Supplementary Information (SI) for CrystEngComm.
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Electronic Supplementary Information

Palladium(II) complexes of 5-acetylmethyl-1,2,4-oxadiazole: versatile ditopic acceptors for halogen bonding

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S1. X-ray diffraction studies

Table S1. Crystal data and structure refinement for **1**·1,3,5-FIB**, 2**·1,4-FIB, and **3**·1,4-FIB.

Identification code	**1**·1,3,5-FIB	**2**·1,4-FIB	**3**·1,4-FIB
CCDC number	2523472	2523473	2523474
Empirical formula	$C_{18}H_{14}F_3I_3N_4O_4Pd$	$C_{20}H_{18}F_4I_2N_4O_4Pd$	$C_{28}H_{18}F_4I_2N_4O_4Pd$
Formula weight	894.43	814.608	910.66
Temperature/K	100.0(3)	100(2)	100(2)
Crystal system	monoclinic	triclinic	triclinic
Space group	C2/c	P-1	P-1
a/Å	4.27490(10)	5.2758(3)	6.0196(2)
b/Å	17.9506(4)	10.3940(13)	10.5726(5)
c/Å	30.5282(8)	11.6124(8)	11.3896(5)
α/°	90	89.207(8)	80.628(4)
β/°	90.086(2)	78.929(5)	88.278(3)
γ/°	90	75.569(7)	76.719(4)
Volume/Å^3	2342.64(10)	604.83(10)	696.04(5)
Z	4	1	1
ρ_{calc}g/cm^3	2.536	2.236	2.173
μ/mm^{-1}	37.962	3.385	2.955
F(000)	1656.0	384.5	434.0
Crystal size/mm^3	0.13 × 0.09 × 0.06	0.28 × 0.16 × 0.1	0.13 × 0.07 × 0.02
Radiation	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.79 to 134.934	7.16 to 64.88	6.956 to 57.998
Index ranges	-4 ≤ h ≤ 5, -21 ≤ k ≤ 21, -34 ≤ l ≤ 36	-7 ≤ h ≤ 7, -12 ≤ k ≤ 14, -16 ≤ l ≤ 16	-8 ≤ h ≤ 8, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	9146	6657	13876
Independent reflections	2057 [R_{int} = 0.0841, R_{sigma} = 0.0618]	3877 [R_{int} = 0.0250, R_{sigma} = 0.0352]	3701 [R_{int} = 0.0614, R_{sigma} = 0.0558]
Data/restraints/parameters	2057/0/155	3877/0/162	3701/0/197
Goodness-of-fit on F^2	1.061	1.069	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0440, wR_2 = 0.1170	R_1 = 0.0243, wR_2 = 0.0538	R_1 = 0.0397, wR_2 = 0.0956
Final R indexes [all data]	R_1 = 0.0602, wR_2 = 0.1249	R_1 = 0.0288, wR_2 = 0.0567	R_1 = 0.0498, wR_2 = 0.1026
Largest diff. peak/hole / e Å^{-3}	1.89/-1.60	0.95/-0.89	2.43/-1.61

Table S2. Plane characteristics and interplane angles for **1–3** and **1**·1,3,5-FIB**, 2**·1,4-FIB, and **3**·1,4-FIB.

	1[1]	**1**·1,3,5-FIB	**2**[1]	**2**·1,4-FIB	**3**[1]	**3**·1,4-FIB
Coordination plane, RMDS (Å)	O1N1O1' N1'Pd1, 0	O1N1O1'N 1'Pd1, 0	O1N1O3N3 Pd1, 0.037	O1N1O1'N 1'Pd1, 0	O1N1O1' N1'Pd1, 0	O1N1O1' N1'Pd1, 0
Ligand plane(s), RMDS (Å)	O1C2C3C 4N1, 0.017	O1C2C3C4 N1, 0.018	O1C2C3C4 N1, 0.009 O3C9C10C 11N3, 0.005	O1C2C3C4 N1, 0.016	O1C2C3C 4N1, 0.030	O1C2C3C 4N1, 0.027
Coordination plane/ligand plane fold angle (°)	9.6(3)	1.5(4)	2.82(9) and 4.66(9)	9.79(9)	23.60(11)	19.74(18)

Table S3. Selected bond distances and angles for **1–3** and **1**·1,3,5-FIB**, 2**·1,4-FIB, and **3**·1,4-FIB.

