Electronic Supplementary Information (ESI)

Remarkable Charge-transfer Mobility from [6] to [10]phenacene as High Performance p-type Organic Semiconductors.

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Table S1: Lattice parameters of phenacene series based on experiment data[1-7] and theoretical calculations.

	3P		4P		5P		6P		7P		8P	
Chemical formula	$C_{14}H_{10}$		$C_{18}H_{12}$		$C_{22}H_{14}$		$C_{26}H_{16}$		$C_{30}H_{18}$		$C_{34}H_{20}$	
	RPG (exp)[1]	vdW	RPG (exp)[2]	vdW	RPG (exp)[3]	vdW	RPG (exp)[4-6]	vdW	RPG (exp)[4-6]	vdW	RPG (exp)[6]	vdW
a [Å]	8.441	8.513	8.386	8.473	8.480	8.595	12.130	8.410	8.438	8.646	8.842	8.854
b[Å]	6.140	6.294	6.196	6.302	6.154	6.238	7.942	6.540	6.177	6.218	6.043	6.084
c [Å]	9.438	9.569	25.203	25.626	13.515	13.641	15.401	15.921	17.829	17.942	19.896	20.097
β [°]	97.960	97.615	116.20	116.18	90.460	90.508	93.160	87.643	93.190	92.864	92.920	92.667

	9P		10P	
Chemical formula	$C_{38}H_{22}$		$C_{42}H_{24}$	
	RPG (exp)[7]	vdW	RPG	vdW
a [Å]	8.844	8.860	8.900	8.998
b[Å]	6.127	6.146	6.170	6.200
c [Å]	22.470	22.569	24.535	24.669
β [°]	92.720	92.845	93.000	92.697

Table S2: Comparison between Kohn-Sham gap (KS), GGA-PBE, G_0W_0 and the previously reported experimental and theoretical data of phenacenes (number benzene rings from 3 to 10, denoted as 3P→ 10P)

	For single molecules			**For lattice structure**			**$E^{exp}_{Optical\ gap}$ (Reported)**	**E^{exp}_{gap} (Ref. 8, 19)**
Name	**E^{KS}_{gap} (This work)**	**E^{KS}_{gap} (Ref. 8)**	**$E^{TD\text{-}DFT}_{gap}$ (Ref. 8)**	**E^{GW}_{gap} (This work)**	**$E^{GGA\text{-}PBE}_{gap}$ (This work)**	**E^{theo}_{gap} (Reported)**		
3P	4.67	4.67	4.19	-	2.89	2.75 (LDA)[12] 2.77 (PBE)[13]	3.16[9] (3.50[20])	4.24
4P	4.20	4.21	3.73	-	2.47	-	3.30[10]	3.89
5P	4.19	4.19	3.70	4.10 (4.08[17, 18])	2.39	2.36 (LDA) [14] 2.20 (PBE)[15]	3.30[11,7]	3.80
6P	4.01	4.00	3.47	3.80	2.29	-	3.10[11,7]	-
7P	4.00	4.00	3.50	3.80	2.15	2.00 (PBE)[16]	3.10[11,7]	-
8P	3.91	-	-	3.70	2.06	-	3.00[11,7]	-
9P	3.91	-	-	3.70	2.08	-	3.00[11,7]	-
10P	3.85	-	-	3.60	2.07	-	-	-

