH}}$ = 405.0 Hz, $^3J_{\text{PH}}$ = 17.2 Hz, $^4J_{\text{HH}}$ = 17.2 Hz, *t*-BuPH), 8.40 ppm (1H, dddq, $^1J_{\text{PH}}$ = 405.0 Hz, $^3J_{\text{PH}}$ = 17.2 Hz, $^4J_{\text{HH}}$ = 17.2 Hz, $^4J_{\text{PH}}$ = 2.8 Hz, 1H, MePH); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ = 12.6 (dd, $^1J_{\text{PC}}$ = 85.6 Hz, $^1J_{\text{PC}}$ = 101.0 Hz, CP_2), 14.8 (dd, $^1J_{\text{PC}}$ = 41.8 Hz, $^3J_{\text{PC}}$ = 6.4 Hz, MeP), 25.4 (d, $^2J_{\text{PC}}$ = 2.5 Hz, PCMe_3), 31.7 (s, *p*- CMe_3), 32.1 (s, *o*- CMe_3), 34.5 (s, *p*- CMe_3), 34.8 (s, *o*- CMe_3), 36.7 (dd, $^1J_{\text{PC}}$ = 41.2 Hz, $^3J_{\text{PC}}$ = 6.5 Hz, PCMe_3), 37.1 (s, *o*- CMe_3), 38.8 (s, *o*- CMe_3), 119.1 (s, *m*-Mes*), 124.0 (s, *m*-Mes*), 137.0 (d, $^2J_{\text{PC}}$ = 1.4 Hz, *ipso*-Mes*), 143.4 (s, *p*-Mes*), 149.7 (dd, $^3J_{\text{PC}}$ = 13.1 Hz, $^3J_{\text{PC}}$ = 6.7 Hz, *o*-Mes*), 151.1 ppm (d, $^3J_{\text{PC}}$ = 6.3 Hz, *o*-Mes*); $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3) δ = 3.3 (d, $^2J_{\text{PP}}$ = 92.0 Hz, MeP), 47.1 ppm (d, $^2J_{\text{PP}}$ = 92.0 Hz, *t*-BuP); IR (KBr) ν = 2286 cm^{-1} ; UV (CH_2Cl_2) λ_{max} (log ϵ) = 400 (4.2) nm; ESI-MS Calcd for $\text{C}_{43}\text{H}_{72}\text{P}_2$, 650.5104; Found, m/z 650.5102.

Compound **2** was characterized by monitoring the mixture of **1** and LiAlH_4 by $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, THF-*benzene-d*₆) δ = -37.1 (ddq, $^2J_{\text{PP}}$ = 49.3 Hz, $^1J_{\text{PH}}$ = 322.1 Hz, $^2J_{\text{PH}}$ = 9.9 Hz, MePH), 143.8 ppm (d, $^2J_{\text{PP}}$ = 49.3 Hz, *t*-BuP).

Preparation of 3-d: To a solution of **1** (20 mg, 0.031 mmol) in THF (0.5 mL) was added a mixture of LiAlD_4 (2 mg, 0.052 mmol) in THF (0.5 mL) and the solution was stirred for 20 min. Methanol (1.0 mL, 0.024 mmol) was added to the solution and stirred for 10 min. The solvent was removed in vacuo and the residue was extracted with hexane. The organic layer was concentrated and the residual solid was washed with ethanol to afford 13 mg of **3-d** as a greenish-yellow solid (64% yield). ^1H NMR (400 MHz, CDCl_3) δ = 0.33 (9H, d, $^3J_{\text{PH}}$ = 16.4 Hz, *t*-BuP), 1.24 (18H, s, *p*-*t*-Bu), 1.49 (18H, s, *o*-*t*-Bu), 1.55 (18H, s, *o*-*t*-Bu), 1.92 (3H, dd, $^2J_{\text{PH}}$ = 13.4 Hz, MeP), 7.02 (2H, s, *m*-Mes*), 7.19 (2H, s, *m*-Mes*), 7.45 ppm (1H, dd, $^1J_{\text{PH}}$ = 389.0 Hz,