Bond/Angle	Bond length (Å)/angle (°)					
	1[1]	**1**·1,3,5-FIB	**2**[1]	**2**·1,4-FIB	**3**[1]	**3**·1,4-FIB
Pd1–O1	1.987(4)	1.976(6)	1.9793(16)	1.9739(16)	1.9835(17)	1.988(3)
Pd1–O3			1.9814(16)			
Pd1–N1	2.047(4)	2.030(7)	2.0447(18)	2.033(2)	2.010(2)	2.017(3)
Pd1–N3			2.0402(19)			
O1–C2	1.302(7)	1.294(10)	1.294(3)	1.284(3)	1.300(3)	1.287(5)
O3–C9			1.297(3)			
N1–C4	1.328(7)	1.335(11)	1.332(3)	1.318(3)	1.340(3)	1.337(5)
N3–C11			1.333(3)			
C2–C3	1.366(8)	1.356(12)	1.370(3)	1.371(3)	1.371(4)	1.387(6)
C9–C10			1.368(3)			
C3–C4	1.402(8)	1.389(13)	1.401(3)	1.406(3)	1.400(3)	1.400(7)
C10–C11			1.404(3)			
O2–N2	1.427(8)	1.430(9)	1.426(3)	1.424(3)	1.434(3)	1.425(6)
O4–N4			1.431(3)			
N2–C5	1.304(9)	1.276(11)	1.303(3)	1.284(4)	1.304(3)	1.294(5)
N4–C12			1.303(3)			
N1–Pd1–O1	91.90(18)	91.8(3)	91.79(7)	91.57(8)	90.61(8)	90.83(13)
N3–Pd1–O3			91.26(7)			

S2. CCDC search

Table S4. Halogen bonds involving 1,2,4-oxadiazles and related heterocycles.

CCDC refcode/structure number	Contact	Interatomic distance, Å (Nc)	C–I···X angle, °	Ref.
HOLSEI01	I···O	3.4474(13) (0.98)	159.45(4)	[2]
TIPZIF	I···N	3.179(2) (0.90)	174.79(7)	[3]
KIDSEY/1824277	I···N I···N I···N I···N	2.991(5) (0.85) 3.146(5) (0.89) 3.142(4) (0.89) 3.020(5) (0.86)	172.5(2) 174.98(19) 173.33(16) 178.41(17)	[4]
KIDSIC/1824278	I···N I···N	3.113(7) (0.88) 3.050(5) (0.86)	173.8(2) 170.46(19)	[4]
CACVEK/1409979	I···N I···N	3.050(12) (0.86) 3.293(11) (0.93)	176.3(5) 169.1(4)	[5]
CACVIO/1409980	I···N I···N	2.954(6) (0.84) 3.400(5) (0.96)	174.5(2) 165.32(18)	[5]
CACVOU/1409981	I···N I···N	2.956(3) (0.84) 3.410(4) (0.97)	173.69(11) 164.05(10)	[5]
CACVUA/1409982	I···N I···N I···N I···N	3.029(6) (0.88) 3.371(7) (0.95) 3.457(7) (0.98) 3.009(6) (0.85)	174.3(2) 166.31(19) 159.96(18) 173.3(2)	[5]
CACWAH/1409983	I···N I···N	3.285(9) (0.93) 3.112(8) (0.88)	169.7(3) 176.9(3)	[5]
2384981	I···N I···O I···O	2.759(4) (0.78) 3.091(3) (0.88) 2.845(3) (0.81)	168.12(16) 142.20(14) 155.91(14)	[6]
1·1,3,5-FIB	I···N	2.956(7) (0.84)	173.6(2)	This work
2·1,4-FIB	I···N	2.987(2) (0.88)	178.60(2)	This work
3·1,4-FIB	I···N	2.938(3) (0.83)	176.88(5)	This work

Nc is normalized contact distance which is determined as a ratio between interatomic distance and sum of corresponding Bondi van der Waals radii, Bondi[7] $\sum_{vdW}I + N = 3.53$, $\sum_{vdW}I + O = 3.50$ Å.