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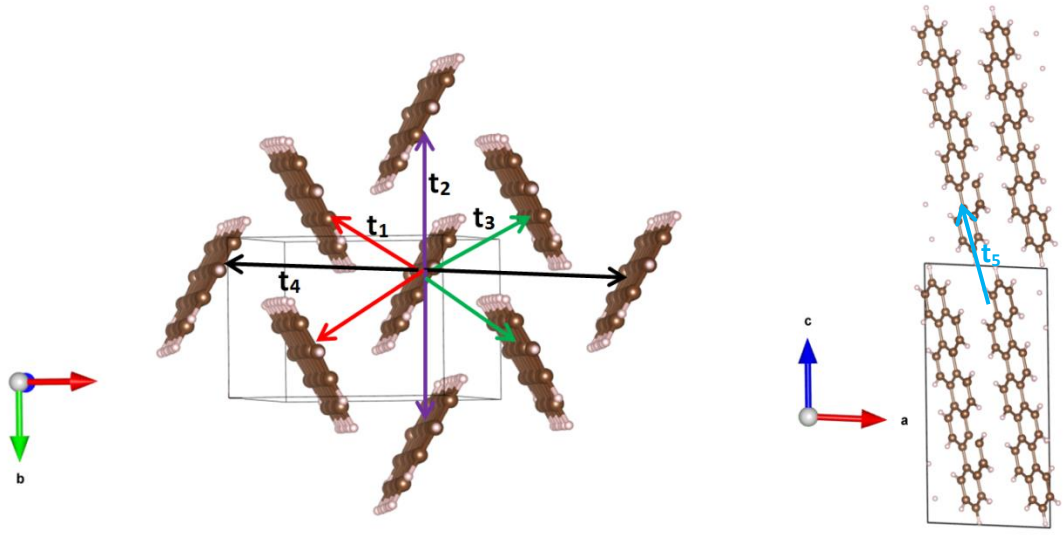
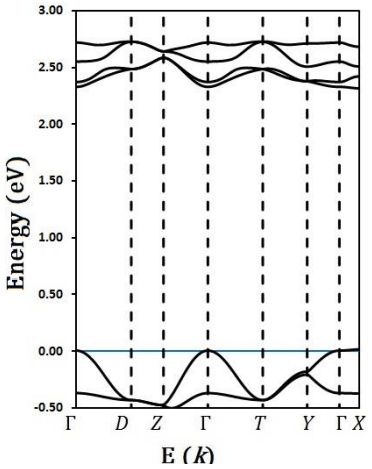
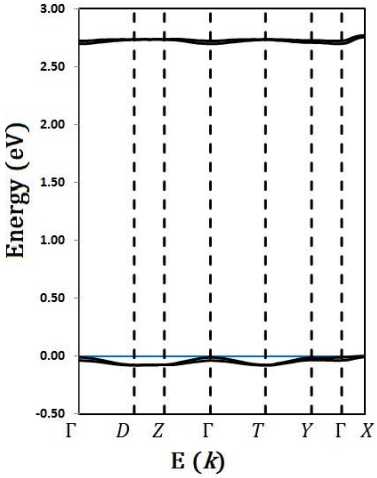


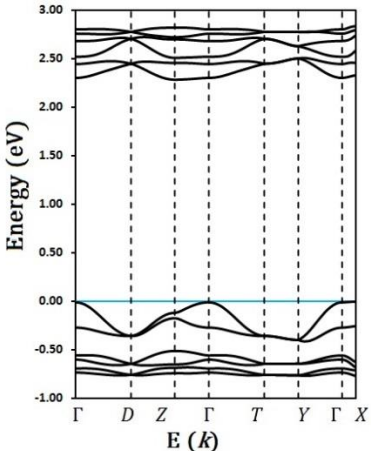
Fig. S1: Directions of hopping pathways for 7P crystal. The surrounding molecules are deleted for the purpose of clarify. *The other members in phenacene series share the same structural features*; thus, have similar hopping pathways as 7P. (C: brown; H: white)



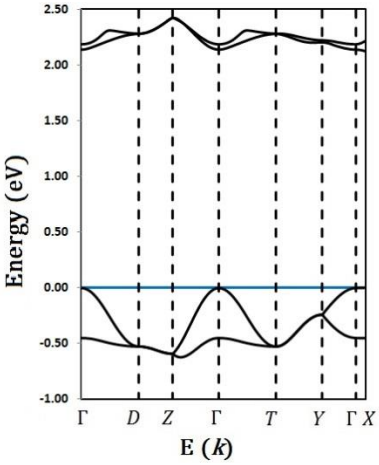
5P-RPG (picene)