$^3J_{\text{PH}} = 14.6$ Hz, *t*-BuPH); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) $\delta = 11.7$ (dd, $^1J_{\text{PC}} = 85.6$ Hz, $^1J_{\text{PC}} = 101.8$ Hz, CP_2), 14.5 (dd, $^1J_{\text{PC}} = 42.3$ Hz, $^3J_{\text{PC}} = 5.5$ Hz, MeP), 25.0 (d, $^2J_{\text{PC}} = 2.6$ Hz, PCMe_3), 31.3 (s, *p*- CMe_3), 32.6 (d, $^5J_{\text{PC}} = 2.7$ Hz, *o*- CMe_3), 34.1 (s, *p*- CMe_3), 34.2 (s, *o*- CMe_3), 36.6 (s, *o*- CMe_3), 36.7 (dd, $^1J_{\text{PC}} = 41.4$ Hz, $^3J_{\text{PC}} = 6.6$ Hz, PCMe_3), 38.3 (s, *o*- CMe_3), 118.4 (s, *m*-Mes*), 123.4 (d, $^2J_{\text{PC}} = 2.5$ Hz, *ipso*-Mes*), 131.7 (s, *m*-Mes*), 142.6 (s, *p*-Mes*), 149.0 (dd, $^3J_{\text{PC}} = 13.1$ Hz, $^3J_{\text{PC}} = 6.6$ Hz, *o*-Mes*), 150.5 ppm (d, $^3J_{\text{PC}} = 6.0$ Hz, *o*-Mes*); $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3) $\delta = 2.6$ (dt, $^2J_{\text{PP}} = 91.5$ Hz, $^1J_{\text{PD}} = 64.6$ Hz MeP), 47.2 ppm (d, $^2J_{\text{PP}} = 91.5$ Hz, *t*-BuP); ESI-MS Calcd for $\text{C}_{43}\text{H}_{71}\text{P}_2\text{D}$, 651.5167; Found, *m/z* 651.5164.

Compound **2-d** was characterized by monitoring the mixture of **1** and LiAlD_4 by $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, THF-*benzene-d*₆) $\delta = -37.4$ (dt, $^2J_{\text{PP}} = 50.3$ Hz, $^1J_{\text{PD}} = 50.3$ Hz, MePD), 144.1 ppm (d, $^2J_{\text{PP}} = 50.3$ Hz, *t*-BuP).

X-Ray Crystallography for **3**

A Rigaku RAXIS-IV imaging plate detector with graphite-monochromated $\text{MoK}\alpha$ radiation ($\lambda = 0.71070$ Å) was used. The structure was solved by direct methods (SIR92)² expanded using Fourier techniques (DIRDIF94),³ and then refined by full-matrix least squares on *F* for variable parameters. The positions of the hydrogen atom on phosphorus were refined. The data were corrected for Lorentz polarization effect. Structure solution, refinement, and graphical representation were carried out using the teXsan package.⁴ CCDC-670462 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Selected bond lengths (Å) and angles (°): P1–C1 1.697(5), P1–C2 1.720(5), P1–C_{*t*-Bu} 1.854(4), P2–C1 1.755(4), P2–C2 1.773(5), P2–C_{Me} 1.828(5), C1–C_{Mes*} 1.484(6), C2–C_{Mes*} 1.496(6), C1–P1–C2 93.3(2), C1–P1–C_{*t*-Bu} 122.2(2), C2–P1–C_{*t*-Bu} 120.6(2), C1–P2–C2 89.6(2), C1–P2–C_{Me} 116.8(2), C2–P2–C_{Me} 116.1(2), P1–C1–P2 89.2(2), P1–C1–C_{Mes*} 126.8(2), P2–C1–C_{Mes*} 143.9(4), P1–C2–P2 87.8(2), P1–C2–C_{Mes*} 127.4(3), P2–C2–C_{Mes*} 144.0(4).

Calculations

Computations were performed with the Gaussian03 (revision D.01) quantum chemical program package.⁵ DFT calculations were performed at the B3LYP/DGDZVP2 level^{6,7} for model compounds **4**, **5**, **6**, and the related compounds, as well as for the “near-experimental” P,P-reduced and C,C-reduced molecules including *t*-Bu and 2,6-*t*-Bu₂C₆H₃ substituents.

Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	DGDZVP2
Charge	0
Spin	Singlet
E(RB+HF-LYP)	-919.73634456 au
RMS Gradient Norm	0.00000424 au
Imaginary Freq	none
Dipole Moment	0.0007 Debye
Point Group	C1
CPU Time	14:44:38.0

4

22	22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.3811	1.1687	0.2439	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.3811	-1.1687	-0.2440	C	0	0	0	0	0	0	0	0	0	0	0	0	0
1.3800	0.8377	-1.7695	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.3799	-0.8378	1.7694	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.0405	-2.5071	0.0019	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.3061	-3.3189	-0.0637	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.7861	-2.7244	-0.7726	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.5455	-2.6104	0.9764	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.0404	2.5072	-0.0017	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.5479	2.6098	-0.9750	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.7838	2.7259	0.7745	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.3052	3.3185	0.0611	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.6776	-0.7879	-0.3578	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.4563	-0.1678	0.1001	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.6121	-0.5733	-1.4268	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.9386	-1.8412	-0.2125	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.6775	0.7879	0.3578	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.9386	1.8412	0.2125	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.6120	0.5733	1.4268	H	0	0	0	0	0	0	0	0	0	0	0	0	0
3.4562	0.1678	-0.1001	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.0557	-0.4381	0.4341	P	0	0	0	0	0	0	0	0	0	0	0	0	0
1.0557	0.4381	-0.4342	P	0	0	0	0	0	0	0	0	0	0	0	0	0
1	9	1	0	0	0	0										
1	21	4	0	0	0	0										
1	22	4	0	0	0	0										
2	5	1	0	0	0	0										
2	21	4	0	0	0	0										
2	22	4	0	0	0	0										
3	22	1	0	0	0	0										
4	21	1	0	0	0	0										
5	6	1	0	0	0	0										
5	7	1	0	0	0	0										
5	8	1	0	0	0	0										
9	10	1	0	0	0	0										
9	11	1	0	0	0	0										
9	12	1	0	0	0	0										
13	14	1	0	0	0	0										
13	15	1	0	0	0	0										

A 3D ball-and-stick model of a complex organic molecule. The central structure is a cyclohexane ring in a chair-like conformation. Several substituents are attached to the ring, including a long alkyl chain, a branched alkyl group, and a group containing a double bond. The atoms are represented by spheres: carbon (grey), hydrogen (white), and oxygen (red). The bonds are shown as sticks, with some highlighting the stereochemistry of the substituents.

4'

[illegible]

FOPT
RB3LYP
DGDZVP2
0
Singlet
-919.73650898 au
0.00000482 au
none
0.4877 Debye
C1
08:42:38.7

4''

Created by RShA

22	22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0001	-1.1711	-0.3818	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0001	1.2884	0.0634	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.0374	0.3214	-1.3970	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0003	2.7520	-0.3266	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.8718	3.2644	0.0980	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.8740	3.2635	0.0957	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0010	2.9565	-1.4102	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0002	-2.6767	-0.4347	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.8762	-3.0950	0.0787	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0023	-3.0922	-1.4525	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.8728	-3.0957	0.0834	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.5563	-0.1972	0.9866	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.1728	-1.0555	0.6975	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.1077	-0.3742	1.9665	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.1935	0.6921	1.0295	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.2227	0.0617	-0.2482	P	0	0	0	0	0	0	0	0	0	0	0	0	0
1.2227	0.0614	-0.2482	P	0	0	0	0	0	0	0	0	0	0	0	0	0
2.0375	0.3208	-1.3971	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.5562	-0.1977	0.9866	C	0	0	0	0	0	0	0	0	0	0	0	0	0
3.1936	0.6915	1.0295	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.1076	-0.3746	1.9665	H	0	0	0	0	0	0	0	0	0	0	0	0	0
3.1727	-1.0560	0.6974	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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8	10	1	0	0	0	0										
8	11	1	0	0	0	0										
12	13	1	0	0	0	0										
12	14	1	0	0	0	0										
12	15	1	0	0