S3. Coordinates of cluster and crystal models

Table S5. Coordinates of cluster models

1·1,3,5-FIB

Pd	-1.091636	4.487650	15.264083
O	-0.972629	5.728036	13.730042
O	1.464623	7.372311	16.775227
N	0.097219	5.677775	16.399731
N	1.413684	6.573510	17.959720
C	0.634507	6.781737	15.874646
C	-0.328298	6.848154	13.661354
C	0.305312	4.609714	18.741241
H	-0.771436	4.622405	18.939857
H	0.847909	4.859586	19.660352
H	0.602367	3.610745	18.404271
C	0.627510	5.605972	17.688019
C	0.456826	7.375902	14.632150
H	0.971893	8.308812	14.429321
C	-0.561502	7.600284	12.385277
H	-0.354955	6.945051	11.533022
H	0.102309	8.469883	12.347544
H	-1.604007	7.934991	12.343911
O	-1.210643	3.247264	16.798123
O	-3.647896	1.602989	13.752939
N	-2.280491	3.297525	14.128435
N	-3.596956	2.401790	12.568446
C	-2.817779	2.193563	14.653519
C	-1.854974	2.127146	16.866811
C	-2.488584	4.365586	11.786925
H	-1.411836	4.352895	11.588308
H	-3.031181	4.115714	10.867813
H	-2.785640	5.364555	12.123895
C	-2.810783	3.369328	12.840146
C	-2.640098	1.599398	15.896016
H	-3.155165	0.666488	16.098845
C	-1.621770	1.375016	18.142889
H	-1.828317	2.030249	18.995144
H	-2.285582	0.505417	18.180622
H	-0.579265	1.040309	18.184254
Pd	-5.366536	4.487650	15.264083
O	-5.247529	5.728036	13.730042
O	-2.810277	7.372311	16.775227
N	-4.177681	5.677775	16.399731
N	-2.861216	6.573510	17.959720
C	-3.640393	6.781737	15.874646
C	-4.603198	6.848154	13.661354
C	-3.969588	4.609714	18.741241
H	-5.046336	4.622405	18.939857
H	-3.426991	4.859586	19.660352
H	-3.672533	3.610745	18.404271
C	-3.647390	5.605972	17.688019

C	-3.818074	7.375902	14.632150
H	-3.303007	8.308812	14.429321
C	-4.836402	7.600284	12.385277
H	-4.629855	6.945051	11.533022
H	-4.172591	8.469883	12.347544
H	-5.878907	7.934991	12.343911
O	-5.485543	3.247264	16.798123
O	-7.922796	1.602989	13.752939
N	-6.555391	3.297525	14.128435
N	-7.871856	2.401790	12.568446
C	-7.092679	2.193563	14.653519
C	-6.129874	2.127146	16.866811
C	-6.763484	4.365586	11.786925
H	-5.686736	4.352895	11.588308
H	-7.306081	4.115714	10.867813
H	-7.060540	5.364555	12.123895
C	-7.085683	3.369328	12.840146
C	-6.914998	1.599398	15.896016
H	-7.430065	0.666488	16.098845
C	-5.896670	1.375016	18.142889
H	-6.103217	2.030249	18.995144
H	-6.560482	0.505417	18.180622
H	-4.854165	1.040309	18.184254

2·1,4-FIB

Pd	1.114937	-0.203934	5.694496
O	3.789520	2.709245	6.890112
O	0.386943	1.382947	4.773468
N	2.569146	0.907858	6.579990
N	4.269123	1.712206	7.786654
C	3.519890	0.690919	7.578235
C	2.769430	2.159898	6.219529
C	3.689193	-0.565405	8.367492
H	3.989136	-1.373325	7.692034
H	2.726724	-0.840054	8.811504
C	2.081321	2.963135	5.292920
H	2.472114	3.948396	5.060038
C	0.932720	2.541377	4.674270
C	0.173944	3.503983	3.794812
H	0.019123	3.053143	2.808833
H	0.748537	4.430087	3.686116
H	-0.796168	3.727787	4.250292
C	4.725059	-0.431832	9.472225
H	5.696557	-0.180961	9.033338
H	4.803812	-1.379625	10.015092
H	4.421338	0.360846	10.163776
O	-1.559646	-3.117114	4.498880
O	1.842932	-1.790815	6.615524
N	-0.339272	-1.315726	4.809002
N	-2.039249	-2.120074	3.602338
C	-1.290016	-1.098788	3.810757
C	-0.539556	-2.567766	5.169463