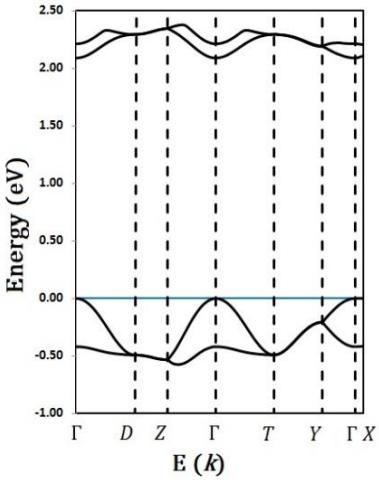
6P-RPG



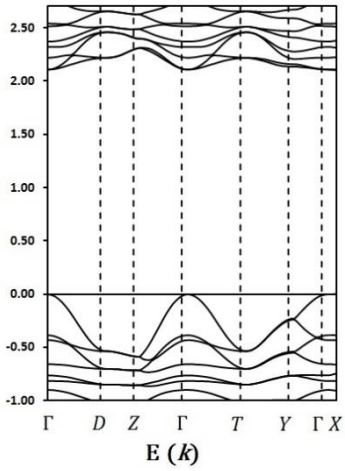
6P-vdW



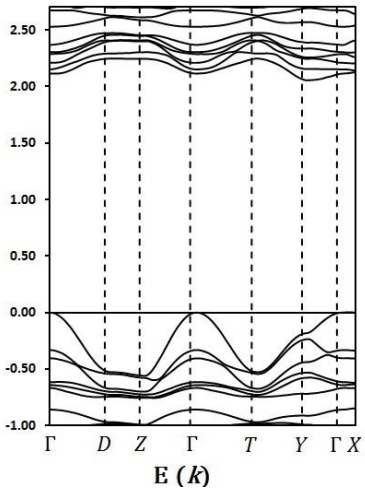
7P-RPG



8P-RPG



9P-RPG



10P-RPG

Fig. S2: Band Structures of phenacene series calculated by GGA-PBE functional.

Crystal Information File (CIF) of 6P-RPG generated by VESTA

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_cell_length_c 15.401000

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_cell_angle_gamma 90.0000

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loop_

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_atom_site_fract_z

_atom_site_occupancy

_atom_site_B_iso_or_equiv

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C3	C	0.667908	0.003603	0.375400	1.0000	0.000
C4	C	0.332092	0.503603	0.624600	1.0000	0.000
C5	C	0.637613	0.001690	0.288582	1.0000	0.000
C6	C	0.362387	0.501690	0.711418	1.0000	0.000
C7	C	0.669146	0.133715	0.232283	1.0000	0.000
C8	C	0.330854	0.633715	0.767717	1.0000	0.000
C9	C	0.734709	0.269787	0.267501	1.0000	0.000
C10	C	0.265291	0.769787	0.732499	1.0000	0.000
C11	C	0.766990	0.270277	0.359687	1.0000	0.000
C12	C	0.233010	0.770277	0.640313	1.0000	0.000
C13	C	0.832003	0.402128	0.398570	1.0000	0.000
C14	C	0.167997	0.902128	0.601430	1.0000	0.000
C15	C	0.861200	0.404405	0.485943	1.0000	0.000
C16	C	0.138800	0.904405	0.514057	1.0000	0.000
C17	C	0.828052	0.274655	0.542817	1.0000	0.000
C18	C	0.171948	0.774655	0.457183	1.0000	0.000
C19	C	0.763630	0.139577	0.506073	1.0000	0.000
C20	C	0.236370	0.639577	0.493927	1.0000	0.000
C21	C	0.730508	0.009512	0.562690	1.0000	0.000
C22	C	0.269492	0.509512	0.437310	1.0000	0.000
C23	C	0.758192	0.012404	0.650173	1.0000	0.000
C24	C	0.241808	0.512404	0.349827	1.0000	0.000
C25	C	0.821711	0.145396	0.689477	1.0000	0.000
C26	C	0.178289	0.645396	0.310523	1.0000	0.000