5

22	22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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0.0017	-1.2711	0.0292	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0034	2.5685	-0.7827	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0030	2.3619	-1.8573	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.8889	3.1763	-0.5600	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.8802	3.1789	-0.5598	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.3887	0.0025	1.1978	C	0	0	0	0	0	0	0	0	0	0	0	0	0
3.0363	0.8854	1.1961	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.7858	0.0042	2.1118	H	0	0	0	0	0	0	0	0	0	0	0	0	0
3.0338	-0.8823	1.1978	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.3525	-0.0016	-0.3531	P	0	0	0	0	0	0	0	0	0	0	0	0	0
1.3525	0.0019	-0.3531	P	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0020	1.4926	1.1037	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0034	-2.5682	-0.7831	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.8803	-3.1785	-0.5604	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0032	-2.3615	-1.8577	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.8888	-3.1762	-0.5604	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0020	-1.4924	1.1034	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.3887	-0.0033	1.1977	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.0336	-0.8883	1.1968	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.7859	-0.0023	2.1119	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.0366	0.8794	1.1969	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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1	12	1	0	0	0	0										
1	13	1	0	0	0	0										
2	11	1	0	0	0	0										
2	12	1	0	0	0	0										
2	14	1	0	0	0	0										
2	18	1	0	0	0	0										
3	4	1	0	0	0	0										
3	5	1	0	0	0	0										
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7	8	1	0	0	0	0										
7	9	1	0	0	0	0										
7	10	1	0	0	0	0										
7	12	1	0	0	0	0										
11	19	1	0	0	0	0										

5'

[illegible]

5''

22	22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0001	-1.1678	-0.7467	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0000	1.1425	0.3351	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0003	2.6666	0.1991	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.8839	3.1096	0.6744	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0008	2.9679	-0.8530	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.8837	3.1099	0.6736	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0002	-2.3227	0.2628	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0006	-1.9826	1.3025	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.8826	-2.9588	0.1255	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.8823	-2.9586	0.1261	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.4789	-0.3982	0.7767	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.1715	-1.1485	0.3829	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.9596	-0.8108	1.6462	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.0741	0.4634	1.0968	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.4787	-0.3988	0.7768	C	0	0	0	0	0	0	0	0	0	0	0	0	0
3.1723	-1.1479	0.3824	H	0	0	0	0	0	0	0	0	0	0	0	0	0
3.0730	0.4630	1.0982	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.9592	-0.8127	1.6454	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.3433	0.1770	-0.5853	P	0	0	0	0	0	0	0	0	0	0	0	0	0
1.3434	0.1768	-0.5853	P	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0002	0.8523	1.3932	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0003	-1.5821	-1.7582	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1	7	1	0	0	0	0										
1	19	1	0	0	0	0										
1	20	1	0	0	0	0										
1	22	1	0	0	0	0										
2	3	1	0	0	0	0										
2	19	1	0	0	0	0										
2	20	1	0	0	0	0										
2	21	1	0	0	0	0										
3	4	1	0	0	0	0										
3	5	1	0	0	0	0										
3	6	1	0	0	0	0										
7	8	1	0	0	0	0										
7	9	1	0	0	0	0										
7	10	1	0	0	0	0										
11	12	1	0	0	0	0										
11	13	1	0	0	0	0										

FOPT
RB3LYP
DGDZVP2
0
Singlet
-919.83834742 au
0.00001165 au
none
1.8790 Debye
C1
3:45:24.3

5''

[illegible]

6

S 13

```
FOPT
RB3LYP
DGDZVP2
0
Singlet
-919.78319875 au
0.00001384 au
none
3.2972 Debye
C1
02:24:15.4
```

6'

[illegible]

6''

[illegible]

6'''

22	22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.1092	1.2074	-0.0263	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.1775	-1.1804	-0.7349	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.0582	-0.0407	-1.5417	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.2854	2.6948	0.1550	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.3649	3.0872	0.9484	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.3104	2.9456	0.4561	H	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0678	3.2742	-0.7546	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.5179	-0.5204	0.8381	C	0	0	0	0	0	0	0	0	0	0	0	0	0
3.1937	0.3311	0.9739	H	0	0	0	0	0	0	0	0	0	0	0	0	0
2.0706	-0.7716	1.8020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
3.0961	-1.3664	0.4509	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1.2101	-0.0306	-0.3735	P	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.3959	0.3084	-0.5716	P	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.3598	-2.4121	0.1579	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.4428	-3.1423	-0.0013	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.3754	-2.1538	1.2198	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.3061	-2.9125	-0.0747	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.1290	-1.4908	-1.7835	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.3223	-0.0577	1.0228	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.8741	0.8514	1.2870	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.0596	-0.8531	0.8623	H	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.6611	-0.3151	1.8559	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1	4	1	0	0	0	0										
1	12	4	0	0	0	0										
1	13	1	0	0	0	0										
2	12	1	0	0	0	0										
2	13	1	0	0	0	0										
2	14	1	0	0	0	0										
2	18	1	0	0	0	0										
3	12	1	0	0	0	0										
4	5	1	0	0	0	0										
4	6	1	0	0	0	0										
4	7	1	0	0	0	0										
8	9	1	0	0	0	0										
8	10	1	0	0	0	0										
8	11	1	0	0	0	0										
8	12	1	0	0	0	0										
13	19	1	0	0	0	0