C	-1.459319	0.157536	3.021500
H	-1.759262	0.965457	3.696958
H	-0.496850	0.432185	2.577488
C	0.148553	-3.371004	6.096072
H	-0.242240	-4.356264	6.328954
C	1.297155	-2.949246	6.714722
C	2.055930	-3.911852	7.594180
H	2.210752	-3.461012	8.580159
H	1.481337	-4.837956	7.702876
H	3.026042	-4.135655	7.138700
C	-2.495185	0.023963	1.916767
H	-3.466682	-0.226907	2.355654
H	-2.573938	0.971757	1.373900
H	-2.191463	-0.768714	1.225216
Pd	-4.160863	-0.203934	5.694496
O	-1.486280	2.709245	6.890112
O	-4.888857	1.382947	4.773468
N	-2.706654	0.907858	6.579990
N	-1.006677	1.712206	7.786654
C	-1.755910	0.690919	7.578235
C	-2.506370	2.159898	6.219529
C	-1.586607	-0.565405	8.367492
H	-1.286664	-1.373325	7.692034
H	-2.549076	-0.840054	8.811504
C	-3.194479	2.963135	5.292920
H	-2.803686	3.948396	5.060038
C	-4.343080	2.541377	4.674270
C	-5.101856	3.503983	3.794812
H	-5.256677	3.053143	2.808833
H	-4.527263	4.430087	3.686116
H	-6.071968	3.727787	4.250292
C	-0.550741	-0.431832	9.472225
H	0.420757	-0.180961	9.033338
H	-0.471988	-1.379625	10.015092
H	-0.854462	0.360846	10.163776
O	-6.835446	-3.117114	4.498880
O	-3.432868	-1.790815	6.615524
N	-5.615072	-1.315726	4.809002
N	-7.315049	-2.120074	3.602338
C	-6.565816	-1.098788	3.810757
C	-5.815356	-2.567766	5.169463
C	-6.735119	0.157536	3.021500
H	-7.035062	0.965457	3.696958
H	-5.772650	0.432185	2.577488
C	-5.127247	-3.371004	6.096072
H	-5.518040	-4.356264	6.328954
C	-3.978645	-2.949246	6.714722
C	-3.219870	-3.911852	7.594180
H	-3.065048	-3.461012	8.580159
H	-3.794463	-4.837956	7.702876
H	-2.249758	-4.135655	7.138700
C	-7.770985	0.023963	1.916767

H	-8.742482	-0.226907	2.355654
H	-7.849738	0.971757	1.373900
H	-7.467263	-0.768714	1.225216

Table S6. Coordinates of crystal models:

1·1,3,5-FIB

I	1.590808	7.825923	25.440036
F	1.295233	10.935506	24.819399
C	0.623370	10.265948	23.863867
C	0.661785	8.865801	23.903554
I	2.615358	7.825923	20.352212
I	4.240533	13.070550	22.896124
F	4.240533	6.885850	22.896124
F	2.910934	10.935506	20.972850
C	4.240533	10.978587	22.896124
C	3.582796	10.265948	21.928381
C	3.544382	8.865801	21.888695
C	4.240533	8.237530	22.896124
I	2.103083	4.095250	22.896124
F	0.773484	1.960206	20.972850
C	2.103083	2.003287	22.896124
C	1.445346	1.290648	21.928381
F	3.432683	1.960206	24.819399
C	2.760820	1.290648	23.863867
I	0.477908	16.801223	20.352212
F	2.103083	15.861150	22.896124
C	1.406932	17.841101	21.888695
C	2.103083	17.212830	22.896124
I	3.728258	16.801223	25.440036
C	2.799235	17.841101	23.903554
I	1.613719	10.124677	10.175953
F	1.318144	7.015094	9.555316
C	0.646281	7.684652	8.599784
C	0.684696	9.084799	8.639471
I	4.263444	4.880050	7.632041
F	4.263444	11.064750	7.632041
C	4.263444	6.972013	7.632041
C	4.263444	9.713070	7.632041
I	2.638269	10.124677	5.088129
F	2.933845	7.015094	5.708767
C	3.605707	7.684652	6.664299
C	3.567293	9.084799	6.624612
I	3.751169	1.149377	10.175953
F	2.125994	2.089450	7.632041
C	2.822146	0.109499	8.639471
C	2.125994	0.737770	7.632041
I	0.500819	1.149377	5.088129
C	1.429843	0.109499	6.624612
I	2.125994	13.855350	7.632041
F	3.455594	15.990394	9.555316
C	2.125994	15.947313	7.632041

C	2.783731	16.659952	8.599784
F	0.796395	15.990394	5.708767
C	1.468257	16.659952	6.664299
O	1.464623	7.372311	16.775227
N	0.097219	5.677775	16.399731
N	1.413684	6.573510	17.959720
C	0.634507	6.781737	15.874646
C	0.305312	4.609714	18.741241
H	0.847909	4.859586	19.660352
H	0.602367	3.610745	18.404271
C	0.627510	5.605972	17.688019
C	0.456826	7.375902	14.632150
H	0.971893	8.308812	14.429321
H	0.102309	8.469883	12.347544
Pd	3.183264	4.487650	15.264083
O	3.302271	5.728036	13.730042
C	3.946602	6.848154	13.661354
H	3.503464	4.622405	18.939857
C	3.713398	7.600284	12.385277
H	3.919945	6.945051	11.533022
H	2.670893	7.934991	12.343911
O	3.064257	3.247264	16.798123
O	0.627004	1.602989	13.752939
N	1.994409	3.297525	14.128435
N	0.677944	2.401790	12.568446
C	1.457121	2.193563	14.653519
C	2.419926	2.127146	16.866811
C	1.786316	4.365586	11.786925
H	2.863064	4.352895	11.588308
H	1.243719	4.115714	10.867813
H	1.489260	5.364555	12.123895
C	1.464117	3.369328	12.840146
C	1.634802	1.599398	15.896016
H	1.119735	0.666488	16.098845
C	2.653130	1.375016	18.142889
H	2.446583	2.030249	18.995144
H	1.989318	0.505417	18.180622
H	3.695635	1.040309	18.184254
O	0.949718	5.728036	1.534040
C	0.305387	6.848154	1.602729
C	0.538591	7.600284	2.878806
H	0.332044	6.945051	3.731061
H	1.581096	7.934991	2.920172
O	3.624984	1.602989	1.511144
N	2.257580	3.297525	1.135648
N	3.574045	2.401790	2.695637
C	2.794868	2.193563	0.610563
C	2.465673	4.365586	3.477158
H	1.388925	4.352895	3.675774
H	3.008270	4.115714	4.396270
H	2.762729	5.364555	3.140188
C	2.787871	3.369328	2.423936