C27	C	0.857484	0.277628	0.635298	1.0000	0.000
C28	C	0.142516	0.777628	0.364702	1.0000	0.000
C29	C	0.921746	0.411570	0.674314	1.0000	0.000
C30	C	0.078255	0.911570	0.325686	1.0000	0.000
C31	C	0.947855	0.416121	0.761841	1.0000	0.000
C32	C	0.052145	0.916121	0.238159	1.0000	0.000
C33	C	0.912300	0.287023	0.818329	1.0000	0.000
C34	C	0.087700	0.787023	0.181671	1.0000	0.000
C35	C	0.849308	0.148975	0.782348	1.0000	0.000
C36	C	0.150692	0.648975	0.217652	1.0000	0.000
C37	C	0.816222	0.021968	0.840204	1.0000	0.000
C38	C	0.183778	0.521968	0.159796	1.0000	0.000
C39	C	0.842465	0.031701	0.928702	1.0000	0.000
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C45	C	0.764344	0.399168	0.209727	1.0000	0.000
C46	C	0.235656	0.899168	0.790273	1.0000	0.000
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C48	C	0.363987	0.632151	0.857359	1.0000	0.000
C49	C	0.730731	0.394855	0.122356	1.0000	0.000
C50	C	0.269269	0.894855	0.877644	1.0000	0.000
C51	C	0.665909	0.260534	0.088174	1.0000	0.000
C52	C	0.334091	0.760534	0.911826	1.0000	0.000
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H2	H	0.139996	0.005172	0.641375	1.0000	0.000
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H6	H	0.048955	0.013130	0.365914	1.0000	0.000
H7	H	0.921904	0.178328	0.033728	1.0000	0.000
H8	H	0.078096	0.678328	0.966272	1.0000	0.000
H9	H	0.997063	0.519923	0.789816	1.0000	0.000
H10	H	0.002937	0.019924	0.210184	1.0000	0.000
H11	H	0.984750	0.401838	0.935450	1.0000	0.000
H12	H	0.015250	0.901838	0.064550	1.0000	0.000
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H14	H	0.184876	0.432506	0.028385	1.0000	0.000
H15	H	0.768831	0.913939	0.815411	1.0000	0.000
H16	H	0.231169	0.413939	0.184589	1.0000	0.000
H17	H	0.729969	0.909216	0.689899	1.0000	0.000
H18	H	0.270031	0.409216	0.310101	1.0000	0.000
H19	H	0.681495	0.904251	0.536906	1.0000	0.000
H20	H	0.318505	0.404251	0.463094	1.0000	0.000
H21	H	0.641111	0.900240	0.415572	1.0000	0.000
H22	H	0.358889	0.400240	0.584428	1.0000	0.000
H23	H	0.587779	0.898182	0.261039	1.0000	0.000
H24	H	0.412221	0.398182	0.738961	1.0000	0.000
H25	H	0.814476	0.505060	0.233575	1.0000	0.000
H26	H	0.185524	0.005060	0.766425	1.0000	0.000
H27	H	0.755321	0.495929	0.079567	1.0000	0.000
H28	H	0.244679	-0.004071	0.920433	1.0000	0.000

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Crystal Information File (CIF) of 6P-vdW generated by VESTA

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C3	1.0	0.604339	0.946069	0.373778	Biso	1.000000	C
C4	1.0	0.395661	0.446069	0.626222	Biso	1.000000	C
C5	1.0	0.569854	0.942683	0.290357	Biso	1.000000	C
C6	1.0	0.430146	0.442683	0.709643	Biso	1.000000	C
C7	1.0	0.609908	0.110326	0.235650	Biso	1.000000	C
C8	1.0	0.390092	0.610326	0.764350	Biso	1.000000	C
C9	1.0	0.688692	0.285644	0.268965	Biso	1.000000	C
C10	1.0	0.311308	0.785644	0.731035	Biso	1.000000	C
C11	1.0	0.726341	0.287211	0.357701	Biso	1.000000	C
C12	1.0	0.273659	0.787211	0.642299	Biso	1.000000	C
C13	1.0	0.805499	0.456086	0.394700	Biso	1.000000	C
C14	1.0	0.194501	0.956086	0.605300	Biso	1.000000	C
C15	1.0	0.839100	0.459354	0.478585	Biso	1.000000	C
C16	1.0	0.160900	0.959354	0.521415	Biso	1.000000	C
C17	1.0	0.797148	0.293577	0.533838	Biso	1.000000	C
C18	1.0	0.202852	0.793577	0.466162	Biso	1.000000	C
C19	1.0	0.718441	0.120859	0.499191	Biso	1.000000	C
C20	1.0	0.281559	0.620859	0.500809	Biso	1.000000	C
C21	1.0	0.675056	0.956096	0.554711	Biso	1.000000	C
C22	1.0	0.324944	0.456096	0.445289	Biso	1.000000	C
C23	1.0	0.707589	0.960130	0.638757	Biso	1.000000	C
C24	1.0	0.292411	0.460130	0.361243	Biso	1.000000	C