Created by AJA

S 17

Data for “near-experimental” molecules

Calculation Type FOPT
 Calculation Method RB3LYP
 Basis Set DGDZVP2
 Charge 0
 Spin Singlet
 E(RB+HF-LYP) -2050.33656470 au
 RMS Gradient Norm 0.00007677 au
 Imaginary Freq none
 Dipole Moment 0.5677 Debye
 Point Group C1
 CPU Time 6:4:17:27.5

P,P-Reduced “Real Molecule”

Created by Agui 8.16.1

93	95	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1.2572	0.0905	-0.3472	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.2561	0.0863	-0.3487	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0071	-2.0277	0.7195	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0023	2.1588	-1.5504	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0038	0.2770	-3.1679	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.8950	0.6859	-3.6534	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0012	-0.8069	-3.2737	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.8795	0.6949	-3.6601	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0002	-0.3214	2.5361	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0004	0.7502	-1.3889	P	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0014	-0.6052	0.6798	P	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0748	1.1725	2.8796	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.0676	1.2887	3.9699	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.7783	1.7228	2.4788	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.9919	1.6261	2.4997	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1.2980	-0.9308	3.1063	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1.2863	-0.8321	4.1985	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1.3890	-1.9972	2.8762	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2.1905	-0.4252	2.7298	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.2226	-1.0566	3.1255	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.1974	-2.1308	2.9153	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.2163	-0.9375	4.2157	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.1675	-0.6575	2.7479	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.7301	0.0540	-0.1343	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.3820	-1.2182	0.0326	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.5246	1.2377	0.1321	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.5400	-1.2827	0.8350	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.7099	1.1010	0.8606	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.1734	-0.1423	1.3019	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.9723	-2.2485	1.0734	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-5.2873	1.9787	1.1177	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-6.0564	-0.2120	1.9304	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2.7324	0.0549	-0.1372	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3.5263	1.2372	0.1373	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3.3853	-1.2181	0.0189	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4.7150	1.0960	0.8595	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4.5475	-1.2874	0.8150	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5.1822	-0.1504	1.2875	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5.2918	1.9723	1.1226	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4.9810	-2.2545	1.0451	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6.0681	-0.2243	1.9115	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.1686	2.6585	-0.3817	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