Pd	1.022903	4.487650	30.528166
H	0.702703	4.622405	26.852391
O	1.141910	3.247264	28.994125
C	1.786241	2.127146	28.925437
C	2.571365	1.599398	29.896233
H	3.086432	0.666488	29.693403
C	1.553036	1.375016	27.649360
H	1.759584	2.030249	26.797105
H	2.216848	0.505417	27.611627
H	0.510532	1.040309	27.607994
C	3.795163	7.375902	0.631933
H	3.280096	8.308812	0.834762
H	4.149679	8.469883	2.916539
O	2.741543	7.372311	29.017021
N	4.108948	5.677775	29.392518
N	2.792483	6.573510	27.832529
C	3.571660	6.781737	29.917602
C	3.900855	4.609714	27.051008
H	3.358257	4.859586	26.131896
H	3.603799	3.610745	27.387977
C	3.578656	5.605972	28.104229
Pd	1.045814	13.462950	15.264083
O	1.164821	14.703336	13.730042
O	3.602073	16.347611	16.775227
N	2.234669	14.653075	16.399731
N	3.551134	15.548810	17.959720
C	2.771957	15.757037	15.874646
C	1.809152	15.823454	13.661354
C	2.442762	13.585014	18.741241
H	1.366014	13.597705	18.939857
H	2.985359	13.834886	19.660352
H	2.739817	12.586045	18.404271
C	2.764960	14.581272	17.688019
C	2.594276	16.351202	14.632150
H	3.109343	17.284112	14.429321
C	1.575948	16.575584	12.385277
H	1.782495	15.920351	11.533022
H	2.239759	17.445183	12.347544
H	0.533443	16.910291	12.343911
O	0.926807	12.222564	16.798123
C	0.282476	11.102446	16.866811
H	0.725614	13.328195	11.588308
C	0.515680	10.350316	18.142889
H	0.309133	11.005549	18.995144
H	1.558185	10.015609	18.184254
O	2.764454	10.578289	13.752939
N	4.131859	12.272825	14.128435
N	2.815394	11.377090	12.568446
C	3.594571	11.168863	14.653519
C	3.923766	13.340886	11.786925
H	3.381169	13.091014	10.867813
H	3.626710	14.339855	12.123895

C	3.601567	12.344628	12.840146
C	3.772252	10.574698	15.896016
H	3.257185	9.641788	16.098845
H	4.126768	9.480717	18.180622
O	1.487534	10.578289	1.511144
N	0.120130	12.272825	1.135648
N	1.436595	11.377090	2.695637
C	0.657418	11.168863	0.610563
C	0.328223	13.340886	3.477158
H	0.870820	13.091014	4.396270
H	0.625279	14.339855	3.140188
C	0.650421	12.344628	2.423936
C	0.433915	10.574698	29.896233
H	0.948982	9.641788	29.693403
H	0.079398	9.480717	27.611627
O	3.087168	14.703336	1.534040
C	2.442837	15.823454	1.602729
C	1.657713	16.351202	0.631933
H	1.142646	17.284112	0.834762
C	2.676041	16.575584	2.878806
H	2.469494	15.920351	3.731061
H	2.012229	17.445183	2.916539
H	3.718546	16.910291	2.920172
H	3.526375	13.328195	3.675774
Pd	3.160353	13.462950	30.528166
O	0.604093	16.347611	29.017021
N	1.971498	14.653075	29.392518
N	0.655033	15.548810	27.832529
C	1.434210	15.757037	29.917602
C	1.763405	13.585014	27.051008
H	2.840153	13.597705	26.852391
H	1.220807	13.834886	26.131896
H	1.466349	12.586045	27.387977
C	1.441206	14.581272	28.104229
O	3.279360	12.222564	28.994125
C	3.923691	11.102446	28.925437
C	3.690486	10.350316	27.649360
H	3.897034	11.005549	26.797105
H	2.647982	10.015609	27.607994

2·1,4-FIB

I	2.418812000	1.572214000	1.970409000
C	0.980900000	0.630796000	0.796660000
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F	3.974393000	8.610923000	1.809597000
C	3.289841000	9.352412000	0.926381000
F	6.121610000	1.047261000	9.579395000
C	6.806162000	0.305772000	10.462611000
F	7.993657000	2.230324000	11.052219000
C	7.772909000	0.927363000	11.235241000
I	7.677191000	8.085970000	9.418582000