C25	1.0	0.787122	0.128853	0.675612	Biso	1.000000 C
C26	1.0	0.212878	0.628853	0.324388	Biso	1.000000 C
C27	1.0	0.831861	0.297577	0.622677	Biso	1.000000 C
C28	1.0	0.168139	0.797577	0.377323	Biso	1.000000 C
C29	1.0	0.909983	0.469722	0.659044	Biso	1.000000 C
C30	1.0	0.090017	0.969722	0.340956	Biso	1.000000 C
C31	1.0	0.942324	0.475131	0.742694	Biso	1.000000 C
C32	1.0	0.057676	0.975131	0.257306	Biso	1.000000 C
C33	1.0	0.900046	0.308945	0.797673	Biso	1.000000 C
C34	1.0	0.099954	0.808945	0.202327	Biso	1.000000 C
C35	1.0	0.821631	0.133015	0.764720	Biso	1.000000 C
C36	1.0	0.178369	0.633015	0.235280	Biso	1.000000 C
C37	1.0	0.781063	0.971349	0.821696	Biso	1.000000 C
C38	1.0	0.218937	0.471349	0.178304	Biso	1.000000 C
C39	1.0	0.816097	0.982989	0.906153	Biso	1.000000 C
C40	1.0	0.183903	0.482989	0.093847	Biso	1.000000 C
C41	1.0	0.893672	0.156988	0.937867	Biso	1.000000 C
C42	1.0	0.106328	0.656988	0.062133	Biso	1.000000 C
C43	1.0	0.934811	0.316794	0.884188	Biso	1.000000 C
C44	1.0	0.065189	0.816794	0.115812	Biso	1.000000 C
C45	1.0	0.725124	0.450747	0.213014	Biso	1.000000 C
C46	1.0	0.274876	0.950747	0.786986	Biso	1.000000 C
C47	1.0	0.571172	0.105824	0.149456	Biso	1.000000 C
C48	1.0	0.428828	0.605824	0.850544	Biso	1.000000 C
C49	1.0	0.684965	0.443290	0.129237	Biso	1.000000 C
C50	1.0	0.315035	0.943290	0.870763	Biso	1.000000 C
C51	1.0	0.607398	0.269842	0.096900	Biso	1.000000 C

C52	1.0	0.392602	0.769842	0.903100	Biso	1.000000 C
H1	1.0	0.840618	0.587247	0.356527	Biso	1.000000 H
H2	1.0	0.159382	0.087247	0.643473	Biso	1.000000 H
H3	1.0	0.899120	0.592885	0.502252	Biso	1.000000 H
H4	1.0	0.100880	0.092885	0.497748	Biso	1.000000 H
H5	1.0	0.944351	0.600022	0.620342	Biso	1.000000 H
H6	1.0	0.055649	0.100022	0.379658	Biso	1.000000 H
H7	1.0	0.919367	0.167012	0.004076	Biso	1.000000 H
H8	1.0	0.080633	0.667012	0.995924	Biso	1.000000 H
H9	1.0	0.001307	0.607583	0.768720	Biso	1.000000 H
H10	1.0	-0.001307	0.107583	0.231280	Biso	1.000000 H
H11	1.0	-0.005379	0.451779	0.907300	Biso	1.000000 H
H12	1.0	0.005379	0.951779	0.092700	Biso	1.000000 H
H13	1.0	0.782314	0.857469	0.948275	Biso	1.000000 H
H14	1.0	0.217686	0.357470	0.051725	Biso	1.000000 H
H15	1.0	0.720528	0.835973	0.800003	Biso	1.000000 H
H16	1.0	0.279472	0.335973	0.199997	Biso	1.000000 H
H17	1.0	0.670644	0.830393	0.677316	Biso	1.000000 H
H18	1.0	0.329356	0.330393	0.322684	Biso	1.000000 H
H19	1.0	0.614035	0.823078	0.531282	Biso	1.000000 H
H20	1.0	0.385965	0.323078	0.468717	Biso	1.000000 H
H21	1.0	0.570780	0.814926	0.412228	Biso	1.000000 H
H22	1.0	0.429220	0.314926	0.587772	Biso	1.000000 H
H23	1.0	0.509786	0.810972	0.264521	Biso	1.000000 H
H24	1.0	0.490214	0.310972	0.735479	Biso	1.000000 H
H25	1.0	0.785273	0.586107	0.235133	Biso	1.000000 H
H26	1.0	0.214727	0.086107	0.764867	Biso	1.000000 H