-3.0347	-2.5641	-0.6786	C	0	0	0	0	0	0	0	0	0	0	0	0
3.1653	2.6629	-0.3593	C	0	0	0	0	0	0	0	0	0	0	0	0
3.0334	-2.5617	-0.6944	C	0	0	0	0	0	0	0	0	0	0	0	0
1.9476	3.2476	0.3887	C	0	0	0	0	0	0	0	0	0	0	0	0
1.0938	2.5775	0.3688	H	0	0	0	0	0	0	0	0	0	0	0	0
2.2066	3.4245	1.4379	H	0	0	0	0	0	0	0	0	0	0	0	0
1.6530	4.2083	-0.0489	H	0	0	0	0	0	0	0	0	0	0	0	0
4.3160	3.6772	-0.1520	C	0	0	0	0	0	0	0	0	0	0	0	0
4.5129	3.8752	0.9058	H	0	0	0	0	0	0	0	0	0	0	0	0
5.2470	3.3505	-0.6247	H	0	0	0	0	0	0	0	0	0	0	0	0
4.0284	4.6305	-0.6085	H	0	0	0	0	0	0	0	0	0	0	0	0
2.9395	2.6160	-1.8904	C	0	0	0	0	0	0	0	0	0	0	0	0
2.2265	1.8511	-2.1914	H	0	0	0	0	0	0	0	0	0	0	0	0
2.5807	3.5831	-2.2603	H	0	0	0	0	0	0	0	0	0	0	0	0
3.8820	2.3856	-2.3981	H	0	0	0	0	0	0	0	0	0	0	0	0
1.9978	-2.4561	-1.8253	C	0	0	0	0	0	0	0	0	0	0	0	0
0.9982	-2.2390	-1.4628	H	0	0	0	0	0	0	0	0	0	0	0	0
2.2767	-1.6768	-2.5399	H	0	0	0	0	0	0	0	0	0	0	0	0
1.9605	-3.4099	-2.3645	H	0	0	0	0	0	0	0	0	0	0	0	0
4.3308	-3.0670	-1.3948	C	0	0	0	0	0	0	0	0	0	0	0	0
4.7103	-2.3157	-2.0946	H	0	0	0	0	0	0	0	0	0	0	0	0
5.1331	-3.3022	-0.6929	H	0	0	0	0	0	0	0	0	0	0	0	0
4.1103	-3.9792	-1.9603	H	0	0	0	0	0	0	0	0	0	0	0	0
2.5820	-3.6495	0.3082	C	0	0	0	0	0	0	0	0	0	0	0	0
1.6328	-3.3907	0.7842	H	0	0	0	0	0	0	0	0	0	0	0	0
2.4441	-4.6074	-0.2068	H	0	0	0	0	0	0	0	0	0	0	0	0
3.3223	-3.8000	1.0995	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.9519	3.2567	0.3577	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.0994	2.5846	0.3576	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.6534	4.2068	-0.1000	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.2143	3.4579	1.4016	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.3227	3.6711	-0.1856	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.2528	3.3353	-0.6540	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.5198	3.8810	0.8698	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.0389	4.6201	-0.6536	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.9451	2.5934	-1.9125	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.5920	3.5575	-2.2955	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.2294	1.8281	-2.2056	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.8875	2.3520	-2.4154	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.3361	-3.0687	-1.3721	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.1204	-3.9836	-1.9349	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.1363	-3.2988	-0.6660	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.7163	-2.3190	-2.0734	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.0037	-2.4630	-1.8144	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.0017	-2.2488	-1.4567	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.9719	-3.4176	-2.3524	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.2830	-1.6837	-2.5289	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.5805	-3.6502	0.3243	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.6311	-3.3893	0.7983	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.3190	-3.8004	1.1173	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.4427	-4.6086	-0.1898	H	0	0	0	0	0	0	0	0	0	0	0	0
1 10	1 0	0 0	0												
1 11	1 0	0 0	0												
1 33	1 0	0 0	0												
2 10	1 0	0 0	0												
2 11	1 0	0 0	0												
2 24	1 0	0 0	0												
3 11	1 0	0 0	0												
4 10	1 0	0 0	0												

5	6	1	0	0	0	0
5	7	1	0	0	0	0
5	8	1	0	0	0	0
5	10	1	0	0	0	0
9	11	1	0	0	0	0
9	12	1	0	0	0	0
9	16	1	0	0	0	0
9	20	1	0	0	0	0
12	13	1	0	0	0	0
12	14	1	0	0	0	0
12	15	1	0	0	0	0
16	17	1	0	0	0	0
16	18	1	0	0	0	0
16	19	1	0	0	0	0
20	21	1	0	0	0	0
20	22	1	0	0	0	0
20	23	1	0	0	0	0
24	25	4	0	0	0	0
24	26	1	0	0	0	0
25	27	4	0	0	0	0
25	43	1	0	0	0	0
26	28	4	0	0	0	0
26	42	1	0	0	0	0
27	29	2	0	0	0	0
27	30	1	0	0	0	0
28	29	4	0	0	0	0
28	31	1	0	0	0	0
29	32	1	0	0	0	0
33	34	1	0	0	0	0
33	35	4	0	0	0	0
34	36	4	0	0	0	0
34	44	1	0	0	0	0
35	37	4	0	0	0	0
35	45	1	0	0	0	0
36	38	4	0	0	0	0
36	39	1	0	0	0	0
37	38	2	0	0	0	0
37	40	1	0	0	0	0
38	41	1	0	0	0	0
42	70	1	0	0	0	0
42	74	1	0	0	0	0
42	78	1	0	0	0	0
43	82	1	0	0	0	0
43	86	1	0	0	0	0
43	90	1	0	0	0	0
44	46	1	0	0	0	0
44	50	1	0	0	0	0
44	54	1	0	0	0	0
45	58	1	0	0	0	0
45	62	1	0	0	0	0
45	66	1	0	0	0	0
46	47	1	0	0	0	0
46	48	1	0	0	0	0
46	49	1	0	0	0	0
50	51	1	0	0	0	0
50	52	1	0	0	0	0
50	53	1	0	0	0	0
54	55	1	0	0	0	0
54	56	1	0	0	0	0