C	9.115103000	9.027388000	10.592332000
Pd	2.410101000	4.829092000	5.694496000
O	5.084684000	7.742271000	6.890112000
N	3.864310000	5.940884000	6.579990000
N	5.564287000	6.745232000	7.786654000
C	4.815054000	5.723945000	7.578235000
C	4.064594000	7.192924000	6.219529000
C	4.984357000	4.467621000	8.367492000
H	5.284301000	3.659701000	7.692034000
H	4.021888000	4.192972000	8.811504000
C	3.376485000	7.996161000	5.292920000
H	3.767279000	8.981422000	5.060038000
C	6.020224000	4.601194000	9.472225000
H	6.991721000	4.852065000	9.033338000
H	6.098976000	3.653401000	10.015092000
H	5.716502000	5.393872000	10.163776000
O	3.138096000	3.242211000	6.615524000
C	2.592319000	2.083780000	6.714722000
C	3.351095000	1.121175000	7.594180000
H	3.505916000	1.572014000	8.580159000
H	2.776502000	0.195070000	7.702876000
H	4.321207000	0.897371000	7.138700000
O	6.957907000	6.415973000	4.773468000
C	7.503684000	7.574404000	4.674270000
C	6.744908000	8.537009000	3.794812000
H	6.590087000	8.086170000	2.808833000
H	7.319501000	9.463114000	3.686116000
H	5.774796000	8.760813000	4.250292000
O	5.011318000	1.915913000	4.498880000
N	6.231693000	3.717300000	4.809002000
N	4.531715000	2.912952000	3.602338000
C	5.280949000	3.934239000	3.810757000
C	6.031408000	2.465260000	5.169463000
C	5.111646000	5.190563000	3.021500000
H	4.811702000	5.998483000	3.696958000
H	6.074115000	5.465212000	2.577488000
C	6.719518000	1.662023000	6.096072000
H	6.328724000	0.676762000	6.328954000
C	4.075779000	5.056990000	1.916767000
H	3.104282000	4.806119000	2.355654000
H	3.997027000	6.004783000	1.373900000
H	4.379501000	4.264312000	1.225216000

3·1,4-FIB

I	2.145147	9.900339	7.636828
F	1.380559	9.451873	4.572433
F	-0.564031	10.424161	3.019446
C	0.616580	10.669092	6.441186
C	0.495333	10.312351	5.106202
C	-0.504419	10.824387	4.311729
I	-2.964865	12.504241	3.600412
F	-2.200278	12.952708	6.664807

F	-0.255687	11.980420	8.217794
C	-1.436299	11.735489	4.796054
C	-1.315052	12.092229	6.131038
C	-0.315300	11.580193	6.925511
Pd	7.576264	6.969825	11.237240
O	4.886614	9.891693	10.157341
O	8.514283	8.586963	11.912598
N	6.191889	8.118162	10.324776
N	4.398732	8.913784	9.242630
C	5.055368	6.732935	8.479621
C	5.201971	7.909488	9.381972
C	5.985221	9.370774	10.745049
C	6.762145	10.170855	11.591213
H	6.377513	11.136177	11.902833
C	4.705445	4.671615	6.646827
H	4.565569	3.868368	5.930577
C	3.840654	6.070274	8.409950
H	3.022531	6.358838	9.061283
C	6.108667	6.367632	7.636828
H	7.064270	6.877048	7.703780
C	8.009063	9.763681	12.042950
C	5.923815	5.347105	6.713127
H	6.730881	5.074898	6.041365
C	8.898010	10.772756	12.725051
H	9.354140	10.318177	13.610185
H	8.301229	11.640144	13.025871
H	9.684064	11.093164	12.032780
C	3.675676	5.032385	7.499734
H	2.731235	4.499779	7.457504
O	10.265913	4.047958	12.317139
O	6.638245	5.352687	10.561882
N	8.960638	5.821488	12.149704
N	10.753796	5.025866	13.231850
C	10.097160	7.206716	13.994859
C	9.950556	6.030163	13.092508
C	9.167307	4.568877	11.729431
C	8.390383	3.768796	10.883267
H	8.775015	2.803474	10.571647
C	10.447083	9.268036	15.827653
H	10.586959	10.071283	16.543903
C	11.311874	7.869377	14.064530
H	12.129997	7.580813	13.413197
C	9.043860	7.572018	14.837652
H	8.088258	7.062603	14.770700
C	7.143465	4.175970	10.431530
C	9.228713	8.592546	15.761353
H	8.421647	8.864753	16.433115
C	6.254518	3.166895	9.749429
H	5.798388	3.621474	8.864294
H	6.851299	2.299506	9.448608
H	5.468464	2.846487	10.441700
C	11.476851	8.907265	14.974746

H	12.421292	9.439872	15.016976

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