H27	1.0	0.714190	0.572346	0.088160	Biso	1.000000 H
H28	1.0	0.285810	0.072346	0.911840	Biso	1.000000 H
H29	1.0	0.576710	0.265713	0.031151	Biso	1.000000 H
H30	1.0	0.423290	0.765713	0.968849	Biso	1.000000 H
H31	1.0	0.510990	-0.029053	0.125828	Biso	1.000000 H
H32	1.0	0.489010	0.470947	0.874172	Biso	1.000000 H

Crystal Information File (CIF) of 10P-vdW generated by VESTA

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_cell_length_a                         8.99751
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_cell_angle_gamma                      90.03498
_symmetry_space_group_name_H-M         'P 1'
_symmetry_Int_Tables_number            1

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_atom_site_fract_y

_atom_site_fract_z

_atom_site_adp_type

_atom_site_B_iso_or_equiv

_atom_site_type_symbol

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C2	1.0	0.414766	0.641464	0.962880	Biso	1.000000	C
C3	1.0	0.291274	0.982512	0.224972	Biso	1.000000	C
C4	1.0	0.496815	0.468060	0.940278	Biso	1.000000	C
C5	1.0	0.243065	0.976996	0.277716	Biso	1.000000	C
C6	1.0	0.530262	0.466407	0.886584	Biso	1.000000	C
C7	1.0	0.276897	0.147474	0.314917	Biso	1.000000	C
C8	1.0	0.483895	0.637717	0.850210	Biso	1.000000	C
C9	1.0	0.407229	0.330215	0.241330	Biso	1.000000	C
C10	1.0	0.364901	0.816064	0.928289	Biso	1.000000	C
C11	1.0	0.400512	0.499136	0.332269	Biso	1.000000	C
C12	1.0	0.354251	0.981598	0.834686	Biso	1.000000	C
C13	1.0	0.361585	0.326628	0.295779	Biso	1.000000	C
C14	1.0	0.400303	0.812529	0.871095	Biso	1.000000	C
C15	1.0	0.144717	0.977020	0.392671	Biso	1.000000	C
C16	1.0	0.606957	0.467532	0.770778	Biso	1.000000	C
C17	1.0	0.105991	0.974548	0.446091	Biso	1.000000	C
C18	1.0	0.641765	0.466808	0.717059	Biso	1.000000	C
C19	1.0	0.151473	0.141725	0.483280	Biso	1.000000	C
C20	1.0	0.594210	0.635392	0.680482	Biso	1.000000	C
C21	1.0	0.231840	0.147183	0.371130	Biso	1.000000	C
C22	1.0	0.521206	0.637000	0.793405	Biso	1.000000	C