54	57	1	0	0	0	0
58	59	1	0	0	0	0
58	60	1	0	0	0	0
58	61	1	0	0	0	0
62	63	1	0	0	0	0
62	64	1	0	0	0	0
62	65	1	0	0	0	0
66	67	1	0	0	0	0
66	68	1	0	0	0	0
66	69	1	0	0	0	0
70	71	1	0	0	0	0
70	72	1	0	0	0	0
70	73	1	0	0	0	0
74	75	1	0	0	0	0
74	76	1	0	0	0	0
74	77	1	0	0	0	0
78	79	1	0	0	0	0
78	80	1	0	0	0	0
78	81	1	0	0	0	0
82	83	1	0	0	0	0
82	84	1	0	0	0	0
82	85	1	0	0	0	0
86	87	1	0	0	0	0
86	88	1	0	0	0	0
86	89	1	0	0	0	0
90	91	1	0	0	0	0
90	92	1	0	0	0	0
90	93	1	0	0	0	0

Created by Agui 8.16.1

2.9636	-2.7164	-0.6026	C	0	0	0	0	0	0	0	0	0	0	0	0
3.3740	2.4554	-0.6334	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.5288	-2.4681	-0.3777	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.7505	2.7621	-0.5553	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.4395	-3.2878	0.3638	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.4263	-3.0412	0.0468	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.5185	-3.1605	1.4482	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.5775	-4.3526	0.1474	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.8305	-3.2987	-0.2396	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.0865	-3.5072	0.8040	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.6859	-2.8145	-0.7192	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.6789	-4.2645	-0.7316	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.2218	-2.4306	-1.8936	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.2870	-1.9170	-2.1145	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.1300	-3.4499	-2.2849	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.0283	-1.9271	-2.4362	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.6543	2.5777	-1.6094	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.7372	2.1777	-1.1860	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.9978	1.9201	-2.4098	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.4083	3.5485	-2.0531	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.9116	3.4628	-1.3226	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.3486	2.7918	-2.0690	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.7158	3.8080	-0.6707	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.5186	4.3418	-1.8449	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.2515	3.7178	0.5531	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.3758	3.3037	1.0569	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.9727	4.6845	0.1173	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.0268	3.9009	1.3031	H	0	0	0	0	0	0	0	0	0	0	0	0
1.7366	-3.4903	-0.0747	C	0	0	0	0	0	0	0	0	0	0	0	0
0.8139	-2.9241	-0.1688	H	0	0	0	0	0	0	0	0	0	0	0	0
1.6097	-4.4165	-0.6472	H	0	0	0	0	0	0	0	0	0	0	0	0
1.8801	-3.7628	0.9754	H	0	0	0	0	0	0	0	0	0	0	0	0
4.1571	-3.7020	-0.4733	C	0	0	0	0	0	0	0	0	0	0	0	0
5.1091	-3.2376	-0.7459	H	0	0	0	0	0	0	0	0	0	0	0	0
4.2502	-4.1266	0.5304	H	0	0	0	0	0	0	0	0	0	0	0	0
3.9853	-4.5408	-1.1558	H	0	0	0	0	0	0	0	0	0	0	0	0
2.8599	-2.4358	-2.1221	C	0	0	0	0	0	0	0	0	0	0	0	0
2.6570	-3.3670	-2.6622	H	0	0	0	0	0	0	0	0	0	0	0	0
2.0681	-1.7346	-2.3769	H	0	0	0	0	0	0	0	0	0	0	0	0
3.8049	-2.0243	-2.4921	H	0	0	0	0	0	0	0	0	0	0	0	0
4.6554	3.3102	-0.4444	C	0	0	0	0	0	0	0	0	0	0	0	0
4.5871	4.1879	-1.0950	H	0	0	0	0	0	0	0	0	0	0	0	0
4.7651	3.6813	0.5788	H	0	0	0	0	0	0	0	0	0	0	0	0
5.5624	2.7628	-0.7165	H	0	0	0	0	0	0	0	0	0	0	0	0
3.2860	2.2227	-2.1662	C	0	0	0	0	0	0	0	0	0	0	0	0
4.1885	1.7140	-2.5198	H	0	0	0	0	0	0	0	0	0	0	0	0
2.4325	1.6220	-2.4805	H	0	0	0	0	0	0	0	0	0	0	0	0
3.2178	3.1860	-2.6836	H	0	0	0	0	0	0	0	0	0	0	0	0
2.2156	3.3501	-0.1332	C	0	0	0	0	0	0	0	0	0	0	0	0
1.2245	2.9349	-0.3029	H	0	0	0	0	0	0	0	0	0	0	0	0
2.3085	3.5245	0.9435	H	0	0	0	0	0	0	0	0	0	0	0	0
2.2618	4.3239	-0.6346	H	0	0	0	0	0	0	0	0	0	0	0	0
1.2720	1.1157	-1.1538	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.2992	-1.2106	0.4614	H	0	0	0	0	0	0	0	0	0	0	0	0
1	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	9	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	31	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	93	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0