C23	1.0	0.236133	0.317084	0.462978	Biso	1.000000 C
C24	1.0	0.509785	0.808927	0.701482	Biso	1.000000 C
C25	1.0	0.359881	0.496024	0.385160	Biso	1.000000 C
C26	1.0	0.388837	0.980442	0.780890	Biso	1.000000 C
C27	1.0	0.275466	0.320833	0.406465	Biso	1.000000 C
C28	1.0	0.473225	0.809998	0.758361	Biso	1.000000 C
C29	1.0	0.114428	0.137893	0.540192	Biso	1.000000 C
C30	1.0	0.630156	0.634163	0.623543	Biso	1.000000 C
C31	1.0	0.162912	0.308803	0.575702	Biso	1.000000 C
C32	1.0	0.581154	0.806622	0.588538	Biso	1.000000 C
C33	1.0	0.029931	0.966360	0.562515	Biso	1.000000 C
C34	1.0	0.714848	0.464054	0.600841	Biso	1.000000 C
C35	1.0	0.127368	0.304841	0.632634	Biso	1.000000 C
C36	1.0	0.616834	0.805372	0.531617	Biso	1.000000 C
C37	1.0	0.996182	0.962466	0.616373	Biso	1.000000 C
C38	1.0	0.748680	0.463001	0.547027	Biso	1.000000 C
C39	1.0	0.043581	0.129682	0.653306	Biso	1.000000 C
C40	1.0	0.701154	0.631851	0.510587	Biso	1.000000 C
C41	1.0	0.282292	0.484482	0.499992	Biso	1.000000 C
C42	1.0	0.462611	0.977906	0.665026	Biso	1.000000 C
C43	1.0	0.247652	0.480439	0.553667	Biso	1.000000 C
C44	1.0	0.496590	0.976844	0.611205	Biso	1.000000 C
C45	1.0	0.175005	0.472052	0.669522	Biso	1.000000 C
C46	1.0	0.568947	0.973843	0.495081	Biso	1.000000 C
C47	1.0	0.141285	0.468350	0.723378	Biso	1.000000 C
C48	1.0	0.604717	0.974197	0.441460	Biso	1.000000 C
C49	1.0	0.008328	0.125596	0.710304	Biso	1.000000 C

C50	1.0	0.737833	0.631153	0.453741	Biso	1.000000	C
C51	1.0	0.924984	0.953056	0.732642	Biso	1.000000	C
C52	1.0	0.820786	0.459569	0.431017	Biso	1.000000	C
C53	1.0	0.056775	0.296909	0.745685	Biso	1.000000	C
C54	1.0	0.691343	0.805671	0.418956	Biso	1.000000	C
C55	1.0	0.890582	0.949516	0.786331	Biso	1.000000	C
C56	1.0	0.858637	0.461644	0.377625	Biso	1.000000	C
C57	1.0	0.020461	0.293335	0.802577	Biso	1.000000	C
C58	1.0	0.731922	0.808317	0.362594	Biso	1.000000	C
C59	1.0	0.935927	0.118322	0.823056	Biso	1.000000	C
C60	1.0	0.817577	0.635503	0.341940	Biso	1.000000	C
C61	1.0	0.067633	0.460097	0.839624	Biso	1.000000	C
C62	1.0	0.688839	0.982706	0.326708	Biso	1.000000	C
C63	1.0	0.028518	0.459485	0.892966	Biso	1.000000	C
C64	1.0	0.732919	0.990645	0.274256	Biso	1.000000	C
C65	1.0	0.895820	0.116741	0.879475	Biso	1.000000	C
C66	1.0	0.864818	0.642651	0.286197	Biso	1.000000	C
C67	1.0	0.938776	0.292047	0.914324	Biso	1.000000	C
C68	1.0	0.824409	0.825427	0.252802	Biso	1.000000	C
C69	1.0	0.810441	0.943424	0.901120	Biso	1.000000	C
C70	1.0	0.954819	0.479959	0.263585	Biso	1.000000	C
C71	1.0	0.888038	0.298709	0.969602	Biso	1.000000	C
C72	1.0	0.880227	0.843874	0.199985	Biso	1.000000	C
C73	1.0	0.765705	0.945990	0.953499	Biso	1.000000	C
C74	1.0	0.007998	0.501460	0.211888	Biso	1.000000	C
C75	1.0	0.800278	0.123454	0.988931	Biso	1.000000	C
C76	1.0	0.973147	0.686951	0.180359	Biso	1.000000	C

C77	1.0	0.384834	0.644662	0.019046	Biso	1.000000	C
C78	1.0	0.284142	0.986404	0.952074	Biso	1.000000	C
C79	1.0	0.307221	0.814504	0.040983	Biso	1.000000	C
C80	1.0	0.255955	0.986075	0.007045	Biso	1.000000	C
C81	1.0	0.913109	0.478381	0.004662	Biso	1.000000	C
C82	1.0	0.742914	0.132342	0.041744	Biso	1.000000	C
C83	1.0	0.850420	0.487337	0.054974	Biso	1.000000	C
C84	1.0	0.766007	0.312902	0.074215	Biso	1.000000	C
H1	1.0	0.887118	0.819662	0.707167	Biso	1.000000	H
H2	1.0	0.855604	0.322461	0.455810	Biso	1.000000	H
H3	1.0	0.826944	0.813669	0.800406	Biso	1.000000	H
H4	1.0	0.921740	0.326516	0.362916	Biso	1.000000	H
H5	1.0	0.265038	0.847947	0.197909	Biso	1.000000	H
H6	1.0	0.533509	0.336400	0.966778	Biso	1.000000	H
H7	1.0	0.409639	0.162940	0.164758	Biso	1.000000	H
H8	1.0	0.179856	0.837846	0.290240	Biso	1.000000	H
H9	1.0	0.593440	0.331461	0.871794	Biso	1.000000	H
H10	1.0	0.107314	0.844476	0.366736	Biso	1.000000	H
H11	1.0	0.646719	0.334257	0.796030	Biso	1.000000	H
H12	1.0	0.039861	0.840007	0.459622	Biso	1.000000	H
H13	1.0	0.706961	0.333044	0.702741	Biso	1.000000	H
H14	1.0	0.392562	0.630539	0.411064	Biso	1.000000	H
H15	1.0	0.350529	0.114267	0.755583	Biso	1.000000	H
H16	1.0	0.990806	0.833733	0.536961	Biso	1.000000	H
H17	1.0	0.754370	0.330634	0.626081	Biso	1.000000	H
H18	1.0	0.932049	0.827031	0.630483	Biso	1.000000	H
H19	1.0	0.813411	0.329027	0.532608	Biso	1.000000	H

H20	1.0	0.286800	0.612270	0.579427	Biso	1.000000 H
H21	1.0	0.457430	0.110303	0.585909	Biso	1.000000 H
H22	1.0	0.347177	0.619408	0.486184	Biso	1.000000 H
H23	1.0	0.398303	0.112226	0.679464	Biso	1.000000 H
H24	1.0	0.239419	0.607140	0.655407	Biso	1.000000 H
H25	1.0	0.502823	0.106646	0.509334	Biso	1.000000 H
H26	1.0	0.180630	0.600658	0.748985	Biso	1.000000 H
H27	1.0	0.565110	0.107344	0.416159	Biso	1.000000 H
H28	1.0	0.779339	0.806360	0.875845	Biso	1.000000 H
H29	1.0	0.985368	0.337117	0.286962	Biso	1.000000 H
H30	1.0	0.851987	0.986833	0.175860	Biso	1.000000 H
H31	1.0	0.700466	0.813146	0.968536	Biso	1.000000 H
H32	1.0	0.078778	0.376307	0.196059	Biso	1.000000 H
H33	1.0	0.021172	0.706798	0.141025	Biso	1.000000 H
H34	1.0	0.135655	0.592407	0.826084	Biso	1.000000 H
H35	1.0	0.621464	0.113701	0.341095	Biso	1.000000 H
H36	1.0	0.067698	0.590891	0.918985	Biso	1.000000 H
H37	1.0	0.700377	0.126267	0.248288	Biso	1.000000 H
H38	1.0	0.470942	0.468739	0.227977	Biso	1.000000 H
H39	1.0	0.464072	0.634142	0.317277	Biso	1.000000 H
H40	1.0	0.290524	0.116264	0.849272	Biso	1.000000 H
H41	1.0	0.977609	0.615589	0.991711	Biso	1.000000 H
H42	1.0	0.864378	0.631806	0.079442	Biso	1.000000 H
H43	1.0	0.718713	0.322627	0.114049	Biso	1.000000 H
H44	1.0	0.676205	0.997337	0.055275	Biso	1.000000 H
H45	1.0	0.425397	0.511334	0.044536	Biso	1.000000 H
H46	1.0	0.285607	0.816184	0.084099	Biso	1.000000 H

H47	1.0	0.194220	0.119355	0.023956	Biso	1.000000 H
H48	1.0	0.244072	0.121260	0.927444	Biso	1.000000 H