2	9	1	0	0	0	0
2	22	1	0	0	0	0
2	92	1	0	0	0	0
3	4	1	0	0	0	0
3	5	1	0	0	0	0
3	6	1	0	0	0	0
3	8	1	0	0	0	0
7	9	1	0	0	0	0
7	10	1	0	0	0	0
7	14	1	0	0	0	0
7	18	1	0	0	0	0
10	11	1	0	0	0	0
10	12	1	0	0	0	0
10	13	1	0	0	0	0
14	15	1	0	0	0	0
14	16	1	0	0	0	0
14	17	1	0	0	0	0
18	19	1	0	0	0	0
18	20	1	0	0	0	0
18	21	1	0	0	0	0
22	23	4	0	0	0	0
22	24	4	0	0	0	0
23	25	4	0	0	0	0
23	41	1	0	0	0	0
24	26	4	0	0	0	0
24	40	1	0	0	0	0
25	27	4	0	0	0	0
25	28	1	0	0	0	0
26	27	4	0	0	0	0
26	29	1	0	0	0	0
27	30	1	0	0	0	0
31	32	1	0	0	0	0
31	33	4	0	0	0	0
32	34	4	0	0	0	0
32	42	1	0	0	0	0
33	35	4	0	0	0	0
33	43	1	0	0	0	0
34	36	4	0	0	0	0
34	37	1	0	0	0	0
35	36	2	0	0	0	0
35	38	1	0	0	0	0
36	39	1	0	0	0	0
40	68	1	0	0	0	0
40	72	1	0	0	0	0
40	76	1	0	0	0	0
41	80	1	0	0	0	0
41	84	1	0	0	0	0
41	88	1	0	0	0	0
42	44	1	0	0	0	0
42	48	1	0	0	0	0
42	52	1	0	0	0	0
43	56	1	0	0	0	0
43	60	1	0	0	0	0
43	64	1	0	0	0	0
44	45	1	0	0	0	0
44	46	1	0	0	0	0
44	47	1	0	0	0	0
48	49	1	0	0	0	0
48	50	1	0	0	0	0

48	51	1	0	0	0	0
52	53	1	0	0	0	0
52	54	1	0	0	0	0
52	55	1	0	0	0	0
56	57	1	0	0	0	0
56	58	1	0	0	0	0
56	59	1	0	0	0	0
60	61	1	0	0	0	0
60	62	1	0	0	0	0
60	63	1	0	0	0	0
64	65	1	0	0	0	0
64	66	1	0	0	0	0
64	67	1	0	0	0	0
68	69	1	0	0	0	0
68	70	1	0	0	0	0
68	71	1	0	0	0	0
72	73	1	0	0	0	0
72	74	1	0	0	0	0
72	75	1	0	0	0	0
76	77	1	0	0	0	0
76	78	1	0	0	0	0
76	79	1	0	0	0	0
80	81	1	0	0	0	0
80	82	1	0	0	0	0
80	83	1	0	0	0	0
84	85	1	0	0	0	0
84	86	1	0	0	0	0
84	87	1	0	0	0	0
88	89	1	0	0	0	0
88	90	1	0	0	0	0
88	91	1	0	0	0	0

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